



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:53 PM GMT

PDB ID : 4Q1S  
Title : Yeast 20S proteasome in Complex with Kendomycin  
Authors : Beck, P.; Heinemeyer, W.; Spaeth, A.; Elnakady, Y.; Mueller, R.; Groll, M.  
Deposited on : 2014-04-04  
Resolution : 2.60 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

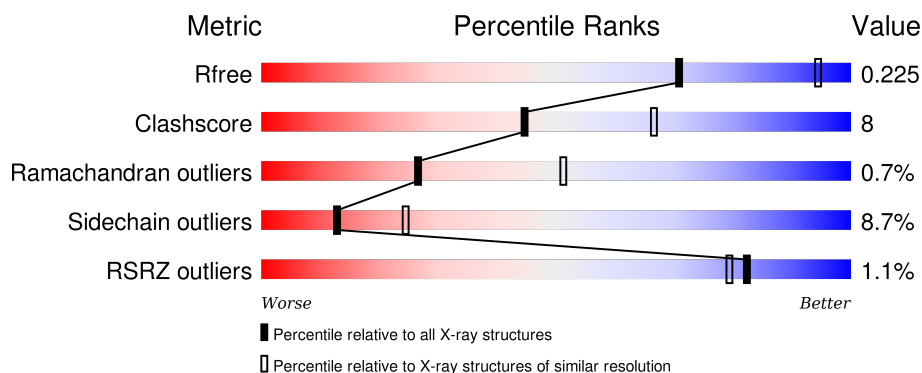
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	A	250	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 14%, yellow 14%, yellow 84%, green 84%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>84%</span> <span>14%</span> </div> </div>
1	O	250	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 13%, yellow 13%, yellow 84%, green 84%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>84%</span> <span>13%</span> </div> </div>
2	B	258	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 22%, yellow 22%, yellow 69%, green 69%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>69%</span> <span>22%</span> </div> </div>
2	P	258	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 18%, yellow 18%, yellow 73%, green 73%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>73%</span> <span>18%</span> </div> </div>
3	C	254	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 19%, yellow 19%, yellow 72%, green 72%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>72%</span> <span>19%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50912 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 type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			
4	R	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
6	T	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1638	1042	279	310	7			

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

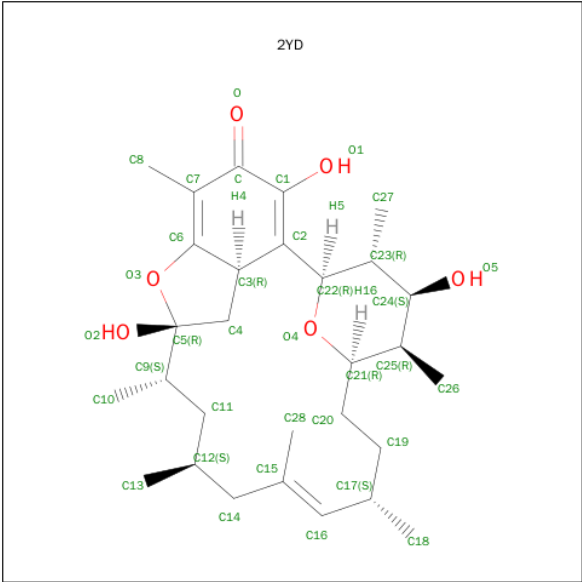
- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is (5R,6R,7S,8R,9R,12S,13E,16S,18S,19R,20AR)-4,7,19-TRIHYDROXY-2,6,8,12,14,16,18-HEPTAMETHYL-6,7,8,9,10,11,12,15,16,17,18,19,20,20A-TETRADECAHYDRO-1,19:5,9-DIEPOXYBENZO[18]ANNULEN-3(5H)-ONE (three-letter code: 2YD) (formula: C<sub>29</sub>H<sub>44</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	H	1	Total	C	O	0	0
			35	29	6		
15	V	1	Total	C	O	0	0
			35	29	6		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	59	Total	O	0	0
			59	59		
16	B	39	Total	O	0	0
			39	39		
16	C	42	Total	O	0	0
			42	42		
16	D	39	Total	O	0	0
			39	39		
16	E	20	Total	O	0	0
			20	20		
16	F	49	Total	O	0	0
			49	49		
16	G	58	Total	O	0	0
			58	58		
16	H	53	Total	O	0	0
			53	53		
16	I	63	Total	O	0	0
			63	63		
16	J	51	Total	O	0	0
			51	51		

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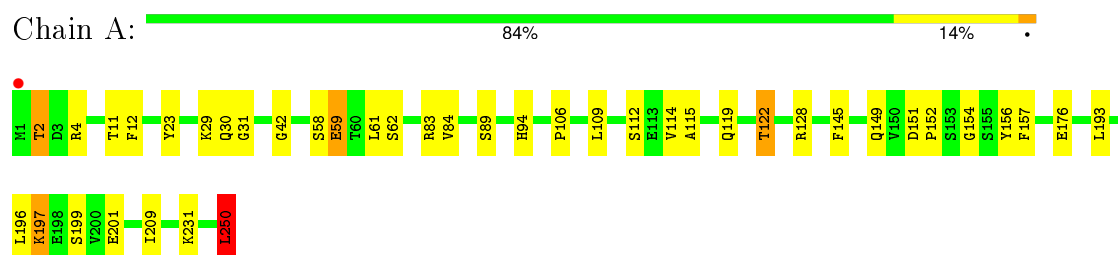
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	K	44	Total 44	O 44	0	0
16	L	58	Total 58	O 58	0	0
16	M	64	Total 64	O 64	0	0
16	N	58	Total 58	O 58	0	0
16	O	31	Total 31	O 31	0	0
16	P	30	Total 30	O 30	0	0
16	Q	25	Total 25	O 25	0	0
16	R	32	Total 32	O 32	0	0
16	S	21	Total 21	O 21	0	0
16	T	38	Total 38	O 38	0	0
16	U	66	Total 66	O 66	0	0
16	V	44	Total 44	O 44	0	0
16	W	62	Total 62	O 62	0	0
16	X	49	Total 49	O 49	0	0
16	Y	48	Total 48	O 48	0	0
16	Z	48	Total 48	O 48	0	0
16	a	62	Total 62	O 62	0	0
16	b	57	Total 57	O 57	0	0



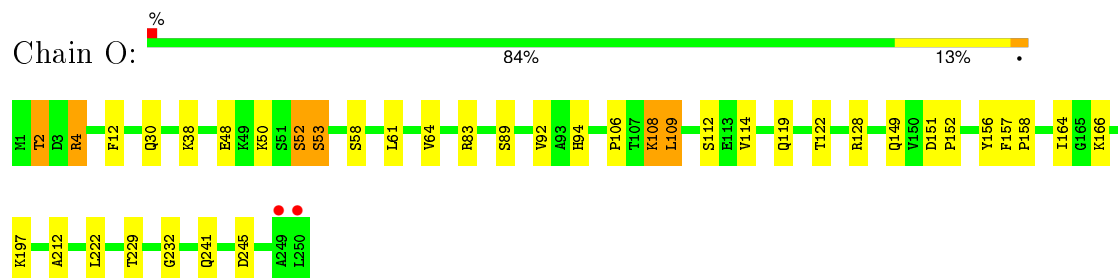
### 3 Residue-property plots [i](#)

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.

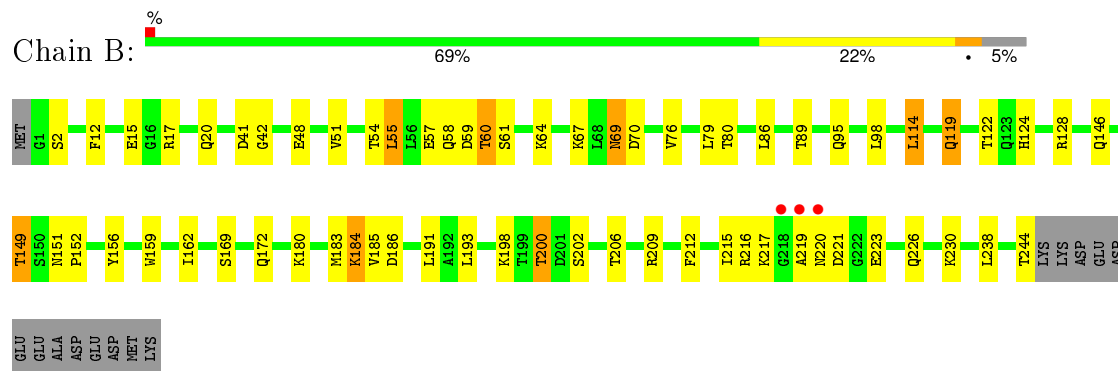
#### • Molecule 1: Proteasome subunit alpha type-2



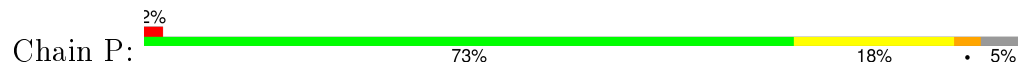
#### • Molecule 1: Proteasome subunit alpha type-2

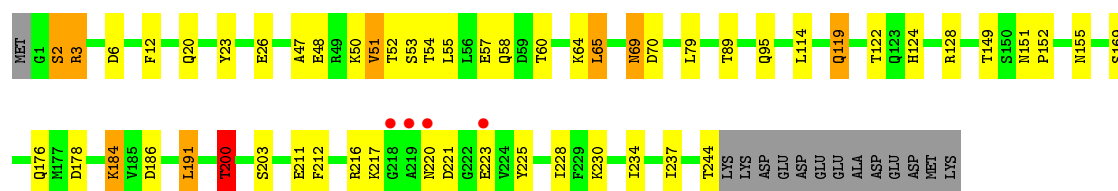


#### • Molecule 2: Proteasome subunit alpha type-3

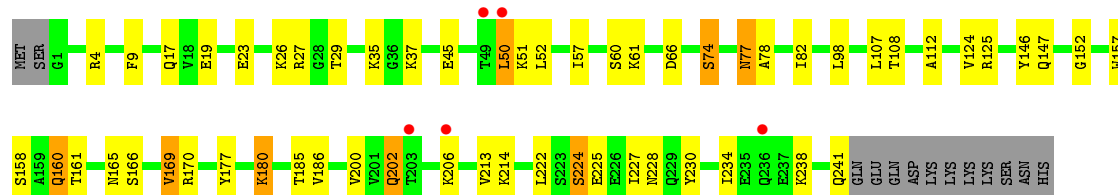
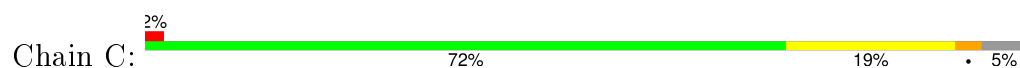


#### • Molecule 2: Proteasome subunit alpha type-3

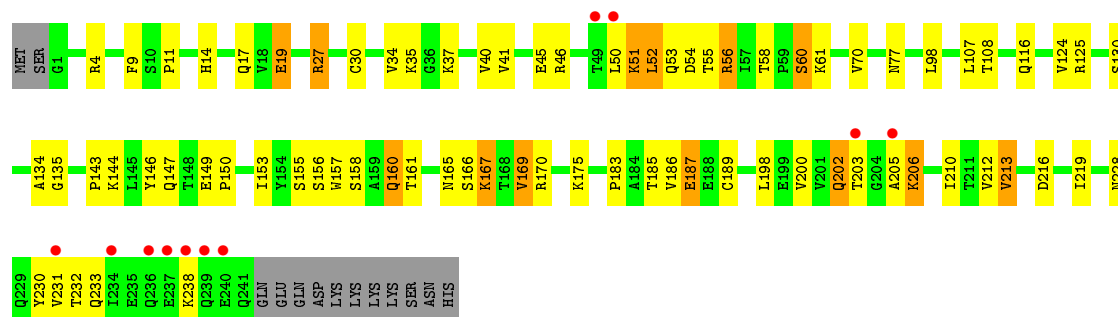




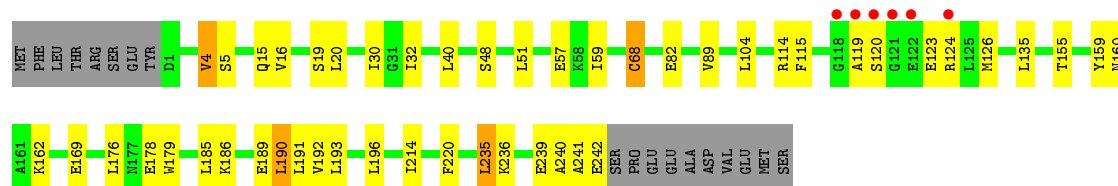
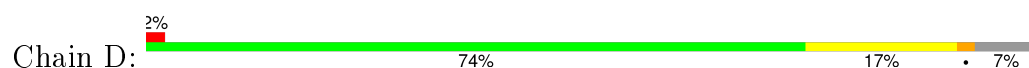
• Molecule 3: Proteasome subunit alpha type-4



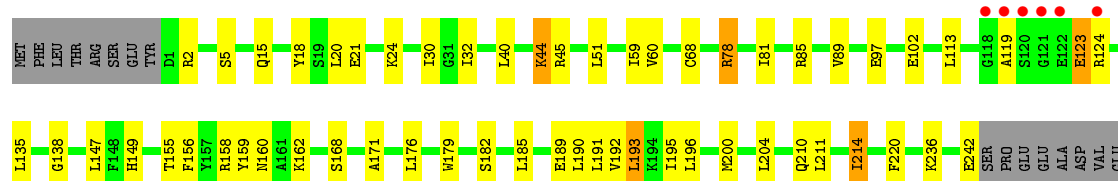
• Molecule 3: Proteasome subunit alpha type-4



• Molecule 4: Proteasome subunit alpha type-5

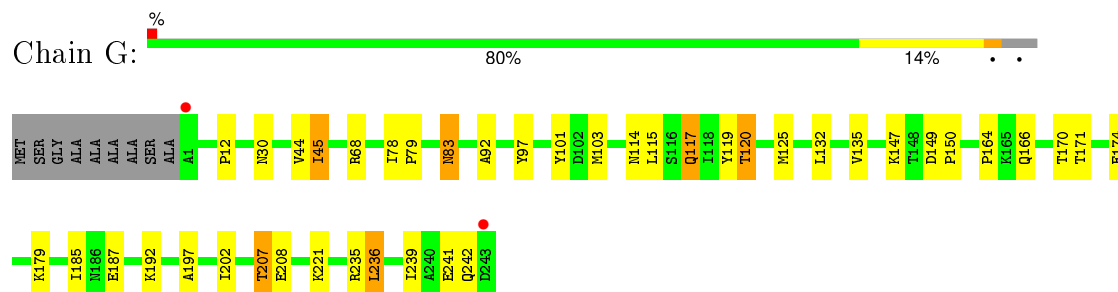


• Molecule 4: Proteasome subunit alpha type-5

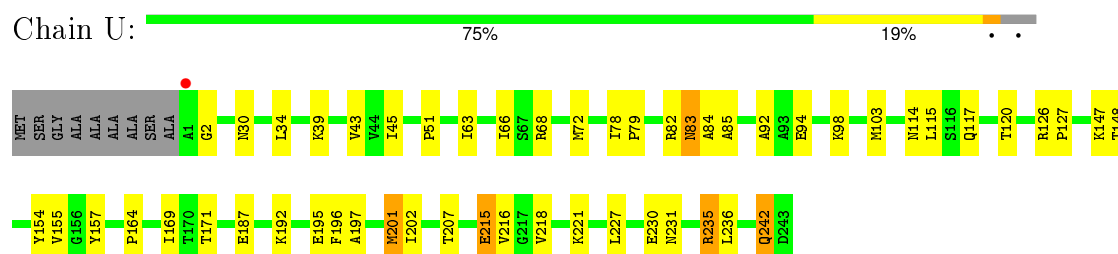




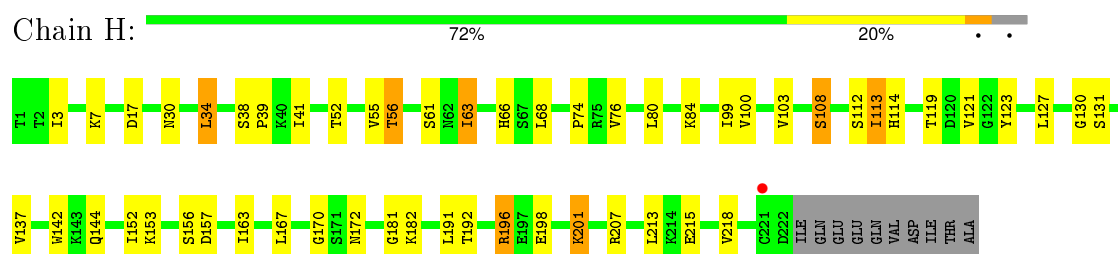
- Molecule 7: Proteasome subunit alpha type-1



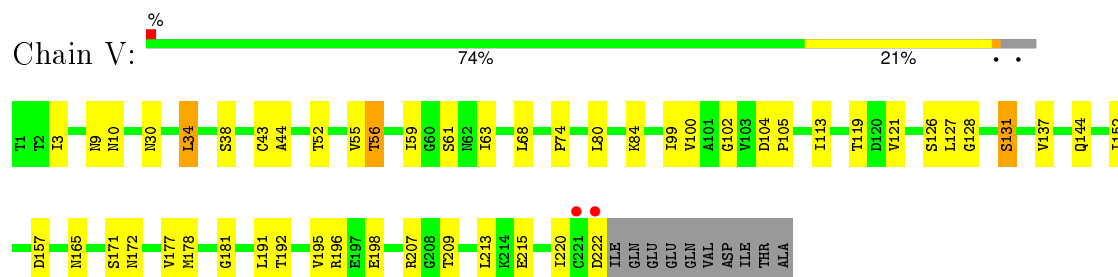
- Molecule 7: Proteasome subunit alpha type-1



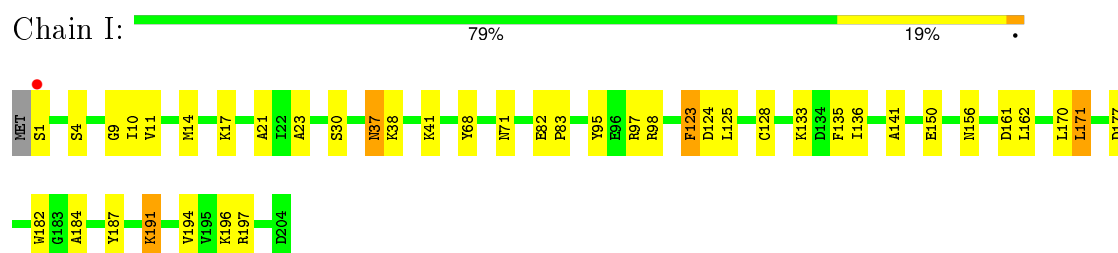
- Molecule 8: Proteasome subunit beta type-2



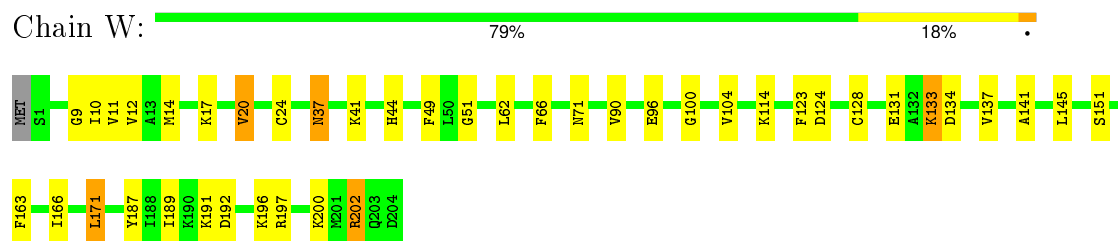
- Molecule 8: Proteasome subunit beta type-2



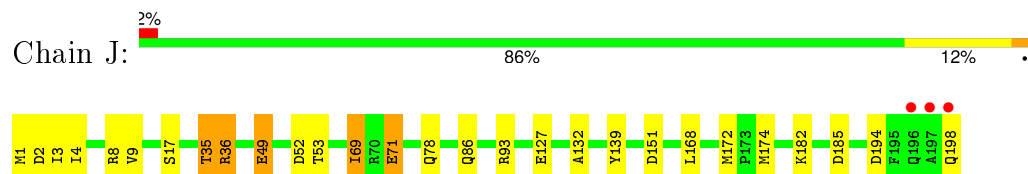
- Molecule 9: Proteasome subunit beta type-3



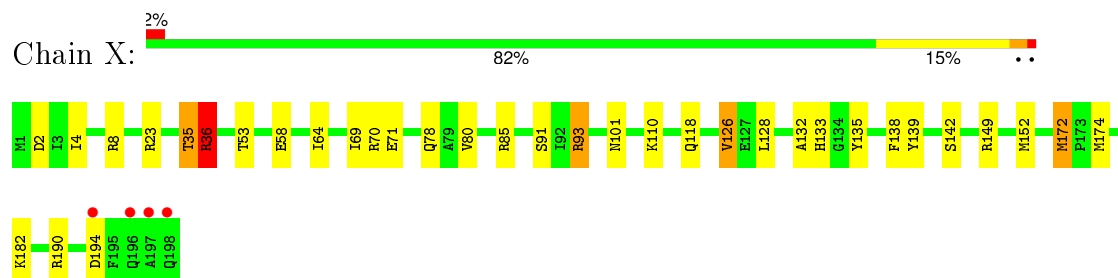
- Molecule 9: Proteasome subunit beta type-3



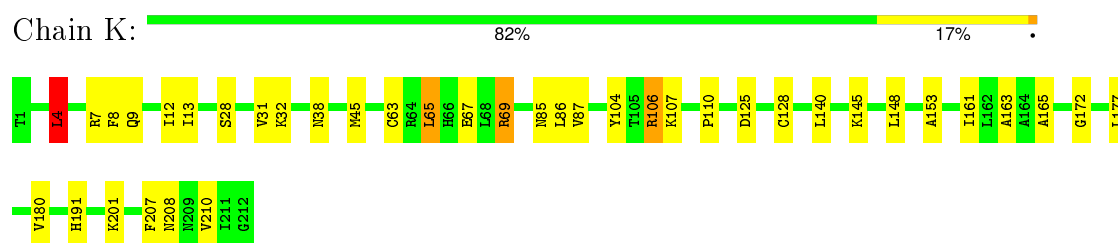
- Molecule 10: Proteasome subunit beta type-4



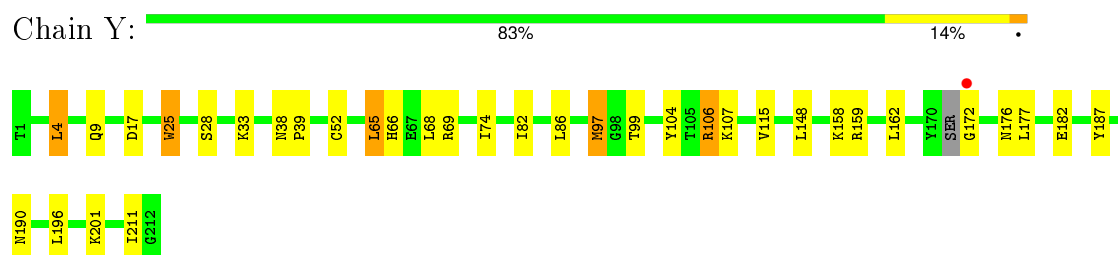
- Molecule 10: Proteasome subunit beta type-4



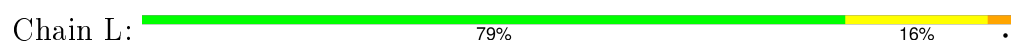
- Molecule 11: Proteasome subunit beta type-5

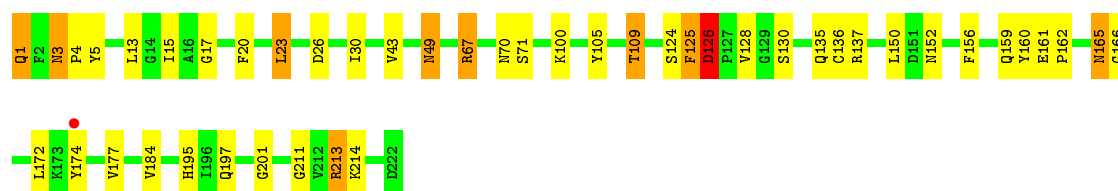


- Molecule 11: Proteasome subunit beta type-5



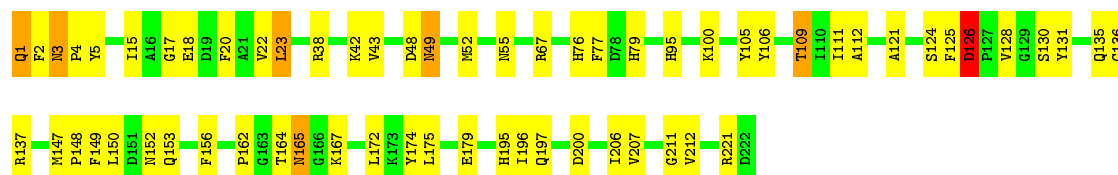
- Molecule 12: Proteasome subunit beta type-6





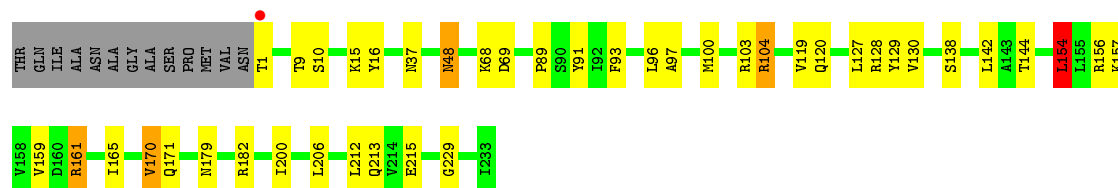
• Molecule 12: Proteasome subunit beta type-6

Chain Z: 72% 25% .



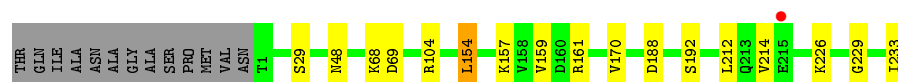
• Molecule 13: Proteasome subunit beta type-7

Chain M: 78% 15% . 5%



• Molecule 13: Proteasome subunit beta type-7

Chain a: 88% 7% 5%



• Molecule 14: Proteasome subunit beta type-1

Chain N: 85% 13% .



• Molecule 14: Proteasome subunit beta type-1

Chain b: 96%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.44Å 301.12Å 145.54Å 90.00° 113.15° 90.00°	Depositor
Resolution (Å)	48.52 – 2.60 48.53 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.52-2.60) 98.4 (48.53-2.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.11 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.175 , 0.224 0.178 , 0.225	Depositor DCC
$R_{free}$ test set	16212 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.5	Xtriage
Anisotropy	0.775	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 324230 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	50912	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2YD

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	A	0.61	0/1952	0.79	1/2642 (0.0%)
1	O	0.54	0/1952	0.76	0/2642
2	B	0.63	0/1934	0.79	0/2618
2	P	0.58	0/1934	0.79	2/2618 (0.1%)
3	C	0.56	0/1919	0.77	1/2598 (0.0%)
3	Q	0.52	0/1919	0.74	2/2598 (0.1%)
4	D	0.57	0/1886	0.79	1/2541 (0.0%)
4	R	0.58	0/1886	0.79	0/2541
5	E	0.57	0/1823	0.77	1/2463 (0.0%)
5	S	0.53	0/1823	0.73	2/2463 (0.1%)
6	F	0.58	0/1936	0.78	1/2614 (0.0%)
6	T	0.57	0/1936	0.78	1/2614 (0.0%)
7	G	0.62	0/1959	0.77	0/2652
7	U	0.60	0/1959	0.76	0/2652
8	H	0.61	0/1715	0.82	0/2326
8	V	0.59	0/1715	0.76	0/2326
9	I	0.66	0/1611	0.79	1/2174 (0.0%)
9	W	0.61	0/1611	0.77	0/2174
10	J	0.64	0/1613	0.84	2/2173 (0.1%)
10	X	0.60	0/1613	0.80	2/2173 (0.1%)
11	K	0.63	0/1681	0.80	3/2274 (0.1%)
11	Y	0.68	0/1674	0.87	5/2263 (0.2%)
12	L	0.64	0/1795	0.80	2/2420 (0.1%)
12	Z	0.67	0/1795	0.81	1/2420 (0.0%)
13	M	0.63	0/1855	0.87	4/2514 (0.2%)
13	a	0.65	0/1855	0.88	2/2514 (0.1%)
14	N	0.63	0/1541	0.79	0/2087
14	b	0.59	0/1541	0.75	0/2087
All	All	0.60	0/50433	0.79	34/68181 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying



if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1
8	H	0	1
8	V	0	1
12	L	0	2
12	Z	0	1
All	All	0	6

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	104	ARG	NE-CZ-NH1	8.33	124.46	120.30
11	Y	172	GLY	N-CA-C	8.08	133.30	113.10
13	M	154	LEU	CA-CB-CG	7.04	131.49	115.30
12	Z	126	ASP	CB-CA-C	-6.60	97.20	110.40
13	M	104	ARG	NE-CZ-NH2	-6.10	117.25	120.30
11	Y	177	LEU	CB-CG-CD1	-5.92	100.94	111.00
10	J	151	ASP	CB-CG-OD1	5.83	123.55	118.30
5	S	205	LEU	CA-CB-CG	5.76	128.55	115.30
4	D	235	LEU	CA-CB-CG	5.74	128.50	115.30
11	Y	159	ARG	NE-CZ-NH1	5.71	123.15	120.30
2	P	200	THR	CB-CA-C	-5.68	96.27	111.60
11	Y	4	LEU	CA-CB-CG	5.67	128.35	115.30
5	E	71	LEU	CA-CB-CG	5.66	128.32	115.30
10	J	36	ARG	NE-CZ-NH1	-5.65	117.47	120.30
13	a	154	LEU	CA-CB-CG	5.64	128.27	115.30
12	L	126	ASP	CB-CA-C	-5.61	99.17	110.40
13	M	103	ARG	NE-CZ-NH2	-5.53	117.53	120.30
10	X	85	ARG	NE-CZ-NH1	5.42	123.01	120.30
10	X	36	ARG	NE-CZ-NH1	5.40	123.00	120.30
11	Y	69	ARG	NE-CZ-NH1	5.31	122.96	120.30
11	K	69	ARG	NE-CZ-NH1	5.31	122.95	120.30
3	C	98	LEU	CA-CB-CG	5.30	127.50	115.30
6	T	172	LEU	CA-CB-CG	5.29	127.48	115.30
11	K	69	ARG	NE-CZ-NH2	-5.28	117.66	120.30
11	K	4	LEU	CA-CB-CG	5.26	127.40	115.30
12	L	67	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	250	LEU	CA-CB-CG	5.23	127.33	115.30
3	Q	98	LEU	CA-CB-CG	5.22	127.32	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	188	ASP	CB-CG-OD1	5.18	122.96	118.30
6	F	126	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	P	6	ASP	CB-CG-OD1	5.12	122.91	118.30
9	I	171	LEU	CA-CB-CG	5.11	127.06	115.30
5	S	71	LEU	CA-CB-CG	5.05	126.92	115.30
3	Q	50	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	201	ARG	Peptide
8	H	181	GLY	Peptide
12	L	125	PHE	Peptide
12	L	174	TYR	Peptide
8	V	181	GLY	Peptide
12	Z	174	TYR	Peptide

## 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	A	1915	0	1929	31	0
1	O	1915	0	1929	30	0
2	B	1904	0	1904	42	0
2	P	1904	0	1904	35	0
3	C	1890	0	1903	35	0
3	Q	1890	0	1903	50	0
4	D	1861	0	1839	26	0
4	R	1861	0	1839	29	0
5	E	1795	0	1800	30	0
5	S	1795	0	1800	44	0
6	F	1896	0	1889	24	0
6	T	1896	0	1889	39	0
7	G	1921	0	1913	34	0
7	U	1921	0	1913	42	0
8	H	1684	0	1688	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	V	1684	0	1688	26	0
9	I	1581	0	1574	25	0
9	W	1581	0	1574	24	0
10	J	1585	0	1590	21	0
10	X	1585	0	1590	26	0
11	K	1644	0	1595	23	0
11	Y	1638	0	1589	22	0
12	L	1757	0	1711	39	0
12	Z	1757	0	1711	50	0
13	M	1824	0	1832	37	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	19	0
14	b	1512	0	1481	0	0
15	H	35	0	40	2	0
15	V	35	0	40	2	0
16	A	59	0	0	1	0
16	B	39	0	0	1	0
16	C	42	0	0	1	0
16	D	39	0	0	0	0
16	E	20	0	0	0	0
16	F	49	0	0	0	0
16	G	58	0	0	1	0
16	H	53	0	0	3	0
16	I	63	0	0	2	0
16	J	51	0	0	3	0
16	K	44	0	0	3	0
16	L	58	0	0	1	0
16	M	64	0	0	6	0
16	N	58	0	0	4	0
16	O	31	0	0	1	0
16	P	30	0	0	0	0
16	Q	25	0	0	2	0
16	R	32	0	0	4	0
16	S	21	0	0	0	0
16	T	38	0	0	2	0
16	U	66	0	0	3	0
16	V	44	0	0	1	0
16	W	62	0	0	2	0
16	X	49	0	0	3	0
16	Y	48	0	0	3	0
16	Z	48	0	0	4	0
16	a	62	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	b	57	0	0	0	0
All	All	50912	0	49370	729	0

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

All (729) 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)
7:U:92:ALA:HA	7:U:103:MET:HE2	1.23	1.15
7:G:92:ALA:HA	7:G:103:MET:CE	1.78	1.13
7:G:92:ALA:HA	7:G:103:MET:HE2	1.21	1.11
2:P:122:THR:HG22	3:Q:125:ARG:HH21	1.25	0.98
2:P:69:ASN:HD22	2:P:70:ASP:H	1.07	0.97
3:C:160:GLN:NE2	3:C:161:THR:H	1.64	0.95
5:E:12:PHE:H	6:F:19:GLN:HE22	1.13	0.95
7:G:187:GLU:HG2	7:G:192:LYS:CB	1.97	0.94
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.32	0.94
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.47	0.94
7:U:92:ALA:HA	7:U:103:MET:CE	1.98	0.94
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.49	0.93
3:C:160:GLN:HE21	3:C:161:THR:N	1.66	0.92
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.35	0.92
1:A:12:PHE:H	2:B:20:GLN:HE22	1.18	0.92
2:P:69:ASN:HD22	2:P:70:ASP:N	1.66	0.92
10:J:174:MET:HG2	10:X:174:MET:CE	2.01	0.90
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.20	0.90
1:O:12:PHE:H	2:P:20:GLN:HE22	1.14	0.89
3:Q:60:SER:HB2	16:Q:303:HOH:O	1.71	0.89
11:K:106:ARG:HH11	11:K:106:ARG:HB2	1.36	0.89
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.54	0.89
14:N:83:LYS:HG3	14:N:119:VAL:HG22	1.56	0.88
5:S:12:PHE:H	6:T:19:GLN:HE22	1.17	0.87
3:C:9:PHE:H	4:D:15:GLN:HE22	1.22	0.87
3:C:160:GLN:HE21	3:C:161:THR:H	0.91	0.86
10:J:174:MET:HG2	10:X:174:MET:HE2	1.55	0.86
2:B:69:ASN:HD22	2:B:70:ASP:H	1.23	0.86
2:P:122:THR:CG2	3:Q:125:ARG:HH21	1.89	0.85
12:L:195:HIS:HD2	12:L:197:GLN:H	1.25	0.84
5:S:49:LYS:HB3	5:S:58:TYR:HB3	1.60	0.83
5:E:53:ASP:HB3	5:E:55:LEU:H	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:122:THR:CG2	2:P:128:ARG:HH21	1.92	0.82
10:X:93:ARG:HG2	10:X:93:ARG:HH11	1.43	0.82
6:F:31:THR:HG21	6:F:47:GLU:O	1.79	0.82
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.25	0.82
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.61	0.81
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.63	0.80
1:O:83:ARG:HE	7:U:114:ASN:HD21	1.28	0.80
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.16	0.80
7:G:92:ALA:CA	7:G:103:MET:CE	2.60	0.80
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.61	0.80
2:B:172:GLN:HG2	3:C:50:LEU:HD21	1.63	0.80
6:T:91:GLU:HG3	6:T:111:ARG:HB3	1.64	0.79
7:U:117:GLN:O	7:U:120:THR:HB	1.83	0.79
6:T:34:ILE:HG12	6:T:196:ILE:HD11	1.64	0.78
1:A:83:ARG:HE	7:G:114:ASN:HD21	1.31	0.78
2:P:155:ASN:ND2	3:Q:77:ASN:HB2	1.99	0.78
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.48	0.78
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.31	0.78
13:M:179:ASN:HD22	13:M:182:ARG:NH1	1.82	0.77
4:D:89:VAL:HG21	11:K:65:LEU:HD13	1.66	0.77
13:M:179:ASN:ND2	13:M:182:ARG:HH11	1.84	0.76
1:A:122:THR:CG2	2:B:128:ARG:HH21	1.97	0.76
14:N:83:LYS:CD	16:N:229:HOH:O	2.33	0.76
10:J:1:MET:HG2	10:J:2:ASP:H	1.49	0.76
13:M:48:ASN:H	13:M:48:ASN:HD22	1.34	0.76
14:N:83:LYS:HD2	16:N:229:HOH:O	1.87	0.75
4:R:45:ARG:HG2	4:R:45:ARG:O	1.84	0.75
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.69	0.74
2:B:119:GLN:O	2:B:122:THR:HB	1.88	0.74
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.68	0.74
1:O:94:HIS:HD2	8:V:61:SER:OG	1.71	0.74
6:T:143:HIS:HD2	16:T:301:HOH:O	1.69	0.74
1:O:128:ARG:HH21	7:U:120:THR:CG2	2.00	0.74
13:M:37:ASN:OD1	16:M:339:HOH:O	2.05	0.74
9:I:187:TYR:OH	9:I:196:LYS:HE3	1.88	0.73
8:V:128:GLY:O	8:V:131:SER:HB2	1.89	0.73
1:O:83:ARG:HH21	7:U:114:ASN:HD22	1.36	0.73
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.71	0.73
2:B:41:ASP:OD2	2:B:184:LYS:HE3	1.89	0.72
12:Z:126:ASP:HB3	12:Z:128:VAL:H	1.54	0.72
6:T:186:ARG:HH11	6:T:186:ARG:HG3	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.89	0.72
14:N:14:LEU:HD11	14:N:100:ALA:HB3	1.70	0.72
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.71	0.71
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.20	0.71
3:Q:160:GLN:HE21	3:Q:161:THR:H	1.36	0.71
7:U:187:GLU:HG2	7:U:192:LYS:CB	2.21	0.71
2:P:69:ASN:ND2	2:P:70:ASP:H	1.85	0.71
14:N:92:ASN:HB2	16:N:245:HOH:O	1.90	0.71
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.73	0.71
12:L:1:GLN:NE2	13:M:1:THR:HG21	2.05	0.71
11:K:4:LEU:HD13	11:K:161:ILE:HD11	1.72	0.70
13:M:161:ARG:CG	13:M:161:ARG:HH11	2.02	0.70
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.21	0.70
3:Q:160:GLN:NE2	3:Q:161:THR:H	1.89	0.70
2:B:42:GLY:HA3	2:B:185:VAL:HG21	1.72	0.70
7:U:83:ASN:C	7:U:83:ASN:HD22	1.95	0.70
1:A:94:HIS:HD2	8:H:61:SER:OG	1.74	0.70
12:L:159:GLN:HG2	8:V:209:THR:HG21	1.74	0.70
1:O:119:GLN:O	1:O:122:THR:HB	1.92	0.70
4:R:97:GLU:OE2	16:R:309:HOH:O	2.10	0.70
6:T:123:ASN:HD22	6:T:123:ASN:C	1.94	0.70
6:T:175:LEU:HD11	6:T:191:GLN:HG3	1.74	0.69
10:X:93:ARG:CG	10:X:93:ARG:HH11	2.04	0.69
11:K:201:LYS:HE3	16:K:332:HOH:O	1.92	0.69
2:P:48:GLU:OE2	2:P:200:THR:HG22	1.92	0.69
1:O:38:LYS:NZ	2:P:57:GLU:OE2	2.25	0.69
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.74	0.69
1:A:128:ARG:HH21	7:G:120:THR:CG2	2.06	0.68
9:I:37:ASN:HD22	9:I:38:LYS:HG2	1.57	0.68
2:B:122:THR:HG22	3:C:125:ARG:HH21	1.58	0.68
12:L:159:GLN:HG2	8:V:209:THR:CG2	2.24	0.68
12:Z:164:THR:O	12:Z:167:LYS:HB2	1.93	0.68
4:R:89:VAL:HG21	11:Y:65:LEU:HD13	1.75	0.68
2:P:119:GLN:O	2:P:122:THR:HB	1.94	0.68
5:E:206:THR:H	5:E:209:ASN:HD22	1.40	0.68
12:Z:3:ASN:ND2	12:Z:5:TYR:H	1.92	0.68
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.74	0.67
3:Q:51:LYS:HG3	3:Q:206:LYS:NZ	2.10	0.67
10:X:35:THR:HG21	10:X:182:LYS:NZ	2.10	0.67
6:F:31:THR:CG2	6:F:47:GLU:O	2.41	0.67
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:109:THR:HG23	16:Z:306:HOH:O	1.95	0.67
13:M:182:ARG:NE	16:M:364:HOH:O	2.27	0.66
10:J:139:TYR:CE2	10:J:172:MET:HG3	2.30	0.66
9:I:14:MET:HB3	9:I:162:LEU:HD11	1.78	0.66
7:U:169:ILE:HD13	7:U:201:MET:HE3	1.78	0.66
2:B:69:ASN:HD22	2:B:70:ASP:N	1.93	0.65
9:I:123:PHE:HA	9:I:128:CYS:O	1.95	0.65
12:L:3:ASN:HD22	12:L:3:ASN:C	1.99	0.65
2:P:48:GLU:OE2	2:P:200:THR:CG2	2.44	0.65
8:H:52:THR:O	8:H:56:THR:HB	1.97	0.65
2:B:122:THR:CG2	3:C:125:ARG:HH21	2.09	0.65
5:S:1:PHE:HZ	5:S:15:THR:HG1	1.42	0.65
14:N:55:ILE:HD11	14:N:93:LEU:HD13	1.79	0.65
10:X:149:ARG:O	10:X:152:MET:HG3	1.97	0.65
8:V:157:ASP:OD2	15:V:301:2YD:H9	1.97	0.64
6:T:31:THR:HG21	6:T:47:GLU:O	1.97	0.64
7:G:125:MET:O	16:G:310:HOH:O	2.14	0.64
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.79	0.64
6:F:181:GLU:H	6:F:181:GLU:CD	2.00	0.64
10:X:35:THR:HG21	10:X:182:LYS:HZ2	1.60	0.64
11:K:4:LEU:CD1	11:K:161:ILE:HD11	2.27	0.64
7:G:187:GLU:HG2	7:G:192:LYS:HB3	1.77	0.64
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.80	0.64
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.18	0.64
9:I:97:ARG:HD2	16:I:361:HOH:O	1.96	0.63
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.64	0.63
5:E:68:HIS:HE1	5:E:102:LEU:O	1.82	0.63
12:L:17:GLY:HA3	12:L:20:PHE:CE1	2.33	0.63
8:H:34:LEU:HB2	16:H:427:HOH:O	1.98	0.63
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.28	0.63
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.63	0.63
3:Q:157:TRP:CE2	4:R:51:LEU:HD23	2.34	0.63
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.47	0.63
2:B:48:GLU:OE2	2:B:209:ARG:NH2	2.32	0.63
5:S:68:HIS:HE1	5:S:102:LEU:O	1.82	0.63
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.62	0.62
11:Y:176:ASN:HD21	11:Y:190:ASN:HD22	1.46	0.62
6:T:91:GLU:CG	6:T:111:ARG:HB3	2.29	0.62
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.65	0.62
12:L:23:LEU:HD13	12:L:43:VAL:CG1	2.30	0.62
1:O:52:SER:O	1:O:53:SER:HB3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:123:ASN:HD22	6:T:124:SER:N	1.98	0.62
5:S:9:THR:HG21	5:S:119:THR:HA	1.81	0.62
10:J:174:MET:HG2	10:X:174:MET:HE1	1.82	0.61
6:T:31:THR:CG2	6:T:47:GLU:O	2.48	0.61
5:S:53:ASP:HB3	5:S:55:LEU:H	1.64	0.61
1:A:83:ARG:HE	7:G:114:ASN:ND2	1.97	0.61
14:N:2:SER:OG	14:N:130:GLY:HA3	2.00	0.61
13:M:182:ARG:CD	16:M:364:HOH:O	2.48	0.61
7:G:117:GLN:O	7:G:120:THR:HB	2.00	0.61
12:Z:49:ASN:ND2	16:Z:324:HOH:O	2.30	0.61
7:U:92:ALA:CA	7:U:103:MET:HE2	2.16	0.61
12:Z:3:ASN:HD22	12:Z:3:ASN:C	2.02	0.61
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.47	0.61
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.82	0.61
1:O:83:ARG:HE	7:U:114:ASN:ND2	1.98	0.60
8:H:137:VAL:HG22	15:H:301:2YD:H46	1.82	0.60
1:O:158:PRO:HB2	2:P:57:GLU:HB3	1.83	0.60
2:P:228:ILE:HD12	2:P:228:ILE:N	2.16	0.60
12:L:152:ASN:O	12:L:156:PHE:HA	2.01	0.60
13:M:48:ASN:ND2	13:M:48:ASN:H	1.96	0.60
8:H:201:LYS:HE2	12:Z:179:GLU:OE2	2.02	0.60
9:W:123:PHE:HA	9:W:128:CYS:O	2.01	0.60
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.83	0.60
12:L:3:ASN:ND2	12:L:5:TYR:H	1.99	0.60
12:Z:3:ASN:HD22	12:Z:4:PRO:N	2.00	0.60
1:A:83:ARG:HH21	7:G:114:ASN:HD22	1.48	0.60
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.00	0.60
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.84	0.59
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.84	0.59
3:Q:160:GLN:HE21	3:Q:161:THR:N	1.99	0.59
5:S:203:GLU:CG	5:S:204:SER:H	2.15	0.59
3:Q:146:TYR:CE2	3:Q:156:SER:HB3	2.37	0.59
4:R:21:GLU:OE1	4:R:24:LYS:NZ	2.35	0.59
7:U:83:ASN:C	7:U:83:ASN:ND2	2.56	0.59
1:A:119:GLN:O	1:A:122:THR:HB	2.02	0.59
3:Q:51:LYS:HD2	3:Q:52:LEU:H	1.67	0.59
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.38	0.59
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.49	0.59
8:H:167:LEU:HD22	12:Z:196:ILE:O	2.02	0.59
6:T:48:LYS:HD2	6:T:211:GLU:OE2	2.03	0.59
10:J:49:GLU:HG2	10:J:52:ASP:OD2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:16:TYR:CZ	13:M:170:VAL:HG13	2.37	0.59
3:Q:51:LYS:HG3	3:Q:206:LYS:HZ3	1.69	0.58
3:C:157:TRP:CZ2	4:D:51:LEU:HD23	2.38	0.58
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.84	0.58
11:K:201:LYS:NZ	11:K:210:VAL:O	2.36	0.58
12:L:15:ILE:HG23	12:L:136:CYS:HB3	1.85	0.58
9:I:37:ASN:ND2	9:I:38:LYS:HG2	2.19	0.58
4:D:104:LEU:C	4:D:104:LEU:HD13	2.24	0.58
13:M:182:ARG:HD2	16:M:364:HOH:O	2.04	0.58
11:K:201:LYS:HG3	11:K:207:PHE:HB2	1.85	0.58
4:D:82:GLU:OE2	11:K:69:ARG:NH1	2.36	0.58
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.39	0.58
10:J:1:MET:HG2	10:J:2:ASP:N	2.18	0.58
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.86	0.58
2:P:234:ILE:HA	2:P:237:ILE:HG22	1.86	0.57
3:Q:165:ASN:HB2	3:Q:200:VAL:HG11	1.87	0.57
5:S:206:THR:OG1	5:S:209:ASN:HB2	2.04	0.57
14:N:195:GLN:NE2	14:N:195:GLN:HA	2.18	0.57
2:B:64:LYS:HE2	2:B:76:VAL:O	2.03	0.57
6:F:123:ASN:C	6:F:123:ASN:HD22	2.06	0.57
7:G:83:ASN:C	7:G:83:ASN:HD22	2.08	0.57
7:U:202:ILE:HG23	7:U:207:THR:O	2.05	0.57
11:K:165:ALA:HB1	11:K:172:GLY:HA2	1.87	0.57
10:J:194:ASP:O	10:J:198:GLN:HB2	2.04	0.57
1:O:83:ARG:HH21	7:U:114:ASN:ND2	2.02	0.56
6:F:75:SER:OG	6:F:161:THR:HG23	2.06	0.56
7:G:92:ALA:CA	7:G:103:MET:HE2	2.15	0.56
11:K:63:CYS:O	11:K:67:GLU:HG3	2.05	0.56
7:U:126:ARG:HG3	7:U:127:PRO:O	2.06	0.56
6:F:32:THR:HG23	6:F:47:GLU:OE2	2.06	0.56
12:Z:22:VAL:HG12	12:Z:206:ILE:HG13	1.88	0.56
10:J:3:ILE:HD13	10:J:168:LEU:HD13	1.88	0.56
5:E:12:PHE:H	6:F:19:GLN:NE2	1.94	0.56
5:E:205:LEU:HA	5:E:209:ASN:ND2	2.21	0.56
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.36	0.56
7:U:82:ARG:HD2	16:U:308:HOH:O	2.05	0.56
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.70	0.56
9:W:133:LYS:NZ	9:W:134:ASP:HB3	2.21	0.56
8:H:7:LYS:HG3	8:H:123:TYR:HA	1.87	0.56
4:R:149:HIS:O	4:R:156:PHE:HA	2.04	0.56
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:213:ARG:NH1	16:L:350:HOH:O	2.36	0.56
12:Z:3:ASN:HD22	12:Z:4:PRO:CD	2.19	0.55
12:L:15:ILE:HG12	12:L:136:CYS:HB2	1.88	0.55
10:X:110:LYS:HB2	10:X:110:LYS:NZ	2.22	0.55
10:J:86:GLN:HB3	16:J:209:HOH:O	2.05	0.55
5:S:156:TYR:OH	6:T:57:PRO:HD2	2.07	0.55
1:O:151:ASP:HB3	1:O:152:PRO:HD2	1.88	0.55
11:Y:66:HIS:HA	16:Y:339:HOH:O	2.05	0.55
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.89	0.55
2:B:15:GLU:O	3:C:27:ARG:NH1	2.39	0.55
7:U:92:ALA:CA	7:U:103:MET:CE	2.79	0.55
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.88	0.55
6:F:32:THR:HG21	6:F:164:GLY:HA3	1.88	0.55
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.54	0.55
11:Y:176:ASN:ND2	11:Y:190:ASN:HD22	2.04	0.55
8:V:34:LEU:HD12	8:V:44:ALA:HB2	1.89	0.55
6:T:91:GLU:HG3	6:T:111:ARG:CB	2.35	0.54
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.42	0.54
2:B:12:PHE:H	3:C:17:GLN:HE22	1.55	0.54
13:M:179:ASN:ND2	13:M:182:ARG:NH1	2.45	0.54
12:Z:109:THR:CG2	16:Z:306:HOH:O	2.54	0.54
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.48	0.54
5:S:155:LEU:CD2	6:T:55:LEU:HD12	2.36	0.54
10:J:35:THR:HG21	10:J:182:LYS:NZ	2.23	0.54
6:T:165:ARG:O	6:T:169:LYS:HG3	2.06	0.54
4:D:68:CYS:HB2	4:D:135:LEU:O	2.07	0.54
8:V:195:VAL:HG23	16:V:418:HOH:O	2.06	0.54
13:M:48:ASN:HD22	13:M:48:ASN:N	2.00	0.54
2:B:42:GLY:HA3	2:B:185:VAL:CG2	2.36	0.54
12:L:3:ASN:HD22	12:L:4:PRO:N	2.04	0.54
2:B:180:LYS:O	2:B:183:MET:HG3	2.08	0.54
6:T:50:ILE:HG22	6:T:50:ILE:O	2.07	0.54
2:B:86:LEU:HB3	2:B:114:LEU:HD21	1.88	0.54
11:K:163:ALA:HB1	10:X:142:SER:HB2	1.89	0.54
8:V:172:ASN:HB3	8:V:191:LEU:O	2.08	0.54
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.90	0.54
1:O:94:HIS:CD2	8:V:61:SER:OG	2.57	0.54
7:U:30:ASN:HD22	7:U:164:PRO:HG2	1.73	0.54
5:E:28:ILE:HD11	5:E:148:PRO:HD3	1.90	0.54
9:W:37:ASN:HD22	9:W:37:ASN:C	2.11	0.54
11:K:86:LEU:HD13	11:K:86:LEU:C	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:28:GLU:HG2	6:T:165:ARG:CZ	2.39	0.53
7:G:44:VAL:HG13	7:G:135:VAL:HG11	1.90	0.53
12:L:125:PHE:HA	12:L:130:SER:O	2.08	0.53
5:E:170:TYR:HB2	5:E:198:GLN:HG2	1.91	0.53
8:H:103:VAL:HG12	8:H:108:SER:HB2	1.89	0.53
8:V:52:THR:O	8:V:56:THR:HB	2.09	0.53
11:Y:106:ARG:HD2	11:Y:182:GLU:OE1	2.08	0.53
2:B:186:ASP:OD1	2:B:216:ARG:NH2	2.38	0.53
3:C:165:ASN:HB2	3:C:200:VAL:HG11	1.90	0.53
5:S:49:LYS:CB	5:S:58:TYR:HB3	2.36	0.53
12:L:109:THR:HG23	12:L:125:PHE:HB2	1.91	0.53
10:X:93:ARG:NH1	10:X:93:ARG:CG	2.69	0.53
2:B:64:LYS:CE	2:B:76:VAL:O	2.57	0.53
12:Z:152:ASN:O	12:Z:156:PHE:HA	2.09	0.53
1:A:89:SER:OG	1:A:114:VAL:HG22	2.08	0.53
2:P:155:ASN:HD22	3:Q:77:ASN:HB2	1.73	0.53
10:J:71:GLU:OE2	10:J:71:GLU:HA	2.08	0.53
3:C:23:GLU:OE1	3:C:26:LYS:HE2	2.09	0.52
1:O:4:ARG:HB2	2:P:2:SER:OG	2.08	0.52
11:K:4:LEU:CD1	11:K:161:ILE:CD1	2.87	0.52
5:E:206:THR:H	5:E:209:ASN:ND2	2.07	0.52
6:F:191:GLN:HE21	6:F:194:LYS:HE3	1.75	0.52
7:U:230:GLU:HG2	16:U:360:HOH:O	2.08	0.52
3:Q:135:GLY:HA2	3:Q:213:VAL:HG21	1.90	0.52
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	1.91	0.52
5:S:1:PHE:HE2	5:S:17:ARG:HH11	1.58	0.52
7:U:43:VAL:HG22	7:U:218:VAL:HG22	1.91	0.52
10:X:190:ARG:HH11	10:X:190:ARG:HG2	1.74	0.52
6:T:168:ALA:O	6:T:172:LEU:HD22	2.10	0.52
4:R:191:LEU:O	4:R:195:ILE:HG13	2.09	0.52
3:Q:213:VAL:HB	3:Q:219:ILE:HG12	1.92	0.52
3:C:60:SER:HB2	16:C:311:HOH:O	2.10	0.52
11:Y:25:TRP:HH2	12:Z:147:MET:HB2	1.75	0.52
10:X:118:GLN:NE2	10:X:132:ALA:H	2.08	0.52
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.92	0.51
4:D:159:TYR:CZ	4:D:162:LYS:HD3	2.45	0.51
12:L:165:ASN:CG	12:L:165:ASN:O	2.48	0.51
2:P:122:THR:HG22	3:Q:125:ARG:NH2	2.09	0.51
11:Y:176:ASN:ND2	11:Y:187:TYR:OH	2.43	0.51
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.92	0.51
3:C:29:THR:HB	3:C:45:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:137:VAL:HG22	15:V:301:2YD:H46	1.92	0.51
3:Q:35:LYS:HD3	3:Q:158:SER:HA	1.93	0.51
9:I:95:TYR:CE1	9:I:98:ARG:HD3	2.46	0.51
13:M:215:GLU:HA	13:M:215:GLU:OE2	2.09	0.51
8:H:207:ARG:O	12:Z:162:PRO:HB3	2.10	0.51
4:R:196:LEU:O	4:R:200:MET:HG3	2.11	0.51
1:A:83:ARG:HH21	7:G:114:ASN:ND2	2.09	0.51
3:Q:187:GLU:HG2	3:Q:230:TYR:OH	2.11	0.51
1:O:108:LYS:HG2	16:O:308:HOH:O	2.09	0.51
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.23	0.51
7:U:227:LEU:HB3	7:U:231:ASN:HB2	1.93	0.50
6:T:75:SER:HB2	6:T:161:THR:HG23	1.92	0.50
10:X:101:ASN:HB3	10:X:133:HIS:CE1	2.46	0.50
13:M:93:PHE:CE1	13:M:128:ARG:HD3	2.46	0.50
3:C:161:THR:HG23	3:C:166:SER:HB2	1.94	0.50
3:Q:160:GLN:NE2	3:Q:160:GLN:HA	2.26	0.50
12:L:1:GLN:HE22	13:M:1:THR:HG21	1.77	0.50
6:T:220:THR:O	6:T:221:ASN:HB2	2.12	0.50
2:P:69:ASN:ND2	2:P:70:ASP:N	2.47	0.50
6:T:110:ASP:O	6:T:114:GLN:HG2	2.11	0.50
11:Y:201:LYS:HE2	16:Y:327:HOH:O	2.09	0.50
6:T:67:ASP:OD1	6:T:68:ARG:N	2.43	0.50
7:U:147:LYS:HB3	7:U:157:TYR:CE2	2.47	0.50
6:T:78:ILE:HB	6:T:79:PRO:HD3	1.93	0.50
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.76	0.50
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.10	0.50
1:A:115:ALA:HB1	1:A:154:GLY:O	2.11	0.50
1:A:151:ASP:HB3	1:A:152:PRO:HD2	1.92	0.50
13:M:9:THR:HG23	13:M:10:SER:N	2.26	0.50
3:C:158:SER:HB3	3:C:177:TYR:CE1	2.47	0.50
13:M:89:PRO:HD2	13:M:120:GLN:OE1	2.11	0.50
8:H:123:TYR:HB3	8:H:142:TRP:CZ2	2.47	0.50
6:T:186:ARG:NH1	6:T:186:ARG:HG3	2.25	0.50
11:Y:17:ASP:OD1	11:Y:33:LYS:NZ	2.42	0.50
9:W:202:ARG:HG3	16:W:307:HOH:O	2.12	0.50
6:T:32:THR:HG23	6:T:47:GLU:OE2	2.12	0.50
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.77	0.50
8:V:172:ASN:HD22	8:V:192:THR:HA	1.77	0.49
4:D:241:ALA:O	4:D:242:GLU:HB2	2.12	0.49
5:S:118:ASN:N	5:S:118:ASN:HD22	2.10	0.49
5:S:61:LYS:O	5:S:72:SER:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:91:GLU:HG2	6:F:111:ARG:CB	2.37	0.49
4:R:185:LEU:O	4:R:189:GLU:HG3	2.12	0.49
4:R:204:LEU:HD23	4:R:204:LEU:C	2.32	0.49
1:A:59:GLU:CD	1:A:59:GLU:H	2.16	0.49
12:Z:3:ASN:ND2	12:Z:3:ASN:C	2.65	0.49
12:L:13:LEU:HD23	12:L:184:VAL:HG22	1.94	0.49
1:A:197:LYS:NZ	1:A:250:LEU:HD11	2.28	0.49
6:T:185:ALA:O	6:T:189:VAL:HG23	2.12	0.49
12:L:161:GLU:HA	12:L:161:GLU:OE1	2.12	0.49
8:H:114:HIS:HB3	16:H:413:HOH:O	2.13	0.49
3:C:161:THR:HG21	3:C:169:VAL:HG22	1.94	0.49
7:G:236:LEU:O	7:G:239:ILE:HG13	2.13	0.49
16:R:316:HOH:O	12:Z:95:HIS:HD2	1.95	0.49
3:C:224:SER:O	3:C:228:ASN:HB2	2.12	0.49
7:G:101:TYR:OH	8:H:66:HIS:HE1	1.96	0.49
8:V:9:ASN:OD1	8:V:10:ASN:N	2.45	0.49
8:H:196:ARG:HH21	9:I:150:GLU:HG3	1.78	0.49
5:S:25:LEU:CD1	5:S:148:PRO:HG2	2.42	0.49
12:Z:48:ASP:OD2	12:Z:76:HIS:HE1	1.96	0.49
2:P:184:LYS:HE2	2:P:186:ASP:OD2	2.12	0.49
12:L:30:ILE:HD12	12:L:30:ILE:C	2.33	0.49
2:P:47:ALA:HB1	2:P:64:LYS:HD3	1.95	0.49
1:A:149:GLN:O	1:A:156:TYR:HA	2.13	0.49
3:Q:166:SER:HA	3:Q:169:VAL:HG13	1.94	0.49
2:B:95:GLN:HE22	2:B:98:LEU:HD23	1.78	0.48
3:Q:30:CYS:H	3:Q:45:GLU:HG2	1.78	0.48
3:Q:40:VAL:HG22	3:Q:143:PRO:HB2	1.94	0.48
5:S:178:PHE:HA	5:S:181:ILE:HG13	1.95	0.48
7:G:45:ILE:HD13	7:G:197:ALA:CB	2.43	0.48
12:L:162:PRO:HB3	8:V:207:ARG:O	2.13	0.48
1:O:106:PRO:HG2	1:O:109:LEU:HB2	1.95	0.48
1:O:122:THR:CG2	2:P:128:ARG:NH2	2.71	0.48
7:G:170:THR:O	7:G:174:GLU:HG3	2.13	0.48
9:W:163:PHE:CE1	9:W:197:ARG:HD2	2.48	0.48
10:X:126:VAL:HG13	10:X:128:LEU:HG	1.94	0.48
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.95	0.48
6:T:86:ASN:ND2	16:T:306:HOH:O	2.45	0.48
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.96	0.48
12:Z:147:MET:N	12:Z:148:PRO:CD	2.76	0.48
10:X:139:TYR:CE2	10:X:172:MET:HG3	2.49	0.48
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:45:ILE:HG13	7:U:216:VAL:HG22	1.95	0.48
12:Z:112:ALA:HA	12:Z:121:ALA:O	2.14	0.48
10:J:139:TYR:CZ	10:J:172:MET:HG3	2.48	0.48
11:Y:82:ILE:HG13	16:Y:343:HOH:O	2.13	0.48
1:A:23:TYR:CD1	7:G:12:PRO:HA	2.48	0.48
12:Z:126:ASP:HB2	12:Z:130:SER:H	1.79	0.47
3:Q:54:ASP:OD1	3:Q:56:ARG:HG3	2.14	0.47
7:U:94:GLU:HG2	7:U:98:LYS:HD3	1.96	0.47
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.95	0.47
5:E:205:LEU:H	5:E:205:LEU:HD23	1.79	0.47
5:S:1:PHE:HZ	5:S:15:THR:OG1	1.96	0.47
8:H:3:ILE:HG13	8:H:99:ILE:HD12	1.96	0.47
9:W:44:HIS:HB3	9:W:49:PHE:CD2	2.49	0.47
5:S:193:VAL:O	5:S:196:ILE:HG22	2.14	0.47
2:P:114:LEU:HA	2:P:114:LEU:HD23	1.71	0.47
6:T:32:THR:HG21	6:T:164:GLY:HA3	1.95	0.47
4:D:59:ILE:HG22	4:D:220:PHE:HZ	1.79	0.47
1:A:31:GLY:HA2	16:A:344:HOH:O	2.14	0.47
2:B:57:GLU:HG2	2:B:60:THR:OG1	2.14	0.47
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.97	0.47
5:S:143:LEU:HD21	5:S:158:THR:HG22	1.97	0.47
2:B:172:GLN:HG3	3:C:50:LEU:HD11	1.96	0.47
1:A:83:ARG:NE	7:G:114:ASN:HD21	2.07	0.47
4:R:45:ARG:O	4:R:45:ARG:CG	2.57	0.47
3:Q:34:VAL:HG23	3:Q:189:CYS:SG	2.54	0.47
8:H:215:GLU:HG3	9:I:197:ARG:HG2	1.97	0.47
9:I:37:ASN:HD22	9:I:37:ASN:C	2.18	0.47
9:I:123:PHE:CD1	9:I:123:PHE:N	2.83	0.47
3:C:66:ASP:HA	10:J:69:ILE:HD13	1.96	0.47
4:D:32:ILE:CD1	4:D:192:VAL:HG23	2.33	0.47
12:Z:195:HIS:CD2	12:Z:197:GLN:H	2.21	0.47
7:G:241:GLU:O	7:G:242:GLN:HB3	2.14	0.47
8:H:38:SER:HB2	8:H:39:PRO:HD2	1.97	0.47
5:S:189:ILE:CG2	5:S:212:ILE:HD13	2.45	0.47
5:S:111:LEU:HD23	5:S:111:LEU:HA	1.73	0.47
12:L:20:PHE:CE2	12:L:177:VAL:HA	2.50	0.47
12:Z:175:LEU:HD22	12:Z:179:GLU:HG2	1.97	0.47
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	1.97	0.47
4:R:159:TYR:CE1	4:R:162:LYS:HD3	2.50	0.47
11:Y:28:SER:HB2	12:Z:137:ARG:HH22	1.80	0.46
6:F:74:TYR:CE1	6:F:81:GLY:HA3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:LEU:HD12	3:C:52:LEU:HA	1.57	0.46
12:Z:126:ASP:HB3	12:Z:128:VAL:N	2.25	0.46
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.50	0.46
7:G:83:ASN:ND2	7:G:83:ASN:C	2.68	0.46
6:F:91:GLU:HG3	6:F:111:ARG:HH11	1.80	0.46
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.45	0.46
8:V:84:LYS:HE2	8:V:119:THR:HG23	1.96	0.46
12:Z:15:ILE:HG12	12:Z:136:CYS:HB2	1.97	0.46
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.51	0.46
3:Q:155:SER:OG	4:R:51:LEU:HD21	2.16	0.46
1:O:48:GLU:HG2	1:O:50:LYS:H	1.81	0.46
14:N:83:LYS:HD3	16:N:229:HOH:O	2.05	0.46
8:V:213:LEU:HD21	9:W:200:LYS:HE3	1.97	0.46
5:E:155:LEU:HD23	6:F:55:LEU:HA	1.98	0.46
13:M:159:VAL:O	13:M:159:VAL:HG23	2.15	0.46
6:F:8:ASN:O	6:F:8:ASN:OD1	2.33	0.46
4:D:185:LEU:O	4:D:189:GLU:HG3	2.16	0.46
3:Q:46:ARG:NH1	3:Q:206:LYS:O	2.48	0.46
8:V:3:ILE:HG13	8:V:99:ILE:HD12	1.98	0.46
7:G:97:TYR:HB2	14:N:61:TYR:HB2	1.96	0.46
1:O:241:GLN:NE2	1:O:245:ASP:OD1	2.48	0.46
3:C:180:LYS:H	3:C:180:LYS:HG2	1.58	0.46
2:P:65:LEU:HD22	2:P:211:GLU:HB3	1.96	0.46
10:J:4:ILE:O	10:J:132:ALA:HA	2.15	0.46
11:Y:66:HIS:CG	11:Y:74:ILE:HD12	2.51	0.46
4:D:82:GLU:OE1	11:K:69:ARG:HD2	2.16	0.46
7:U:148:THR:HG22	7:U:154:TYR:CB	2.46	0.46
11:Y:158:LYS:HD3	11:Y:196:LEU:HD11	1.98	0.46
5:E:136:TYR:CE2	5:E:217:LYS:HA	2.51	0.46
11:K:28:SER:HB2	12:L:137:ARG:HH22	1.80	0.46
6:F:220:THR:HB	6:F:225:LYS:HD3	1.97	0.46
4:D:30:ILE:HG22	4:D:192:VAL:HG22	1.98	0.46
12:Z:125:PHE:HA	12:Z:130:SER:O	2.16	0.46
6:F:36:ILE:HG12	6:F:172:LEU:HD11	1.98	0.46
12:Z:207:VAL:HG22	12:Z:212:VAL:HG22	1.98	0.45
13:M:154:LEU:HD21	13:M:179:ASN:OD1	2.16	0.45
9:I:135:PHE:O	9:I:136:ILE:HD13	2.16	0.45
9:W:62:LEU:CD1	9:W:104:VAL:HG21	2.46	0.45
5:S:44:VAL:HG23	5:S:188:LEU:HD13	1.98	0.45
5:S:216:GLY:O	5:S:217:LYS:C	2.54	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:52:MET:HB2	12:Z:111:ILE:HG22	1.97	0.45
3:C:77:ASN:N	3:C:77:ASN:HD22	2.14	0.45
4:D:178:GLU:HG3	4:D:191:LEU:HD11	1.97	0.45
13:M:16:TYR:CE1	13:M:170:VAL:HG13	2.51	0.45
5:S:62:ILE:HG21	5:S:213:ALA:HB2	1.99	0.45
5:S:63:ILE:HB	5:S:71:LEU:CD2	2.46	0.45
3:C:186:VAL:HG21	3:C:214:LYS:HE3	1.98	0.45
12:Z:23:LEU:HD13	12:Z:43:VAL:CG1	2.44	0.45
1:A:2:THR:O	1:A:4:ARG:HG3	2.17	0.45
11:Y:99:THR:HG22	11:Y:115:VAL:O	2.17	0.45
7:U:34:LEU:C	7:U:34:LEU:HD12	2.37	0.45
7:G:132:LEU:O	7:G:147:LYS:HA	2.16	0.45
2:B:184:LYS:HE2	2:B:186:ASP:H	1.82	0.45
2:P:48:GLU:OE2	2:P:200:THR:HG23	2.16	0.45
8:V:126:SER:O	8:V:127:LEU:HD23	2.16	0.45
12:L:126:ASP:HB3	12:L:128:VAL:H	1.81	0.45
10:X:23:ARG:HD3	10:X:23:ARG:HA	1.79	0.45
7:U:83:ASN:HD22	7:U:84:ALA:N	2.15	0.45
6:T:123:ASN:ND2	6:T:123:ASN:C	2.64	0.45
11:K:13:ILE:HG13	11:K:153:ALA:HB1	1.99	0.45
4:D:239:GLU:C	4:D:241:ALA:H	2.20	0.45
2:B:95:GLN:NE2	16:B:307:HOH:O	2.44	0.45
6:F:110:ASP:O	6:F:114:GLN:HG2	2.17	0.45
12:Z:149:PHE:CE1	12:Z:153:GLN:HG3	2.52	0.44
5:E:84:SER:O	5:E:88:ARG:HG3	2.17	0.44
16:R:313:HOH:O	12:Z:79:HIS:CD2	2.69	0.44
10:J:172:MET:CE	10:J:174:MET:HB2	2.48	0.44
1:A:94:HIS:CD2	8:H:61:SER:OG	2.62	0.44
12:L:3:ASN:HD22	12:L:5:TYR:H	1.64	0.44
13:M:170:VAL:HG22	16:M:327:HOH:O	2.17	0.44
6:F:175:LEU:HD11	6:F:191:GLN:HG3	2.00	0.44
2:B:159:TRP:CD2	2:B:162:ILE:HD13	2.52	0.44
5:S:205:LEU:HA	5:S:209:ASN:ND2	2.33	0.44
11:K:38:ASN:HB3	16:K:337:HOH:O	2.16	0.44
2:B:198:LYS:HE2	2:B:198:LYS:HB3	1.60	0.44
12:Z:38:ARG:HD3	12:Z:200:ASP:OD1	2.17	0.44
12:Z:5:TYR:CE1	12:Z:106:TYR:HB2	2.52	0.44
2:B:57:GLU:O	2:B:61:SER:HB2	2.17	0.44
11:K:31:VAL:CG1	11:K:45:MET:HE2	2.48	0.44
5:S:166:GLY:HA3	5:S:198:GLN:O	2.17	0.44
9:W:66:PHE:CZ	9:W:90:VAL:HG22	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:185:ASP:HB2	16:J:224:HOH:O	2.16	0.44
2:P:178:ASP:HB2	2:P:191:LEU:HD21	2.00	0.44
1:O:61:LEU:HG	7:U:155:VAL:HG23	1.99	0.44
3:Q:51:LYS:HG3	3:Q:206:LYS:HZ1	1.83	0.44
8:V:215:GLU:HG3	9:W:197:ARG:HG2	1.99	0.44
16:R:320:HOH:O	12:Z:79:HIS:HE1	2.00	0.44
13:M:161:ARG:CG	13:M:161:ARG:NH1	2.68	0.44
7:U:231:ASN:HB3	16:U:302:HOH:O	2.17	0.44
11:K:7:ARG:NE	11:K:125:ASP:OD1	2.45	0.44
5:S:81:ARG:O	5:S:85:ASN:HB2	2.18	0.44
10:X:8:ARG:NE	16:X:202:HOH:O	2.36	0.44
2:B:215:ILE:HG12	2:B:226:GLN:HG2	1.99	0.44
9:W:62:LEU:HD11	9:W:104:VAL:HG21	1.99	0.44
1:O:61:LEU:HA	1:O:61:LEU:HD23	1.52	0.44
8:H:172:ASN:HD22	8:H:192:THR:HA	1.82	0.44
4:R:60:VAL:HG21	4:R:81:ILE:HG13	1.99	0.44
4:R:44:LYS:HE3	4:R:210:GLN:HB2	2.00	0.44
3:Q:27:ARG:HB3	3:Q:27:ARG:HH11	1.82	0.44
13:M:48:ASN:ND2	13:M:48:ASN:N	2.61	0.44
9:W:41:LYS:O	9:W:51:GLY:HA2	2.18	0.44
5:S:71:LEU:HA	5:S:132:LEU:O	2.17	0.44
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.51	0.44
5:E:87:LEU:HD12	5:E:87:LEU:HA	1.76	0.44
2:B:149:THR:O	2:B:156:TYR:HA	2.19	0.43
6:F:33:SER:HB3	6:F:46:VAL:HG23	1.99	0.43
5:E:98:PHE:O	13:M:91:TYR:HA	2.18	0.43
9:I:21:ALA:HA	9:I:187:TYR:O	2.17	0.43
4:R:193:LEU:HD22	4:R:211:LEU:HD11	2.00	0.43
10:X:135:TYR:O	10:X:138:PHE:HB2	2.17	0.43
9:I:191:LYS:HB3	9:I:191:LYS:HE3	1.64	0.43
4:D:4:VAL:HG12	4:D:15:GLN:HG3	1.99	0.43
2:B:119:GLN:HG3	3:C:78:ALA:HB1	1.99	0.43
5:S:70:GLY:HA3	5:S:221:PHE:CZ	2.53	0.43
6:T:9:SER:HB2	7:U:126:ARG:HD3	2.00	0.43
3:Q:186:VAL:HG13	3:Q:212:VAL:HG11	2.00	0.43
5:E:70:GLY:HA3	5:E:221:PHE:CE2	2.52	0.43
12:L:26:ASP:HA	12:L:201:GLY:O	2.17	0.43
14:N:114:PRO:HD2	14:N:118:SER:O	2.17	0.43
1:A:196:LEU:HD23	1:A:209:ILE:HD12	1.99	0.43
7:U:196:PHE:O	7:U:197:ALA:C	2.55	0.43
1:A:193:LEU:HA	1:A:193:LEU:HD23	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.00	0.43
12:L:1:GLN:HE21	13:M:1:THR:HG21	1.80	0.43
12:Z:42:LYS:NZ	16:Z:320:HOH:O	2.37	0.43
5:E:155:LEU:HD13	5:E:158:THR:HB	1.99	0.43
1:A:231:LYS:HE3	1:A:231:LYS:HB2	1.79	0.43
12:Z:1:GLN:HE21	12:Z:2:PHE:H	1.67	0.43
5:S:206:THR:H	5:S:209:ASN:HB3	1.81	0.43
5:S:134:ILE:HD12	5:S:215:VAL:HG12	1.99	0.43
2:P:23:TYR:O	2:P:26:GLU:HB3	2.17	0.43
11:K:191:HIS:N	11:K:191:HIS:CD2	2.87	0.43
1:A:11:THR:HB	2:B:20:GLN:NE2	2.34	0.43
7:G:30:ASN:HA	7:G:164:PRO:HG2	2.00	0.43
5:E:137:ASP:HB2	16:M:345:HOH:O	2.18	0.43
12:L:17:GLY:HA3	12:L:20:PHE:CZ	2.53	0.43
6:T:171:GLU:HB3	6:T:195:ILE:HG12	1.99	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.81	0.43
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.49	0.43
8:H:213:LEU:HD13	11:Y:211:ILE:HG22	2.01	0.43
12:L:1:GLN:NE2	13:M:1:THR:CG2	2.80	0.43
4:D:159:TYR:CE1	4:D:162:LYS:HD3	2.54	0.43
10:X:23:ARG:HD2	16:X:217:HOH:O	2.19	0.43
11:K:7:ARG:HG2	11:K:110:PRO:HB2	2.00	0.43
5:E:2:ARG:O	5:E:3:ASN:C	2.57	0.43
9:I:11:VAL:HA	9:I:23:ALA:O	2.19	0.43
5:E:231:LYS:HD3	5:E:232:TYR:CE2	2.53	0.43
5:S:206:THR:H	5:S:209:ASN:CB	2.32	0.43
1:O:64:VAL:HG11	1:O:212:ALA:HB3	2.01	0.43
9:W:187:TYR:OH	9:W:196:LYS:HE3	2.19	0.43
3:C:29:THR:O	3:C:74:SER:OG	2.36	0.43
4:D:120:SER:HB2	5:E:124:GLY:HA3	2.01	0.43
11:Y:52:CYS:SG	11:Y:97:MET:HB3	2.58	0.43
5:E:173:ARG:HB3	5:E:173:ARG:NH1	2.34	0.43
10:X:194:ASP:N	10:X:194:ASP:OD1	2.52	0.43
3:Q:51:LYS:HB3	3:Q:51:LYS:HE3	1.81	0.42
11:K:12:ILE:HB	11:K:180:VAL:HB	2.00	0.42
9:W:14:MET:HG3	9:W:166:ILE:HD12	2.01	0.42
11:K:85:ASN:ND2	16:K:322:HOH:O	2.51	0.42
13:M:96:LEU:O	13:M:100:MET:HG2	2.19	0.42
5:E:214:ILE:HG13	5:E:215:VAL:N	2.34	0.42
1:O:149:GLN:O	1:O:156:TYR:HA	2.19	0.42
9:I:170:LEU:HD21	9:I:184:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:8:ARG:HG2	10:J:8:ARG:O	2.18	0.42
3:C:160:GLN:HE22	3:C:170:ARG:HH21	1.68	0.42
10:J:3:ILE:O	10:J:17:SER:HA	2.19	0.42
4:R:159:TYR:CZ	4:R:162:LYS:HD3	2.55	0.42
7:U:148:THR:HG22	7:U:154:TYR:HB2	2.02	0.42
9:W:11:VAL:HG22	9:W:24:CYS:HB3	2.01	0.42
9:W:171:LEU:HA	9:W:171:LEU:HD12	1.92	0.42
3:Q:149:GLU:HB2	3:Q:150:PRO:CD	2.50	0.42
16:H:444:HOH:O	9:I:161:ASP:HA	2.20	0.42
8:V:152:ILE:HD11	8:V:177:VAL:HG21	2.02	0.42
7:G:119:TYR:CD1	7:G:119:TYR:N	2.86	0.42
6:T:57:PRO:O	6:T:58:GLN:HB2	2.20	0.42
4:D:191:LEU:HD12	4:D:191:LEU:HA	1.87	0.42
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.54	0.42
1:A:42:GLY:HA2	1:A:145:PHE:CE1	2.54	0.42
5:S:2:ARG:O	5:S:3:ASN:C	2.58	0.42
3:Q:198:LEU:HA	3:Q:198:LEU:HD23	1.87	0.42
4:R:78:ARG:HD3	4:R:78:ARG:HA	1.72	0.42
5:E:68:HIS:O	5:E:135:GLY:HA2	2.19	0.42
12:Z:48:ASP:OD2	12:Z:76:HIS:CE1	2.73	0.42
12:Z:38:ARG:NH1	12:Z:221:ARG:O	2.51	0.42
1:A:196:LEU:HD12	1:A:196:LEU:HA	1.70	0.42
8:H:112:SER:O	8:H:119:THR:HA	2.19	0.42
6:T:41:GLY:HA3	6:T:215:CYS:O	2.19	0.42
12:Z:49:ASN:ND2	12:Z:211:GLY:HA2	2.32	0.42
6:T:50:ILE:O	6:T:51:THR:C	2.58	0.42
7:U:147:LYS:HB3	7:U:157:TYR:HE2	1.84	0.42
4:R:135:LEU:HB3	4:R:147:LEU:HD11	2.02	0.42
1:O:89:SER:OG	1:O:114:VAL:HG22	2.19	0.42
3:C:82:ILE:CD1	3:C:82:ILE:N	2.83	0.42
9:I:1:SER:HB3	16:I:363:HOH:O	2.20	0.42
8:H:17:ASP:HA	8:H:172:ASN:O	2.20	0.42
8:H:130:GLY:O	8:H:131:SER:C	2.58	0.42
14:N:15:GLY:HA2	14:N:174:ARG:O	2.20	0.42
5:S:170:TYR:CD1	5:S:170:TYR:C	2.93	0.42
7:U:63:ILE:HD12	7:U:215:GLU:HG3	2.02	0.42
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.00	0.41
8:H:157:ASP:OD2	15:H:301:2YD:H9	2.20	0.41
5:S:205:LEU:HA	5:S:209:ASN:HD22	1.83	0.41
5:S:155:LEU:HD23	6:T:55:LEU:HA	2.01	0.41
8:H:172:ASN:HB3	8:H:191:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:44:VAL:HG23	5:E:188:LEU:HD13	2.01	0.41
13:M:15:LYS:HD2	13:M:165:ILE:HD13	2.02	0.41
10:J:93:ARG:NH1	16:J:228:HOH:O	2.50	0.41
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.41
7:U:66:ILE:HD11	7:U:72:MET:HE1	2.02	0.41
11:Y:162:LEU:HD13	11:Y:196:LEU:HD23	2.02	0.41
3:Q:134:ALA:HA	3:Q:144:LYS:O	2.20	0.41
4:D:16:VAL:O	4:D:19:SER:HB3	2.20	0.41
7:U:169:ILE:CD1	7:U:201:MET:HE3	2.48	0.41
12:L:3:ASN:ND2	12:L:3:ASN:C	2.67	0.41
14:N:84:GLU:O	14:N:88:GLU:HB2	2.19	0.41
3:Q:14:HIS:HB3	3:Q:19:GLU:OE1	2.21	0.41
4:D:190:LEU:HD12	4:D:190:LEU:HA	1.96	0.41
13:M:129:TYR:HE2	13:M:144:THR:HG22	1.85	0.41
4:R:113:LEU:HD13	5:S:125:ARG:HH21	1.85	0.41
14:N:161:GLN:HE22	14:N:165:TRP:HE1	1.67	0.41
5:S:203:GLU:CG	5:S:204:SER:N	2.83	0.41
7:U:72:MET:HE1	7:U:85:ALA:HA	2.02	0.41
2:B:193:LEU:HD21	2:B:212:PHE:CE1	2.55	0.41
5:S:88:ARG:NH1	12:Z:77:PHE:HB3	2.36	0.41
5:E:202:ASP:HB3	5:E:203:GLU:H	1.60	0.41
6:T:30:GLY:O	6:T:163:LYS:HB2	2.21	0.41
7:G:185:ILE:HD13	7:G:185:ILE:N	2.36	0.41
8:H:41:ILE:HG12	8:H:76:VAL:HG22	2.01	0.41
2:B:42:GLY:CA	2:B:185:VAL:CG2	2.98	0.41
12:Z:164:THR:O	12:Z:165:ASN:CB	2.69	0.41
4:D:115:PHE:HB3	4:D:126:MET:HE3	2.03	0.41
10:X:70:ARG:NH1	16:X:218:HOH:O	2.45	0.41
9:W:137:VAL:HG11	9:W:145:LEU:HB3	2.01	0.41
6:F:117:GLN:HE21	6:F:117:GLN:HB3	1.76	0.41
14:N:193:TYR:CD1	14:N:193:TYR:C	2.94	0.41
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.68	0.41
9:I:141:ALA:HB2	9:I:177:ASP:CB	2.51	0.41
5:S:71:LEU:HD23	5:S:71:LEU:O	2.21	0.41
8:H:152:ILE:O	8:H:156:SER:HB2	2.21	0.41
4:R:59:ILE:HG22	4:R:220:PHE:HZ	1.84	0.41
8:V:102:GLY:HA2	8:V:178:MET:SD	2.61	0.41
10:X:110:LYS:HB2	10:X:110:LYS:HZ3	1.84	0.41
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.56	0.41
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.03	0.41
7:G:202:ILE:HG23	7:G:207:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:LEU:HA	2:B:55:LEU:HD12	1.90	0.41
12:L:3:ASN:HD22	12:L:4:PRO:CD	2.34	0.41
11:Y:86:LEU:C	11:Y:86:LEU:CD1	2.88	0.41
3:Q:200:VAL:O	3:Q:200:VAL:HG12	2.21	0.41
1:O:109:LEU:O	1:O:112:SER:HB3	2.20	0.41
12:L:160:TYR:CG	12:L:166:GLY:HA2	2.56	0.41
4:R:85:ARG:HG2	11:Y:68:LEU:HD13	2.03	0.41
13:M:119:VAL:HG23	13:M:200:ILE:HG22	2.03	0.41
3:C:230:TYR:O	3:C:234:ILE:HG13	2.21	0.41
14:N:161:GLN:NE2	14:N:165:TRP:HE1	2.19	0.41
12:L:49:ASN:ND2	12:L:211:GLY:HA2	2.34	0.41
2:B:209:ARG:HB3	2:B:209:ARG:CZ	2.51	0.41
5:S:188:LEU:HA	5:S:188:LEU:HD23	1.89	0.41
3:Q:228:ASN:O	3:Q:231:VAL:HB	2.21	0.41
13:M:213:GLN:HE21	13:M:213:GLN:HB3	1.59	0.41
6:T:241:LYS:HG2	6:T:241:LYS:O	2.21	0.41
9:W:12:VAL:HG23	9:W:137:VAL:HG12	2.03	0.40
3:C:222:LEU:HB3	3:C:227:ILE:HG13	2.03	0.40
12:Z:17:GLY:HA3	12:Z:20:PHE:CZ	2.56	0.40
9:I:17:LYS:HE2	9:I:156:ASN:HB3	2.02	0.40
10:X:64:ILE:HD12	10:X:80:VAL:HG22	2.04	0.40
3:Q:167:LYS:HB2	16:Q:315:HOH:O	2.21	0.40
3:C:112:ALA:HB1	3:C:152:GLY:O	2.21	0.40
3:Q:160:GLN:NE2	3:Q:170:ARG:HE	2.05	0.40
11:Y:86:LEU:O	11:Y:86:LEU:HD13	2.21	0.40
1:O:2:THR:O	1:O:4:ARG:HG2	2.21	0.40
9:I:82:GLU:HB3	9:I:83:PRO:HD2	2.04	0.40
3:C:108:THR:HG21	3:C:146:TYR:HB3	2.04	0.40
6:F:139:LYS:HG2	6:F:139:LYS:O	2.20	0.40
2:P:50:LYS:O	2:P:51:VAL:O	2.39	0.40
1:A:128:ARG:HH21	7:G:120:THR:HG23	1.82	0.40
10:J:4:ILE:HD12	10:J:4:ILE:HG23	1.84	0.40
7:U:63:ILE:CD1	7:U:215:GLU:HG3	2.52	0.40
13:M:129:TYR:CE2	13:M:144:THR:HG22	2.56	0.40
4:R:168:SER:HA	4:R:171:ALA:HB3	2.03	0.40
3:Q:41:VAL:CG1	3:Q:210:ILE:HG23	2.52	0.40
9:W:96:GLU:HG2	16:W:355:HOH:O	2.21	0.40
6:F:210:LEU:HD21	6:F:212:ILE:HD11	2.02	0.40
1:A:106:PRO:HG2	1:A:109:LEU:HG	2.03	0.40
10:X:4:ILE:HD13	10:X:4:ILE:HA	1.65	0.40
8:H:218:VAL:HB	9:I:194:VAL:HG12	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	A	248/250 (99%)	234 (94%)	13 (5%)	1 (0%)	39	65
1	O	248/250 (99%)	232 (94%)	13 (5%)	3 (1%)	16	33
2	B	242/258 (94%)	228 (94%)	10 (4%)	4 (2%)	11	22
2	P	242/258 (94%)	228 (94%)	10 (4%)	4 (2%)	11	22
3	C	239/254 (94%)	226 (95%)	12 (5%)	1 (0%)	39	65
3	Q	239/254 (94%)	223 (93%)	11 (5%)	5 (2%)	9	16
4	D	240/260 (92%)	226 (94%)	11 (5%)	3 (1%)	15	30
4	R	240/260 (92%)	220 (92%)	17 (7%)	3 (1%)	15	30
5	E	231/234 (99%)	216 (94%)	9 (4%)	6 (3%)	7	11
5	S	231/234 (99%)	210 (91%)	16 (7%)	5 (2%)	8	15
6	F	242/288 (84%)	233 (96%)	9 (4%)	0	100	100
6	T	242/288 (84%)	229 (95%)	12 (5%)	1 (0%)	39	65
7	G	241/252 (96%)	233 (97%)	8 (3%)	0	100	100
7	U	241/252 (96%)	230 (95%)	8 (3%)	3 (1%)	16	33
8	H	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
8	V	220/232 (95%)	209 (95%)	10 (4%)	1 (0%)	34	60
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	193 (96%)	8 (4%)	1 (0%)	34	60
10	J	196/198 (99%)	188 (96%)	7 (4%)	1 (0%)	34	60
10	X	196/198 (99%)	187 (95%)	9 (5%)	0	100	100
11	K	210/212 (99%)	200 (95%)	10 (5%)	0	100	100
11	Y	207/212 (98%)	200 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	34	60
12	Z	220/222 (99%)	207 (94%)	13 (6%)	0	100	100
13	M	231/246 (94%)	225 (97%)	5 (2%)	1 (0%)	39	65
13	a	231/246 (94%)	219 (95%)	11 (5%)	1 (0%)	39	65
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6309/6614 (95%)	5988 (95%)	276 (4%)	45 (1%)	26	51

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
5	E	2	ARG
5	E	3	ASN
2	P	51	VAL
3	Q	52	LEU
3	Q	205	ALA
4	R	119	ALA
5	S	2	ARG
5	S	3	ASN
7	U	51	PRO
2	B	221	ASP
4	D	119	ALA
4	D	240	ALA
5	E	202	ASP
1	O	2	THR
1	O	166	LYS
2	P	221	ASP
3	Q	183	PRO
3	Q	202	GLN
7	U	2	GLY
7	U	242	GLN
1	A	2	THR
5	E	203	GLU
5	E	227	GLU
3	Q	203	THR
4	R	2	ARG
5	S	203	GLU
5	S	217	LYS
6	T	51	THR

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Mol	Chain	Res	Type
8	V	171	SER
2	B	200	THR
2	B	219	ALA
4	D	114	ARG
4	R	123	GLU
3	C	202	GLN
1	O	53	SER
2	P	3	ARG
12	L	126	ASP
2	P	200	THR
5	E	181	ILE
9	W	100	GLY
10	J	9	VAL
13	a	229	GLY
5	S	181	ILE
13	M	229	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	195 (93%)	14 (7%)	20	40
1	O	209/209 (100%)	198 (95%)	11 (5%)	28	53
2	B	203/216 (94%)	176 (87%)	27 (13%)	5	8
2	P	203/216 (94%)	175 (86%)	28 (14%)	4	7
3	C	213/226 (94%)	191 (90%)	22 (10%)	9	16
3	Q	213/226 (94%)	183 (86%)	30 (14%)	4	7
4	D	198/215 (92%)	180 (91%)	18 (9%)	12	22
4	R	198/215 (92%)	180 (91%)	18 (9%)	12	22
5	E	192/193 (100%)	165 (86%)	27 (14%)	4	7
5	S	192/193 (100%)	169 (88%)	23 (12%)	6	11
6	F	201/239 (84%)	178 (89%)	23 (11%)	7	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	T	201/239 (84%)	175 (87%)	26 (13%)	5	9
7	G	207/210 (99%)	193 (93%)	14 (7%)	20	39
7	U	207/210 (99%)	196 (95%)	11 (5%)	28	53
8	H	181/190 (95%)	164 (91%)	17 (9%)	11	20
8	V	181/190 (95%)	165 (91%)	16 (9%)	12	24
9	I	172/173 (99%)	161 (94%)	11 (6%)	22	43
9	W	172/173 (99%)	160 (93%)	12 (7%)	19	37
10	J	175/175 (100%)	167 (95%)	8 (5%)	33	61
10	X	175/175 (100%)	164 (94%)	11 (6%)	22	44
11	K	169/169 (100%)	154 (91%)	15 (9%)	12	23
11	Y	168/169 (99%)	159 (95%)	9 (5%)	27	52
12	L	185/185 (100%)	170 (92%)	15 (8%)	15	28
12	Z	185/185 (100%)	172 (93%)	13 (7%)	19	37
13	M	199/208 (96%)	187 (94%)	12 (6%)	24	47
13	a	199/208 (96%)	184 (92%)	15 (8%)	17	33
14	N	162/162 (100%)	152 (94%)	10 (6%)	23	45
14	b	162/162 (100%)	154 (95%)	8 (5%)	31	57
All	All	5331/5540 (96%)	4867 (91%)	464 (9%)	13	24

All (464) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	30	GLN
1	A	58	SER
1	A	59	GLU
1	A	61	LEU
1	A	62	SER
1	A	84	VAL
1	A	112	SER
1	A	122	THR
1	A	157	PHE
1	A	197	LYS
1	A	199	SER
1	A	201	GLU
1	A	250	LEU

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Mol	Chain	Res	Type
2	B	2	SER
2	B	17	ARG
2	B	54	THR
2	B	55	LEU
2	B	58	GLN
2	B	59	ASP
2	B	60	THR
2	B	67	LYS
2	B	69	ASN
2	B	79	LEU
2	B	80	THR
2	B	89	THR
2	B	114	LEU
2	B	119	GLN
2	B	149	THR
2	B	169	SER
2	B	184	LYS
2	B	191	LEU
2	B	200	THR
2	B	202	SER
2	B	206	THR
2	B	217	LYS
2	B	220	ASN
2	B	223	GLU
2	B	230	LYS
2	B	238	LEU
2	B	244	THR
3	C	4	ARG
3	C	19	GLU
3	C	35	LYS
3	C	37	LYS
3	C	50	LEU
3	C	51	LYS
3	C	61	LYS
3	C	74	SER
3	C	77	ASN
3	C	107	LEU
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	185	THR

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Mol	Chain	Res	Type
3	C	202	GLN
3	C	206	LYS
3	C	213	VAL
3	C	224	SER
3	C	225	GLU
3	C	238	LYS
3	C	241	GLN
4	D	4	VAL
4	D	5	SER
4	D	20	LEU
4	D	40	LEU
4	D	48	SER
4	D	57	GLU
4	D	68	CYS
4	D	123	GLU
4	D	124	ARG
4	D	155	THR
4	D	169	GLU
4	D	176	LEU
4	D	186	LYS
4	D	190	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
5	E	1	PHE
5	E	3	ASN
5	E	8	ASP
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	53	ASP
5	E	55	LEU
5	E	61	LYS
5	E	71	LEU
5	E	99	ASN
5	E	116	GLN
5	E	121	SER
5	E	144	LEU
5	E	178	PHE
5	E	184	ASN
5	E	187	GLU

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Mol	Chain	Res	Type
5	E	188	LEU
5	E	198	GLN
5	E	202	ASP
5	E	205	LEU
5	E	207	VAL
5	E	208	ASP
5	E	219	THR
5	E	222	THR
5	E	227	GLU
5	E	231	LYS
6	F	32	THR
6	F	39	ASN
6	F	72	CYS
6	F	75	SER
6	F	94	SER
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	165	ARG
6	F	167	SER
6	F	172	LEU
6	F	181	GLU
6	F	186	ARG
6	F	187	GLU
6	F	191	GLN
6	F	198	LEU
6	F	201	GLU
6	F	205	GLU
6	F	207	ASP
6	F	214	TRP
6	F	221	ASN
6	F	228	LYS
6	F	241	LYS
7	G	45	ILE
7	G	68	ARG
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	120	THR
7	G	166	GLN
7	G	171	THR
7	G	179	LYS

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Mol	Chain	Res	Type
7	G	207	THR
7	G	208	GLU
7	G	221	LYS
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	56	THR
8	H	63	ILE
8	H	68	LEU
8	H	84	LYS
8	H	100	VAL
8	H	108	SER
8	H	113	ILE
8	H	121	VAL
8	H	144	GLN
8	H	153	LYS
8	H	182	LYS
8	H	196	ARG
8	H	198	GLU
8	H	201	LYS
9	I	4	SER
9	I	30	SER
9	I	37	ASN
9	I	68	TYR
9	I	123	PHE
9	I	124	ASP
9	I	125	LEU
9	I	133	LYS
9	I	171	LEU
9	I	182	TRP
9	I	191	LYS
10	J	35	THR
10	J	36	ARG
10	J	49	GLU
10	J	53	THR
10	J	69	ILE
10	J	71	GLU
10	J	78	GLN
10	J	127	GLU
11	K	4	LEU

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Mol	Chain	Res	Type
11	K	8	PHE
11	K	9	GLN
11	K	32	LYS
11	K	65	LEU
11	K	87	VAL
11	K	104	TYR
11	K	106	ARG
11	K	107	LYS
11	K	128	CYS
11	K	140	LEU
11	K	145	LYS
11	K	148	LEU
11	K	177	LEU
11	K	208	ASN
12	L	1	GLN
12	L	3	ASN
12	L	23	LEU
12	L	49	ASN
12	L	67	ARG
12	L	71	SER
12	L	109	THR
12	L	124	SER
12	L	126	ASP
12	L	135	GLN
12	L	150	LEU
12	L	165	ASN
12	L	172	LEU
12	L	213	ARG
12	L	214	LYS
13	M	48	ASN
13	M	68	LYS
13	M	69	ASP
13	M	104	ARG
13	M	138	SER
13	M	154	LEU
13	M	157	LYS
13	M	161	ARG
13	M	170	VAL
13	M	171	GLN
13	M	206	LEU
13	M	212	LEU
14	N	10	ASP

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Mol	Chain	Res	Type
14	N	22	THR
14	N	36	ARG
14	N	83	LYS
14	N	104	ASP
14	N	105	LYS
14	N	107	LYS
14	N	119	VAL
14	N	178	LEU
14	N	195	GLN
1	O	4	ARG
1	O	30	GLN
1	O	52	SER
1	O	58	SER
1	O	92	VAL
1	O	108	LYS
1	O	109	LEU
1	O	157	PHE
1	O	164	ILE
1	O	197	LYS
1	O	229	THR
2	P	2	SER
2	P	3	ARG
2	P	52	THR
2	P	53	SER
2	P	54	THR
2	P	55	LEU
2	P	58	GLN
2	P	60	THR
2	P	65	LEU
2	P	69	ASN
2	P	79	LEU
2	P	89	THR
2	P	119	GLN
2	P	149	THR
2	P	169	SER
2	P	176	GLN
2	P	184	LYS
2	P	191	LEU
2	P	200	THR
2	P	203	SER
2	P	212	PHE
2	P	216	ARG

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Mol	Chain	Res	Type
2	P	217	LYS
2	P	220	ASN
2	P	223	GLU
2	P	225	TYR
2	P	230	LYS
2	P	244	THR
3	Q	4	ARG
3	Q	19	GLU
3	Q	27	ARG
3	Q	37	LYS
3	Q	51	LYS
3	Q	53	GLN
3	Q	55	THR
3	Q	56	ARG
3	Q	58	THR
3	Q	60	SER
3	Q	61	LYS
3	Q	70	VAL
3	Q	107	LEU
3	Q	116	GLN
3	Q	130	SER
3	Q	147	GLN
3	Q	153	ILE
3	Q	160	GLN
3	Q	167	LYS
3	Q	169	VAL
3	Q	175	LYS
3	Q	185	THR
3	Q	187	GLU
3	Q	202	GLN
3	Q	206	LYS
3	Q	213	VAL
3	Q	216	ASP
3	Q	232	THR
3	Q	233	GLN
3	Q	238	LYS
4	R	5	SER
4	R	20	LEU
4	R	40	LEU
4	R	44	LYS
4	R	68	CYS
4	R	78	ARG

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Mol	Chain	Res	Type
4	R	102	GLU
4	R	123	GLU
4	R	124	ARG
4	R	155	THR
4	R	158	ARG
4	R	176	LEU
4	R	182	SER
4	R	190	LEU
4	R	193	LEU
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	1	PHE
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	197	SER
5	S	198	GLN
5	S	203	GLU
5	S	205	LEU
5	S	207	VAL
5	S	208	ASP
5	S	211	SER
5	S	217	LYS
5	S	219	THR
5	S	222	THR
5	S	231	LYS
6	T	32	THR
6	T	39	ASN
6	T	47	GLU
6	T	52	SER
6	T	91	GLU
6	T	94	SER
6	T	117	GLN

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Mol	Chain	Res	Type
6	T	123	ASN
6	T	126	ARG
6	T	139	LYS
6	T	148	GLU
6	T	161	THR
6	T	165	ARG
6	T	167	SER
6	T	172	LEU
6	T	181	GLU
6	T	186	ARG
6	T	191	GLN
6	T	198	LEU
6	T	201	GLU
6	T	205	GLU
6	T	207	ASP
6	T	214	TRP
6	T	228	LYS
6	T	231	LEU
6	T	240	GLN
7	U	39	LYS
7	U	68	ARG
7	U	83	ASN
7	U	115	LEU
7	U	171	THR
7	U	201	MET
7	U	215	GLU
7	U	221	LYS
7	U	235	ARG
7	U	236	LEU
7	U	242	GLN
8	V	30	ASN
8	V	34	LEU
8	V	38	SER
8	V	43	CYS
8	V	55	VAL
8	V	56	THR
8	V	59	ILE
8	V	68	LEU
8	V	100	VAL
8	V	121	VAL
8	V	131	SER
8	V	144	GLN

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Mol	Chain	Res	Type
8	V	196	ARG
8	V	198	GLU
8	V	220	ILE
8	V	222	ASP
9	W	17	LYS
9	W	20	VAL
9	W	37	ASN
9	W	114	LYS
9	W	124	ASP
9	W	131	GLU
9	W	133	LYS
9	W	151	SER
9	W	171	LEU
9	W	191	LYS
9	W	192	ASP
9	W	202	ARG
10	X	2	ASP
10	X	35	THR
10	X	36	ARG
10	X	53	THR
10	X	69	ILE
10	X	71	GLU
10	X	78	GLN
10	X	91	SER
10	X	93	ARG
10	X	126	VAL
10	X	172	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	25	TRP
11	Y	65	LEU
11	Y	97	MET
11	Y	104	TYR
11	Y	106	ARG
11	Y	107	LYS
11	Y	148	LEU
12	Z	1	GLN
12	Z	3	ASN
12	Z	18	GLU
12	Z	23	LEU
12	Z	49	ASN
12	Z	67	ARG

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Mol	Chain	Res	Type
12	Z	109	THR
12	Z	124	SER
12	Z	126	ASP
12	Z	135	GLN
12	Z	150	LEU
12	Z	165	ASN
12	Z	172	LEU
13	a	29	SER
13	a	48	ASN
13	a	68	LYS
13	a	69	ASP
13	a	104	ARG
13	a	154	LEU
13	a	157	LYS
13	a	159	VAL
13	a	161	ARG
13	a	170	VAL
13	a	192	SER
13	a	212	LEU
13	a	214	VAL
13	a	226	LYS
13	a	233	ILE
14	b	83	LYS
14	b	104	ASP
14	b	105	LYS
14	b	107	LYS
14	b	115	LEU
14	b	119	VAL
14	b	144	GLU
14	b	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (154) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
2	B	20	GLN
2	B	69	ASN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN

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Mol	Chain	Res	Type
2	B	220	ASN
3	C	17	GLN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	207	ASN
4	D	15	GLN
4	D	100	ASN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
5	E	198	GLN
5	E	209	ASN
6	F	19	GLN
6	F	39	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	143	HIS
6	F	191	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	30	ASN
8	H	66	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
9	I	172	ASN
10	J	55	GLN
10	J	86	GLN
10	J	118	GLN
10	J	191	GLN

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Mol	Chain	Res	Type
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	95	HIS
12	L	135	GLN
12	L	158	ASN
12	L	195	HIS
13	M	18	ASN
13	M	48	ASN
13	M	171	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	38	HIS
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
14	N	195	GLN
1	O	30	GLN
1	O	94	HIS
2	P	20	GLN
2	P	69	ASN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
3	Q	17	GLN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	225	ASN
5	S	30	GLN

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Mol	Chain	Res	Type
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
5	S	198	GLN
5	S	209	ASN
6	T	19	GLN
6	T	39	ASN
6	T	83	HIS
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
7	U	175	ASN
7	U	184	HIS
7	U	186	ASN
8	V	30	ASN
8	V	66	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	37	ASN
9	W	88	GLN
10	X	55	GLN
10	X	86	GLN
10	X	118	GLN
10	X	191	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN

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Mol	Chain	Res	Type
12	Z	55	ASN
12	Z	70	ASN
12	Z	76	HIS
12	Z	79	HIS
12	Z	135	GLN
12	Z	165	ASN
12	Z	195	HIS
13	a	2	GLN
13	a	18	ASN
13	a	26	ASN
13	a	37	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	213	GLN
14	b	38	HIS
14	b	69	GLN
14	b	145	ASN
14	b	161	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 ⓘ

2 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	$\# Z  > 2$
15	2YD	H	301	8	34,38,38	1.42	7 (20%)	39,59,59	1.47	9 (23%)
15	2YD	V	301	8	34,38,38	1.37	4 (11%)	39,59,59	1.36	6 (15%)

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
15	2YD	H	301	8	-	0/21/81/81	0/1/4/4
15	2YD	V	301	8	-	0/21/81/81	0/1/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	301	2YD	C25-C21	2.10	1.57	1.53
15	V	301	2YD	C16-C15	2.16	1.36	1.33
15	H	301	2YD	C14-C15	2.21	1.54	1.51
15	V	301	2YD	O2-C5	2.30	1.44	1.41
15	H	301	2YD	C23-C24	2.34	1.57	1.53
15	H	301	2YD	C4-C5	2.37	1.57	1.52
15	H	301	2YD	O2-C5	2.53	1.45	1.41
15	H	301	2YD	C25-C24	2.61	1.58	1.53
15	V	301	2YD	C4-C5	2.64	1.58	1.52
15	V	301	2YD	C23-C24	2.66	1.58	1.53
15	H	301	2YD	C16-C15	2.74	1.37	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	301	2YD	C5-C4-C3	-2.75	98.84	104.02
15	H	301	2YD	C28-C15-C14	-2.71	111.64	115.50
15	H	301	2YD	C2-C1-C	-2.56	121.12	123.55
15	V	301	2YD	C28-C15-C14	-2.53	111.88	115.50
15	H	301	2YD	O4-C22-C2	-2.51	103.78	107.87
15	H	301	2YD	C5-C4-C3	-2.38	99.53	104.02
15	V	301	2YD	C11-C12-C14	-2.21	108.12	111.54
15	V	301	2YD	O5-C24-C25	-2.11	105.49	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	301	2YD	O4-C21-C20	-2.08	102.69	108.38
15	H	301	2YD	C26-C25-C24	2.10	114.41	111.93
15	H	301	2YD	C21-O4-C22	2.43	117.40	112.89
15	H	301	2YD	C1-C-C7	2.48	121.36	119.78
15	V	301	2YD	C25-C24-C23	2.88	115.23	111.84
15	V	301	2YD	C4-C3-C2	3.42	129.74	116.50
15	H	301	2YD	C4-C3-C2	3.67	130.69	116.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	301	2YD	2	0
15	V	301	2YD	2	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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-0.60	1 (0%) 93 91	31, 45, 76, 130	0
1	O	250/250 (100%)	-0.46	2 (0%) 87 85	35, 51, 87, 116	0
2	B	244/258 (94%)	-0.60	3 (1%) 81 77	29, 49, 90, 147	0
2	P	244/258 (94%)	-0.34	4 (1%) 74 69	37, 53, 102, 151	0
3	C	241/254 (94%)	-0.36	5 (2%) 67 61	35, 55, 114, 135	0
3	Q	241/254 (94%)	-0.09	11 (4%) 36 29	36, 59, 126, 145	0
4	D	242/260 (93%)	-0.32	6 (2%) 61 54	36, 54, 93, 186	0
4	R	242/260 (93%)	-0.37	6 (2%) 61 54	38, 55, 92, 184	0
5	E	233/234 (99%)	-0.43	3 (1%) 79 75	36, 56, 86, 137	0
5	S	233/234 (99%)	-0.27	4 (1%) 73 68	42, 61, 91, 142	0
6	F	244/288 (84%)	-0.55	3 (1%) 81 77	33, 51, 93, 126	0
6	T	244/288 (84%)	-0.33	2 (0%) 87 85	37, 56, 101, 130	0
7	G	243/252 (96%)	-0.65	2 (0%) 87 85	33, 46, 82, 156	0
7	U	243/252 (96%)	-0.60	1 (0%) 93 91	35, 49, 81, 131	0
8	H	222/232 (95%)	-0.55	1 (0%) 91 90	33, 45, 67, 122	0
8	V	222/232 (95%)	-0.62	2 (0%) 85 83	34, 48, 72, 127	0
9	I	204/205 (99%)	-0.59	1 (0%) 91 90	30, 41, 76, 107	0
9	W	204/205 (99%)	-0.46	0 100 100	34, 44, 79, 121	0
10	J	198/198 (100%)	-0.60	3 (1%) 76 71	31, 43, 71, 173	0
10	X	198/198 (100%)	-0.60	4 (2%) 68 63	33, 47, 69, 158	0
11	K	212/212 (100%)	-0.68	0 100 100	31, 43, 62, 77	0
11	Y	211/212 (99%)	-0.68	1 (0%) 91 90	29, 43, 63, 85	0
12	L	222/222 (100%)	-0.63	1 (0%) 91 90	32, 45, 69, 115	0
12	Z	222/222 (100%)	-0.60	0 100 100	32, 43, 66, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.65	1 (0%) 93 91	29, 46, 69, 101	0
13	a	233/246 (94%)	-0.63	1 (0%) 93 91	29, 44, 67, 105	0
14	N	196/196 (100%)	-0.69	0 100 100	32, 42, 65, 96	0
14	b	196/196 (100%)	-0.58	0 100 100	31, 44, 68, 90	0
All	All	6367/6614 (96%)	-0.51	68 (1%) 82 79	29, 48, 86, 186	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	119	ALA	16.0
4	D	121	GLY	12.1
4	R	121	GLY	11.3
4	D	120	SER	8.7
10	X	197	ALA	7.4
4	D	122	GLU	7.3
2	P	219	ALA	6.3
10	J	197	ALA	6.2
4	R	119	ALA	6.0
7	U	1	ALA	5.7
5	E	1	PHE	5.7
10	J	198	GLN	5.5
1	A	1	MET	5.5
10	X	198	GLN	5.2
4	R	124	ARG	4.9
6	F	1	GLY	4.8
3	C	49	THR	4.8
3	Q	50	LEU	4.6
5	S	1	PHE	4.4
3	Q	203	THR	4.3
4	R	120	SER	4.2
6	T	243	ILE	4.1
2	B	219	ALA	3.9
10	X	196	GLN	3.9
2	B	220	ASN	3.8
5	S	2	ARG	3.8
1	O	250	LEU	3.6
2	P	218	GLY	3.6
4	D	124	ARG	3.6
9	I	1	SER	3.4
3	C	50	LEU	3.0
2	P	220	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
8	H	221	CYS	3.0
3	Q	49	THR	3.0
5	S	233	ILE	2.9
7	G	1	ALA	2.9
3	Q	236	GLN	2.8
10	X	194	ASP	2.8
4	D	118	GLY	2.7
3	Q	238	LYS	2.7
3	Q	240	GLU	2.7
3	C	203	THR	2.7
5	E	233	ILE	2.7
1	O	249	ALA	2.7
8	V	221	CYS	2.6
11	Y	172	GLY	2.6
3	Q	237	GLU	2.5
13	a	215	GLU	2.5
3	Q	234	ILE	2.5
13	M	1	THR	2.5
8	V	222	ASP	2.5
4	R	118	GLY	2.4
3	Q	231	VAL	2.4
3	Q	205	ALA	2.3
3	Q	239	GLN	2.3
3	C	206	LYS	2.3
5	E	2	ARG	2.3
7	G	243	ASP	2.3
12	L	174	TYR	2.3
2	B	218	GLY	2.3
10	J	196	GLN	2.2
2	P	223	GLU	2.2
6	F	202	ASP	2.1
5	S	190	LYS	2.1
4	R	122	GLU	2.1
6	T	198	LEU	2.1
6	F	205	GLU	2.0
3	C	236	GLN	2.0

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

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
15	2YD	V	301	35/35	0.96	0.15	0.90	41,56,62,66	0
15	2YD	H	301	35/35	0.97	0.14	0.41	45,50,57,66	0

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

There are no such residues in this entry.