



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:14 PM GMT

PDB ID : 4R17  
Title : Ligand-induced aziridine-formation at subunit beta5 of the yeast 20S proteasome  
Authors : Dubiella, C.; Cui, H.; Gersch, M.; Brouwer, A.J.; Sieber, S.A.; Krueger, A.; Liskamp, R.; Groll, M.  
Deposited on : 2014-08-04  
Resolution : 2.10 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

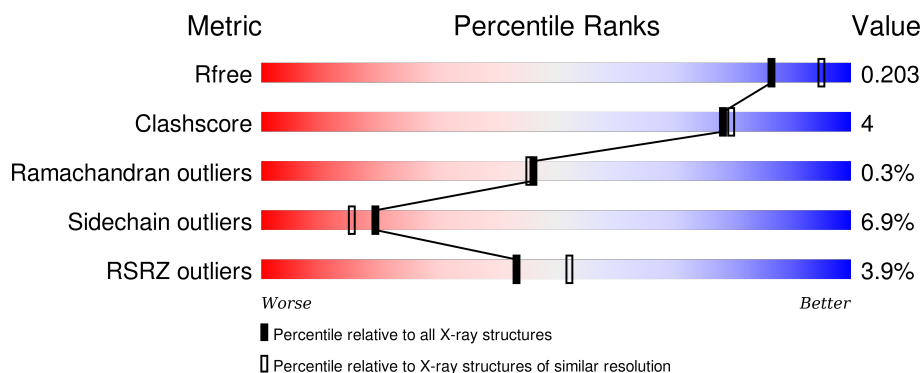
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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>4%</div> <div>94%</div> <div>• •</div> </div>
1	O	250	<div> <div>4%</div> <div>94%</div> <div>5% •</div> </div>
2	B	258	<div> <div>5%</div> <div>79%</div> <div>14% • 5%</div> </div>
2	P	258	<div> <div>5%</div> <div>81%</div> <div>12% • 5%</div> </div>
3	C	254	<div> <div>8%</div> <div>79%</div> <div>11% 5% 6%</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	

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
15	MG	I	302	-	-	-	X
15	MG	J	201	-	-	-	X
15	MG	K	303	-	-	-	X
16	3K4	K	301	-	-	-	X

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 52831 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	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			
1	O	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			

- 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	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	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	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1637	1041	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

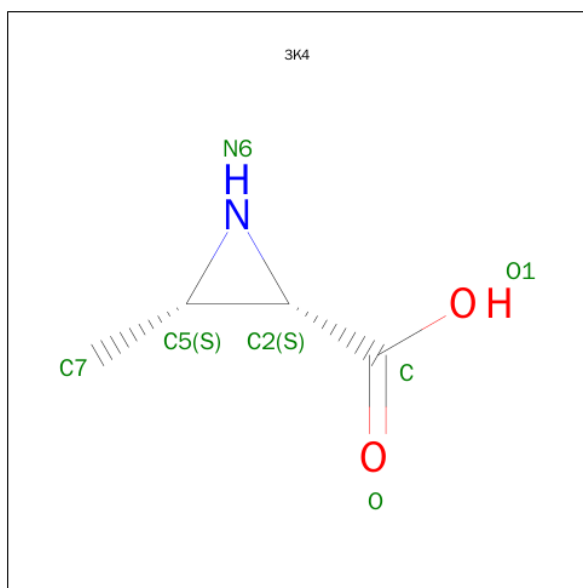
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	J	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	K	2	Total	Mg	0	0
			2	2		
15	H	1	Total	Mg	0	0
			1	1		
15	I	2	Total	Mg	0	0
			2	2		
15	V	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		
15	Y	1	Total	Mg	0	0
			1	1		

- Molecule 16 is (2S,3S)-3-METHYLAZIRIDINE-2-CARBOXYLIC ACID (three-letter code: 3K4) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	K	1	Total	C	N	O	0	0
			6	4	1	1		
16	Y	1	Total	C	N	O	0	0
			6	4	1	1		

- Molecule 17 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	167	Total O 167 167	0	0
17	B	115	Total O 115 115	0	0
17	C	105	Total O 105 105	0	0
17	D	123	Total O 123 123	0	0
17	E	69	Total O 69 69	0	0
17	F	117	Total O 117 117	0	0
17	G	158	Total O 158 158	0	0
17	H	135	Total O 135 135	0	0
17	I	140	Total O 140 140	0	0
17	J	123	Total O 123 123	0	0
17	K	152	Total O 152 152	0	0
17	L	158	Total O 158 158	0	0
17	M	168	Total O 168 168	0	0
17	N	112	Total O 112 112	0	0
17	O	118	Total O 118 118	0	0
17	P	91	Total O 91 91	0	0
17	Q	79	Total O 79 79	0	0
17	R	107	Total O 107 107	0	0
17	S	55	Total O 55 55	0	0
17	T	94	Total O 94 94	0	0
17	U	133	Total O 133 133	0	0
17	V	111	Total O 111 111	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	W	128	Total 128	O 128	0	0
17	X	118	Total 118	O 118	0	0
17	Y	148	Total 148	O 148	0	0
17	Z	166	Total 166	O 166	0	0
17	a	165	Total 165	O 165	0	0
17	b	117	Total 117	O 117	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.

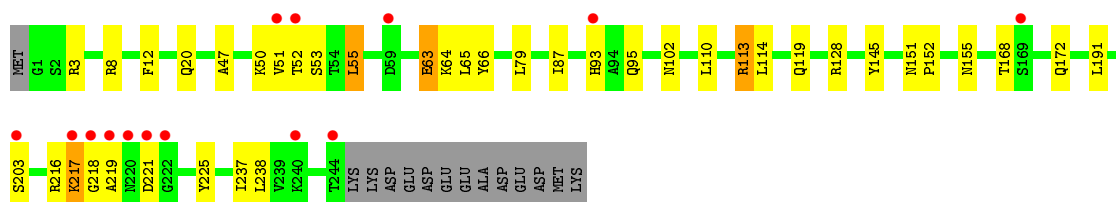
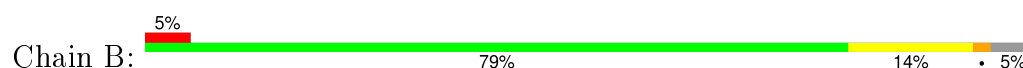
- Molecule 1: Proteasome subunit alpha type-2



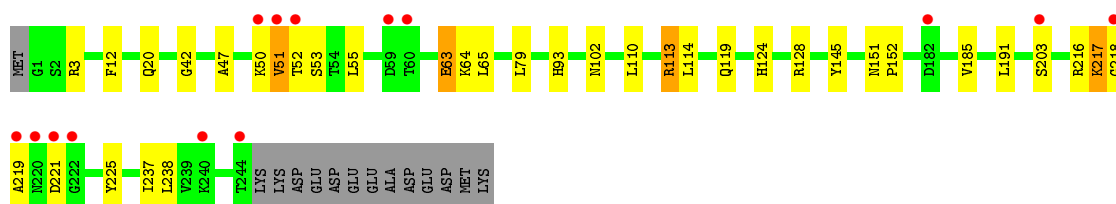
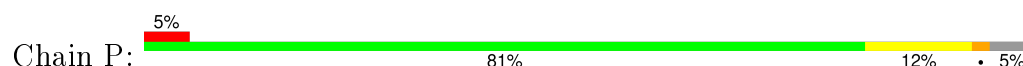
- Molecule 1: Proteasome subunit alpha type-2



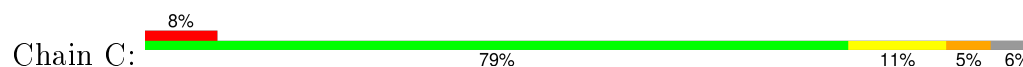
- Molecule 2: Proteasome subunit alpha type-3

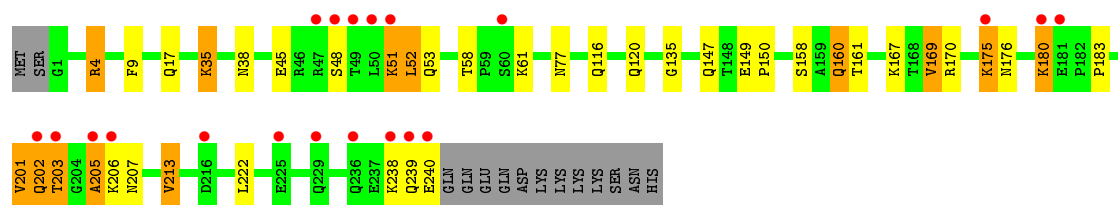


- Molecule 2: Proteasome subunit alpha type-3

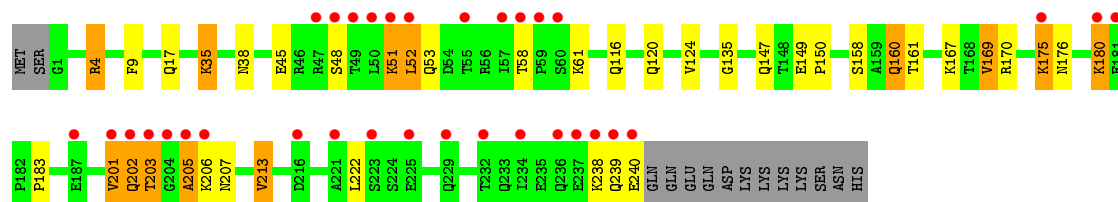
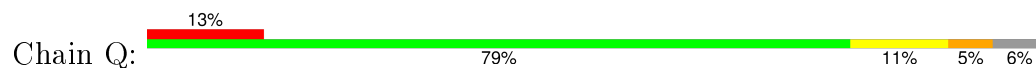


- Molecule 3: Proteasome subunit alpha type-4

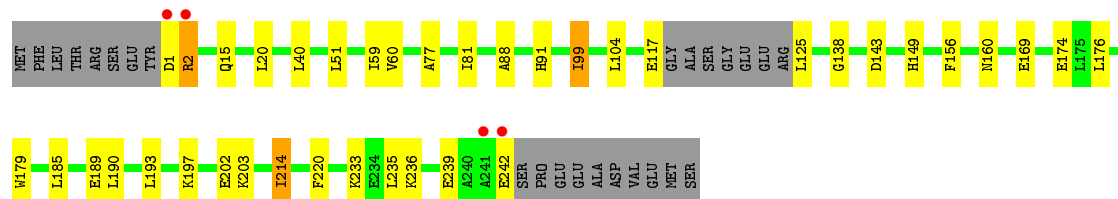
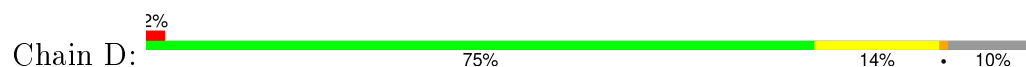




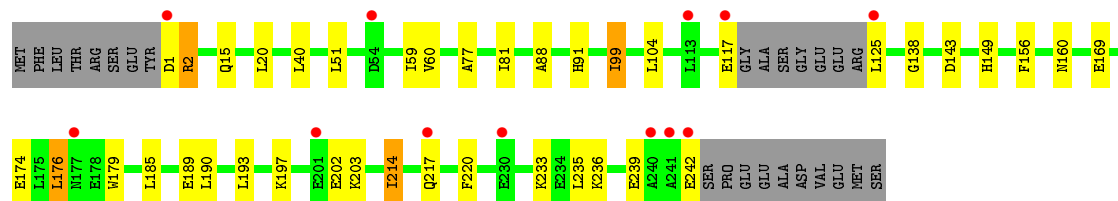
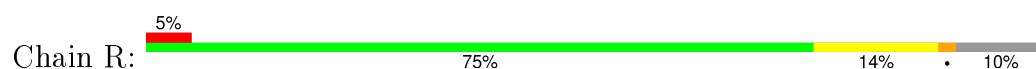
• Molecule 3: Proteasome subunit alpha type-4



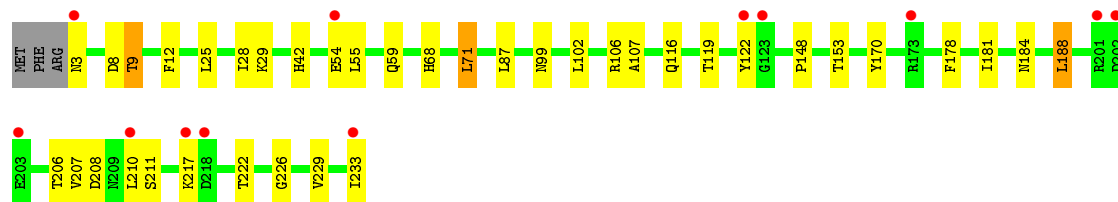
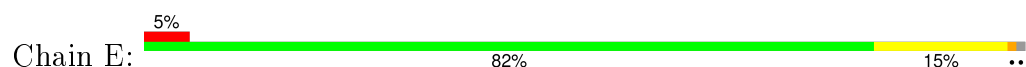
• Molecule 4: Proteasome subunit alpha type-5



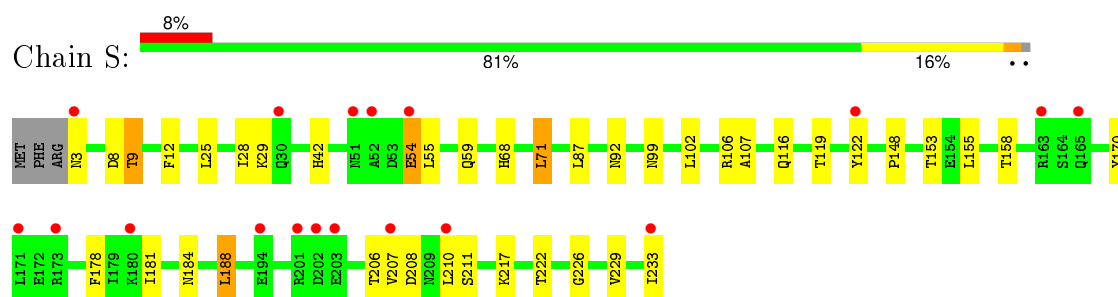
• Molecule 4: Proteasome subunit alpha type-5



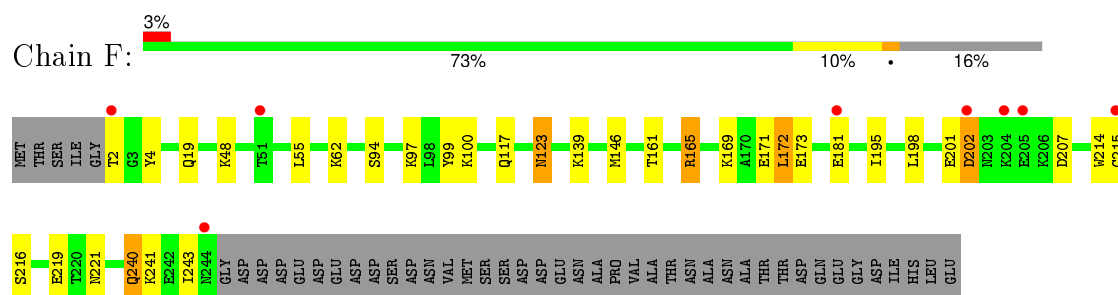
• Molecule 5: Proteasome subunit alpha type-6



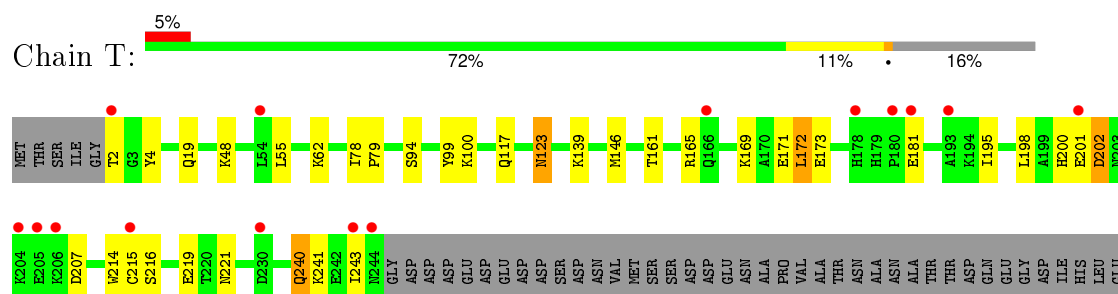
• Molecule 5: Proteasome subunit alpha type-6



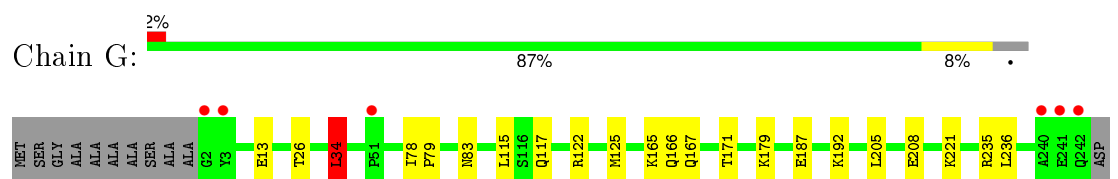
- Molecule 6: Proteasome subunit alpha type-7



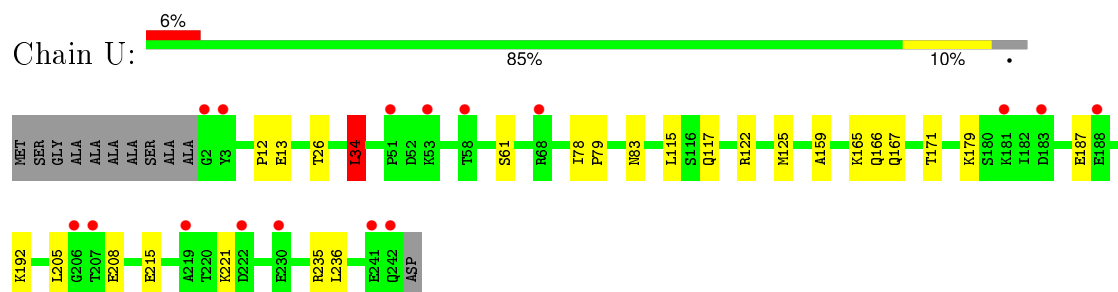
- Molecule 6: Proteasome subunit alpha type-7



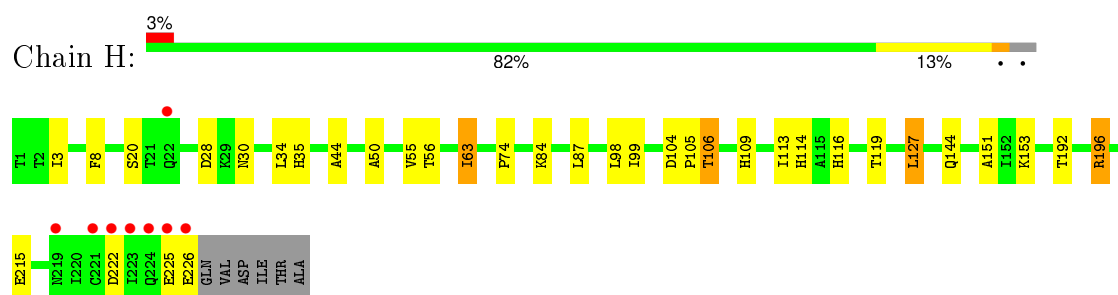
- Molecule 7: Proteasome subunit alpha type-1



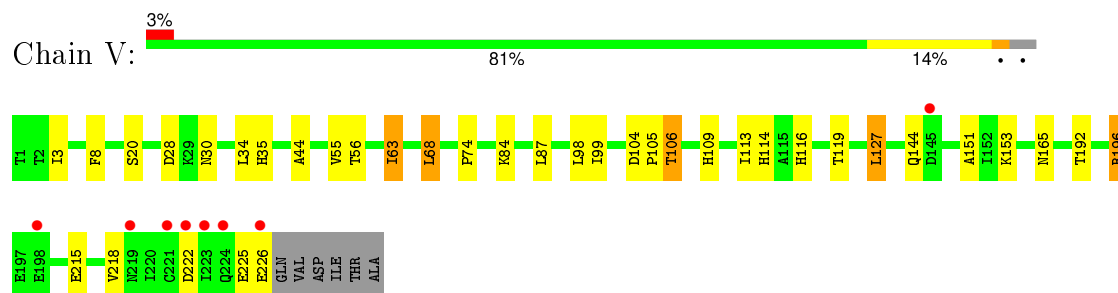
- Molecule 7: Proteasome subunit alpha type-1



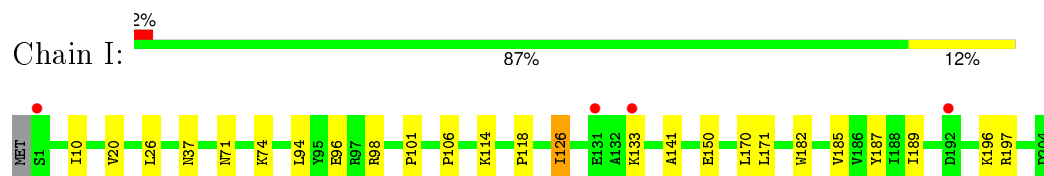
- Molecule 8: Proteasome subunit beta type-2



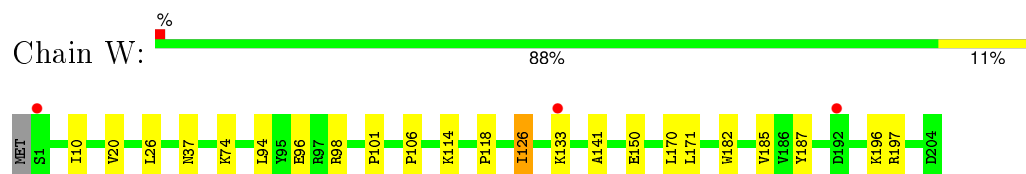
- Molecule 8: Proteasome subunit beta type-2



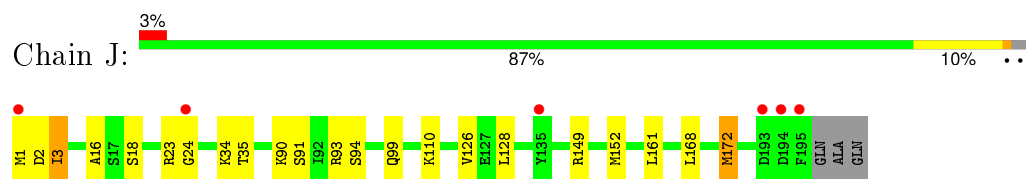
- Molecule 9: Proteasome subunit beta type-3



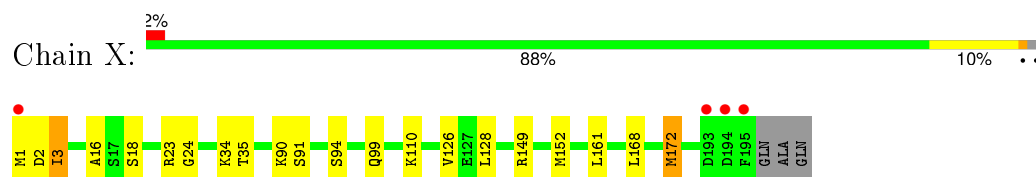
- Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-4

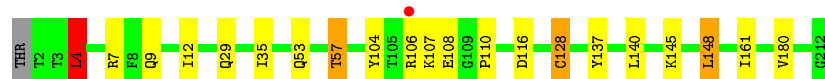


- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-5

Chain K:  90% 8% .




- Molecule 11: Proteasome subunit beta type-5

Chain Y:  90% 8% .




- Molecule 12: Proteasome subunit beta type-6

Chain L:  89% 9% .



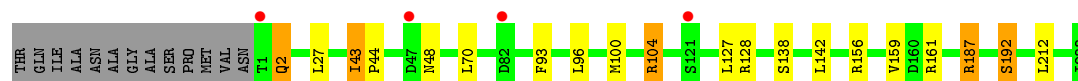
- Molecule 12: Proteasome subunit beta type-6

Chain Z:  89% 9% .




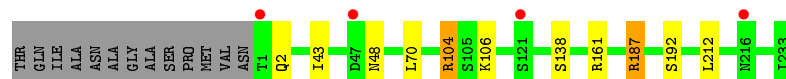
- Molecule 13: Proteasome subunit beta type-7

Chain M:  87% 6% 5% .



- Molecule 13: Proteasome subunit beta type-7

Chain a:  90% 5% .

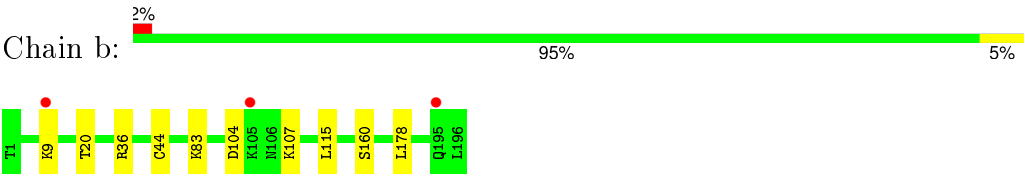


- Molecule 14: Proteasome subunit beta type-1

Chain N:  90% 8% .



- Molecule 14: Proteasome subunit beta type-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.72Å 301.36Å 144.74Å 90.00° 112.81° 90.00°	Depositor
Resolution (Å)	15.00 – 2.10 15.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (15.00-2.10) 98.9 (15.00-2.10)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.185 , 0.198 0.191 , 0.203	Depositor DCC
$R_{free}$ test set	30359 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.1	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 607186 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	52831	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: 3K4, MG

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	0.29	0/1944	0.54	0/2632
1	O	0.28	0/1944	0.54	0/2632
2	B	0.30	0/1934	0.58	0/2618
2	P	0.31	0/1934	0.57	0/2618
3	C	0.29	0/1910	0.59	0/2586
3	Q	0.29	0/1910	0.59	0/2586
4	D	0.28	0/1837	0.57	0/2475
4	R	0.28	0/1837	0.57	0/2475
5	E	0.28	0/1800	0.55	1/2433 (0.0%)
5	S	0.28	0/1800	0.56	1/2433 (0.0%)
6	F	0.29	0/1932	0.54	0/2609
6	T	0.29	0/1932	0.54	0/2609
7	G	0.29	0/1945	0.56	1/2634 (0.0%)
7	U	0.29	0/1945	0.55	1/2634 (0.0%)
8	H	0.33	0/1750	0.55	0/2373
8	V	0.27	0/1750	0.56	1/2373 (0.0%)
9	I	0.28	0/1611	0.54	0/2174
9	W	0.28	0/1611	0.54	0/2174
10	J	0.27	0/1589	0.54	0/2142
10	X	0.27	0/1589	0.54	0/2142
11	K	0.27	0/1674	0.59	1/2264 (0.0%)
11	Y	0.27	0/1674	0.59	1/2264 (0.0%)
12	L	0.34	0/1795	0.55	0/2420
12	Z	0.28	0/1795	0.56	1/2420 (0.0%)
13	M	0.36	0/1855	0.66	3/2514 (0.1%)
13	a	0.34	0/1855	0.64	3/2514 (0.1%)
14	N	0.27	0/1541	0.54	0/2087
14	b	0.27	0/1541	0.54	0/2087
All	All	0.29	0/50234	0.57	14/67922 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	104	ARG	NE-CZ-NH1	10.95	125.77	120.30
13	a	104	ARG	NE-CZ-NH1	8.21	124.41	120.30
13	a	104	ARG	NE-CZ-NH2	-8.11	116.25	120.30
13	M	104	ARG	NE-CZ-NH2	-7.98	116.31	120.30
11	Y	4	LEU	CA-CB-CG	5.83	128.70	115.30
11	K	4	LEU	CA-CB-CG	5.81	128.67	115.30
12	Z	150	LEU	CB-CG-CD1	5.62	120.55	111.00
8	V	68	LEU	CB-CG-CD1	5.48	120.31	111.00
7	G	34	LEU	CA-CB-CG	5.45	127.83	115.30
7	U	34	LEU	CA-CB-CG	5.44	127.81	115.30
5	E	71	LEU	CA-CB-CG	5.35	127.61	115.30
5	S	71	LEU	CA-CB-CG	5.32	127.53	115.30
13	a	187	ARG	NE-CZ-NH1	5.27	122.94	120.30
13	M	187	ARG	NE-CZ-NH1	5.20	122.90	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1907	0	1917	6	0
1	O	1907	0	1917	6	0
2	B	1904	0	1904	27	0
2	P	1904	0	1904	20	0
3	C	1881	0	1895	21	0
3	Q	1881	0	1895	20	0
4	D	1813	0	1797	14	0
4	R	1813	0	1797	15	0
5	E	1773	0	1775	13	0
5	S	1773	0	1775	17	0
6	F	1892	0	1883	20	0
6	T	1892	0	1883	21	0
7	G	1907	0	1901	7	0
7	U	1907	0	1901	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1719	0	1719	25	0
8	V	1719	0	1719	27	0
9	I	1581	0	1574	15	0
9	W	1581	0	1574	13	0
10	J	1561	0	1569	14	0
10	X	1561	0	1569	13	0
11	K	1637	0	1585	9	0
11	Y	1637	0	1585	9	0
12	L	1757	0	1711	11	0
12	Z	1757	0	1711	10	0
13	M	1824	0	1832	8	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	11	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	K	2	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	K	6	0	5	0	0
16	Y	6	0	5	0	0
17	A	167	0	0	0	0
17	B	115	0	0	0	0
17	C	105	0	0	1	0
17	D	123	0	0	0	0
17	E	69	0	0	0	0
17	F	117	0	0	0	0
17	G	158	0	0	0	0
17	H	135	0	0	0	0
17	I	140	0	0	0	0
17	J	123	0	0	1	0
17	K	152	0	0	1	0
17	L	158	0	0	0	0
17	M	168	0	0	1	0
17	N	112	0	0	0	0
17	O	118	0	0	0	0
17	P	91	0	0	0	0
17	Q	79	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	R	107	0	0	0	0
17	S	55	0	0	0	0
17	T	94	0	0	0	0
17	U	133	0	0	0	0
17	V	111	0	0	0	0
17	W	128	0	0	0	0
17	X	118	0	0	0	0
17	Y	148	0	0	0	0
17	Z	166	0	0	0	0
17	a	165	0	0	0	0
17	b	117	0	0	0	0
All	All	52831	0	49096	336	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 4.

All (336) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:THR:HG22	2:B:53:SER:H	1.22	1.03
2:B:52:THR:HG22	2:B:53:SER:N	1.80	0.97
14:N:35:THR:HG21	14:N:45:ARG:HE	1.36	0.90
2:P:52:THR:HG22	2:P:53:SER:N	1.88	0.89
2:P:52:THR:CG2	2:P:53:SER:N	2.39	0.86
6:F:146:MET:CE	6:F:161:THR:HB	2.09	0.83
6:T:146:MET:CE	6:T:161:THR:HB	2.10	0.81
2:P:52:THR:CG2	2:P:53:SER:H	1.93	0.80
2:B:52:THR:CG2	2:B:53:SER:H	1.94	0.80
2:B:12:PHE:H	3:C:17:GLN:HE22	1.34	0.74
11:K:53:GLN:O	11:K:57:THR:HG23	1.89	0.73
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.88	0.72
2:B:219:ALA:HB2	2:B:225:TYR:HB2	1.73	0.69
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.23	0.69
2:P:219:ALA:HB2	2:P:225:TYR:HB2	1.73	0.68
6:T:240:GLN:HA	6:T:240:GLN:HE21	1.59	0.68
6:F:240:GLN:HA	6:F:240:GLN:HE21	1.59	0.67
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.77	0.66
2:B:3:ARG:HB3	5:E:122:TYR:OH	1.95	0.66
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.76	0.66
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.76	0.65
6:T:146:MET:HE1	6:T:161:THR:HB	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.77	0.64
6:F:146:MET:HE3	6:F:161:THR:HB	1.78	0.64
4:R:176:LEU:HD11	5:S:54:GLU:HB2	1.81	0.63
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.80	0.63
14:N:35:THR:CG2	14:N:45:ARG:HE	2.12	0.62
1:O:12:PHE:H	2:P:20:GLN:HE22	1.47	0.62
8:H:3:ILE:HG22	8:H:99:ILE:HD12	1.82	0.62
3:C:51:LYS:O	3:C:52:LEU:HB2	1.99	0.62
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.00	0.61
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.65	0.61
8:V:3:ILE:HG22	8:V:99:ILE:HD12	1.82	0.61
2:B:52:THR:HG22	2:B:53:SER:O	2.01	0.60
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.65	0.60
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.47	0.60
10:X:1:MET:CB	10:X:34:LYS:HE3	2.32	0.60
6:T:146:MET:HE3	6:T:161:THR:HB	1.83	0.60
2:P:52:THR:HG23	2:P:53:SER:H	1.64	0.60
5:E:12:PHE:H	6:F:19:GLN:HE22	1.50	0.60
5:S:12:PHE:H	6:T:19:GLN:HE22	1.48	0.60
6:F:146:MET:HE1	6:F:161:THR:HB	1.84	0.60
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.84	0.60
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.84	0.59
10:J:1:MET:CB	10:J:34:LYS:HE3	2.32	0.59
4:R:197:LYS:NZ	4:R:239:GLU:OE2	2.35	0.59
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.85	0.59
4:D:197:LYS:NZ	4:D:239:GLU:OE2	2.35	0.58
7:G:165:LYS:HD2	7:G:205:LEU:HD22	1.86	0.58
1:A:12:PHE:H	2:B:20:GLN:HE22	1.52	0.58
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.86	0.58
2:P:216:ARG:HB3	2:P:218:GLY:H	1.69	0.58
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.85	0.58
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.86	0.57
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.87	0.57
3:C:201:VAL:O	3:C:202:GLN:CB	2.53	0.57
7:U:165:LYS:HD2	7:U:205:LEU:HD22	1.85	0.57
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.51	0.57
2:B:216:ARG:HB3	2:B:218:GLY:H	1.69	0.57
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.87	0.57
14:N:35:THR:HG21	14:N:45:ARG:NE	2.16	0.56
3:C:9:PHE:H	4:D:15:GLN:HE22	1.52	0.56
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.87	0.56
8:H:114:HIS:HD2	8:H:116:HIS:H	1.54	0.56
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.53	0.56
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.36	0.56
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.87	0.56
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.36	0.56
11:K:106:ARG:HG2	11:K:106:ARG:HH11	1.72	0.55
11:Y:106:ARG:HH11	11:Y:106:ARG:HG2	1.71	0.55
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.88	0.55
6:T:172:LEU:HD13	6:T:195:ILE:CD1	2.37	0.55
8:V:114:HIS:HD2	8:V:116:HIS:H	1.54	0.55
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.89	0.55
8:V:3:ILE:HG21	8:V:44:ALA:HB3	1.90	0.54
14:N:20:THR:CG2	14:N:31:THR:OG1	2.55	0.54
8:H:3:ILE:HG21	8:H:44:ALA:HB3	1.89	0.54
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.20	0.54
7:U:187:GLU:HG2	7:U:192:LYS:CB	2.37	0.54
2:B:155:ASN:ND2	3:C:77:ASN:HB2	2.23	0.54
6:F:172:LEU:HD13	6:F:195:ILE:CD1	2.37	0.54
7:G:34:LEU:HD23	7:G:34:LEU:C	2.28	0.54
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.88	0.54
10:J:1:MET:HB3	10:J:34:LYS:HE3	1.90	0.54
10:X:1:MET:CG	10:X:34:LYS:HE3	2.39	0.53
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.91	0.53
7:U:34:LEU:C	7:U:34:LEU:HD23	2.28	0.53
7:G:187:GLU:HG2	7:G:192:LYS:CB	2.37	0.53
10:X:1:MET:HB3	10:X:34:LYS:HE3	1.89	0.53
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.90	0.53
10:J:168:LEU:O	10:J:172:MET:HB2	2.09	0.53
2:P:217:LYS:C	2:P:219:ALA:H	2.12	0.53
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.90	0.53
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	1.90	0.53
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.91	0.53
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.22	0.52
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.92	0.52
5:E:206:THR:C	5:E:233:ILE:HD11	2.30	0.52
12:L:189:THR:HG22	8:V:196:ARG:HH11	1.74	0.52
2:B:217:LYS:C	2:B:219:ALA:H	2.12	0.52
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.92	0.52
10:X:168:LEU:O	10:X:172:MET:HB2	2.09	0.52
10:J:1:MET:CG	10:J:34:LYS:HE3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:201:VAL:O	3:C:202:GLN:HB2	2.09	0.52
3:C:175:LYS:HG3	3:C:176:ASN:ND2	2.25	0.52
9:W:98:ARG:HD2	9:W:126:ILE:HG12	1.93	0.51
3:Q:175:LYS:HG3	3:Q:176:ASN:ND2	2.25	0.51
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.09	0.51
5:E:9:THR:HG21	5:E:119:THR:HA	1.92	0.51
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.93	0.51
2:B:110:LEU:HD23	2:B:110:LEU:C	2.31	0.51
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.93	0.51
2:P:110:LEU:HD23	2:P:110:LEU:C	2.31	0.51
5:S:9:THR:HG21	5:S:119:THR:HA	1.92	0.51
5:S:206:THR:C	5:S:233:ILE:HD11	2.30	0.51
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.93	0.51
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.93	0.50
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.92	0.50
14:N:83:LYS:HG3	14:N:119:VAL:HG23	1.93	0.50
9:W:187:TYR:OH	9:W:196:LYS:HE3	2.11	0.50
12:L:189:THR:HG22	8:V:196:ARG:NH1	2.26	0.50
3:C:203:THR:C	3:C:205:ALA:H	2.14	0.50
9:I:98:ARG:HD2	9:I:126:ILE:HG12	1.93	0.50
11:K:29:GLN:NE2	17:K:476:HOH:O	2.30	0.50
3:C:4:ARG:HG2	4:D:117:GLU:OE1	2.11	0.50
9:W:170:LEU:C	9:W:170:LEU:HD23	2.32	0.50
8:V:215:GLU:HG2	9:W:197:ARG:HG2	1.93	0.50
8:H:196:ARG:HH11	12:Z:189:THR:HG22	1.77	0.49
8:H:63:ILE:HG23	8:H:74:PRO:HB3	1.93	0.49
3:Q:203:THR:C	3:Q:205:ALA:H	2.14	0.49
8:V:222:ASP:OD1	9:W:74:LYS:NZ	2.45	0.49
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.60	0.49
2:B:63:GLU:HG2	2:B:64:LYS:HG2	1.94	0.49
2:P:63:GLU:HG2	2:P:64:LYS:HG2	1.94	0.49
1:A:122:THR:HG23	2:B:128:ARG:HH21	1.78	0.49
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.94	0.49
6:F:198:LEU:HD12	6:F:243:ILE:HG22	1.93	0.49
9:I:187:TYR:OH	9:I:196:LYS:HE3	2.12	0.49
9:I:170:LEU:C	9:I:170:LEU:HD23	2.33	0.49
8:H:222:ASP:OD1	9:I:74:LYS:NZ	2.45	0.49
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.60	0.49
3:C:202:GLN:HG3	3:C:203:THR:H	1.78	0.48
10:X:1:MET:HB3	10:X:34:LYS:CE	2.43	0.48
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:215:GLU:HG2	9:I:197:ARG:HG2	1.95	0.48
10:J:1:MET:HB3	10:J:34:LYS:CE	2.44	0.48
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.78	0.48
6:T:198:LEU:HD12	6:T:243:ILE:HG22	1.93	0.48
6:T:202:ASP:N	6:T:202:ASP:OD1	2.44	0.48
10:J:93:ARG:NH1	17:J:407:HOH:O	2.43	0.48
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.78	0.48
8:H:196:ARG:NH1	12:Z:189:THR:HG22	2.29	0.48
13:M:2:GLN:NE2	17:M:459:HOH:O	2.47	0.48
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.96	0.48
6:F:202:ASP:OD1	6:F:202:ASP:N	2.43	0.48
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.96	0.47
7:U:187:GLU:HG2	7:U:192:LYS:HB3	1.96	0.47
11:Y:32:LYS:HB3	11:Y:32:LYS:HE2	1.72	0.47
6:F:123:ASN:C	6:F:123:ASN:HD22	2.17	0.47
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.50	0.47
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.80	0.47
6:T:123:ASN:HD22	6:T:123:ASN:C	2.17	0.47
7:G:187:GLU:HG2	7:G:192:LYS:HB3	1.96	0.47
10:J:91:SER:O	10:J:94:SER:HB2	2.15	0.47
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.29	0.47
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.45	0.47
9:W:26:LEU:HD21	9:W:185:VAL:HG23	1.96	0.47
10:X:149:ARG:O	10:X:152:MET:HG3	2.15	0.47
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.97	0.47
8:V:35:HIS:CB	8:V:56:THR:HG21	2.45	0.46
3:C:120:GLN:NE2	17:C:323:HOH:O	2.47	0.46
9:I:26:LEU:HD21	9:I:185:VAL:HG23	1.96	0.46
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.50	0.46
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.45	0.46
8:H:35:HIS:CB	8:H:56:THR:HG21	2.45	0.46
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.96	0.46
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.51	0.46
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.51	0.46
10:J:149:ARG:O	10:J:152:MET:HG3	2.16	0.46
10:X:91:SER:O	10:X:94:SER:HB2	2.15	0.46
3:Q:45:GLU:HG3	3:Q:201:VAL:HG23	1.99	0.45
1:A:176:GLU:CG	2:B:55:LEU:HD22	2.46	0.45
5:E:68:HIS:HE1	5:E:102:LEU:O	1.99	0.45
4:R:1:ASP:O	4:R:2:ARG:HB2	2.16	0.45
8:H:192:THR:HG22	8:H:192:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.98	0.45
5:S:68:HIS:HE1	5:S:102:LEU:O	1.99	0.45
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.97	0.45
5:E:178:PHE:HA	5:E:181:ILE:HG13	1.99	0.45
8:H:84:LYS:HA	8:H:113:ILE:HD11	1.99	0.45
4:R:59:ILE:HG22	4:R:220:PHE:HZ	1.81	0.45
5:S:153:THR:HG21	6:T:55:LEU:CD2	2.47	0.45
5:S:42:HIS:HB2	5:S:188:LEU:HD12	1.99	0.45
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.63	0.45
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.99	0.45
5:S:178:PHE:HA	5:S:181:ILE:HG13	1.99	0.45
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.97	0.45
3:C:45:GLU:HG3	3:C:201:VAL:HG23	1.99	0.45
8:V:192:THR:HG22	8:V:192:THR:O	2.16	0.45
6:F:97:LYS:NZ	14:N:84:GLU:OE1	2.48	0.45
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.31	0.44
6:T:2:THR:HA	6:T:4:TYR:CD2	2.52	0.44
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.47	0.44
2:P:3:ARG:HB3	5:S:122:TYR:OH	2.17	0.44
6:T:240:GLN:CA	6:T:240:GLN:HE21	2.28	0.44
4:D:59:ILE:HG22	4:D:220:PHE:HZ	1.82	0.44
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.99	0.44
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.47	0.44
3:C:205:ALA:C	3:C:207:ASN:H	2.21	0.44
13:M:93:PHE:CZ	13:M:128:ARG:HG2	2.52	0.44
2:P:145:TYR:OH	2:P:217:LYS:N	2.50	0.44
3:Q:205:ALA:C	3:Q:207:ASN:H	2.21	0.44
7:U:61:SER:OG	7:U:215:GLU:OE2	2.28	0.44
8:H:98:LEU:HB2	8:H:113:ILE:CG2	2.48	0.44
2:B:52:THR:CG2	2:B:53:SER:N	2.49	0.44
10:X:1:MET:CB	10:X:34:LYS:CE	2.95	0.44
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.31	0.44
8:V:98:LEU:HB2	8:V:113:ILE:CG2	2.48	0.44
4:D:1:ASP:O	4:D:2:ARG:HB2	2.16	0.44
10:J:1:MET:CB	10:J:34:LYS:CE	2.95	0.44
5:S:226:GLY:O	5:S:229:VAL:HG22	2.18	0.44
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.53	0.44
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.53	0.44
8:V:196:ARG:NH2	9:W:150:GLU:HG3	2.32	0.43
8:V:106:THR:HG22	8:V:109:HIS:NE2	2.33	0.43
3:Q:135:GLY:HA2	3:Q:213:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.54	0.43
3:C:135:GLY:HA2	3:C:213:VAL:HG21	2.01	0.43
5:E:42:HIS:HB2	5:E:188:LEU:HD12	1.99	0.43
8:V:84:LYS:HA	8:V:113:ILE:HD11	1.99	0.43
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.53	0.43
13:M:159:VAL:HG23	13:M:159:VAL:O	2.18	0.43
6:F:240:GLN:CA	6:F:240:GLN:HE21	2.28	0.43
1:O:122:THR:HG23	2:P:128:ARG:HH21	1.82	0.43
3:Q:120:GLN:NE2	17:Q:330:HOH:O	2.51	0.43
6:F:2:THR:HA	6:F:4:TYR:CD2	2.53	0.43
5:S:28:ILE:HD11	5:S:148:PRO:CD	2.48	0.43
8:H:106:THR:HG22	8:H:109:HIS:NE2	2.33	0.43
2:B:145:TYR:OH	2:B:217:LYS:N	2.50	0.43
8:V:99:ILE:HG13	8:V:127:LEU:HD22	2.01	0.43
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.33	0.43
8:H:196:ARG:NH2	9:I:150:GLU:O	2.52	0.43
1:O:55:LEU:HB3	7:U:159:ALA:O	2.19	0.43
8:V:114:HIS:CD2	8:V:116:HIS:H	2.35	0.43
8:H:225:GLU:O	8:H:226:GLU:HB2	2.19	0.43
8:H:84:LYS:HE2	8:H:119:THR:HG23	2.01	0.43
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	2.01	0.43
12:L:71:SER:OG	12:L:92:ASN:OD1	2.32	0.42
5:E:226:GLY:O	5:E:229:VAL:HG22	2.18	0.42
5:E:170:TYR:C	5:E:170:TYR:CD1	2.93	0.42
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.66	0.42
3:Q:180:LYS:HB2	3:Q:180:LYS:NZ	2.34	0.42
5:S:170:TYR:CD1	5:S:170:TYR:C	2.93	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42
8:H:99:ILE:HG13	8:H:127:LEU:HD22	2.01	0.42
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.02	0.42
3:Q:4:ARG:HG2	4:R:117:GLU:OE1	2.19	0.42
13:M:27:LEU:HB2	13:M:192:SER:HB3	2.02	0.42
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.01	0.42
13:M:43:ILE:HA	13:M:44:PRO:HD3	1.93	0.42
3:C:35:LYS:HG2	3:C:158:SER:O	2.19	0.42
6:F:165:ARG:HB3	6:F:165:ARG:HE	1.61	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.49	0.42
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.19	0.42
10:J:3:ILE:HD12	10:J:168:LEU:HD13	2.02	0.42
6:T:198:LEU:CD1	6:T:243:ILE:HG22	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:7:ARG:HD2	11:K:110:PRO:O	2.20	0.42
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.49	0.42
5:S:210:LEU:HD23	5:S:229:VAL:HB	2.02	0.42
11:K:12:ILE:HB	11:K:180:VAL:HB	2.02	0.42
14:N:13:ILE:HG21	14:N:175:MET:CE	2.49	0.42
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.02	0.42
3:C:180:LYS:HB2	3:C:180:LYS:NZ	2.34	0.42
4:R:185:LEU:O	4:R:189:GLU:HG3	2.19	0.42
5:E:210:LEU:HD23	5:E:229:VAL:HB	2.02	0.41
4:D:185:LEU:O	4:D:189:GLU:HG3	2.20	0.41
8:H:87:LEU:HD12	8:H:113:ILE:HD11	2.02	0.41
8:V:196:ARG:NH2	9:W:150:GLU:O	2.53	0.41
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.02	0.41
11:Y:7:ARG:HD2	11:Y:110:PRO:O	2.20	0.41
4:R:77:ALA:O	4:R:81:ILE:HG12	2.20	0.41
6:F:198:LEU:CD1	6:F:243:ILE:HG22	2.50	0.41
8:H:87:LEU:HD12	8:H:113:ILE:CD1	2.50	0.41
8:V:87:LEU:HD12	8:V:113:ILE:CD1	2.50	0.41
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.68	0.41
4:D:149:HIS:O	4:D:156:PHE:HA	2.20	0.41
1:A:194:LEU:HD23	1:A:250:LEU:HD13	2.03	0.41
12:L:23:LEU:HD13	12:L:43:VAL:HG13	2.02	0.41
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.67	0.41
4:R:149:HIS:O	4:R:156:PHE:HA	2.20	0.41
5:S:155:LEU:HD13	5:S:158:THR:HB	2.03	0.41
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.01	0.41
8:V:20:SER:OG	8:V:28:ASP:HB3	2.20	0.41
13:M:96:LEU:O	13:M:100:MET:HG2	2.21	0.41
6:T:99:TYR:O	6:T:100:LYS:HB3	2.20	0.41
2:P:93:HIS:CE1	2:P:113:ARG:HG2	2.55	0.41
4:D:77:ALA:O	4:D:81:ILE:HG12	2.20	0.41
6:T:169:LYS:O	6:T:173:GLU:HG3	2.21	0.41
10:X:3:ILE:HD12	10:X:168:LEU:HD13	2.02	0.41
8:V:225:GLU:O	8:V:226:GLU:HB2	2.19	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.21	0.41
6:F:99:TYR:O	6:F:100:LYS:HB3	2.20	0.41
5:E:153:THR:HG21	6:F:55:LEU:CD2	2.50	0.41
2:P:42:GLY:HA3	2:P:185:VAL:HG21	2.03	0.41
9:W:94:LEU:HD11	9:W:106:PRO:HG2	2.03	0.41
12:L:195:HIS:HD2	12:L:197:GLN:H	1.68	0.41
11:K:4:LEU:HD13	11:K:161:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:20:SER:OG	8:H:28:ASP:HB3	2.20	0.41
2:P:47:ALA:HB1	2:P:64:LYS:HD3	2.03	0.41
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.03	0.41
3:Q:161:THR:HG21	3:Q:169:VAL:HG22	2.03	0.41
6:F:169:LYS:O	6:F:173:GLU:HG3	2.20	0.41
2:B:47:ALA:HB1	2:B:64:LYS:HD3	2.04	0.40
6:T:48:LYS:HG2	6:T:62:LYS:HD2	2.03	0.40
12:Z:213:ARG:HG2	12:Z:214:LYS:N	2.36	0.40
2:B:93:HIS:CE1	2:B:113:ARG:HG2	2.56	0.40
5:S:153:THR:CG2	6:T:55:LEU:CD2	3.00	0.40
12:L:213:ARG:HG2	12:L:214:LYS:N	2.36	0.40
6:T:200:HIS:O	6:T:200:HIS:CG	2.74	0.40
12:L:173:LYS:HA	12:L:173:LYS:HD3	1.89	0.40
6:T:78:ILE:HB	6:T:79:PRO:HD3	2.04	0.40
6:F:48:LYS:HG2	6:F:62:LYS:HD2	2.03	0.40
2:B:168:THR:O	2:B:172:GLN:HB2	2.21	0.40
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.03	0.40
2:B:66:TYR:CG	2:B:87:ILE:HD13	2.56	0.40
2:B:12:PHE:N	3:C:17:GLN:HE22	2.11	0.40
8:V:218:VAL:CG2	9:W:196:LYS:HB2	2.52	0.40
8:V:87:LEU:HD12	8:V:113:ILE:HD11	2.02	0.40
3:Q:149:GLU:HB2	3:Q:150:PRO:CD	2.51	0.40
3:C:161:THR:HG21	3:C:169:VAL:HG22	2.03	0.40
1:O:194:LEU:HD23	1:O:250:LEU:HD13	2.03	0.40
9:I:94:LEU:HD11	9:I:106:PRO:HG2	2.03	0.40
11:Y:4:LEU:HD13	11:Y:161:ILE:HD11	2.03	0.40
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	247/250 (99%)	241 (98%)	5 (2%)	1 (0%)	39	37
1	O	247/250 (99%)	240 (97%)	6 (2%)	1 (0%)	39	37
2	B	242/258 (94%)	232 (96%)	9 (4%)	1 (0%)	39	37
2	P	242/258 (94%)	232 (96%)	9 (4%)	1 (0%)	39	37
3	C	238/254 (94%)	228 (96%)	6 (2%)	4 (2%)	11	5
3	Q	238/254 (94%)	228 (96%)	6 (2%)	4 (2%)	11	5
4	D	231/260 (89%)	230 (100%)	0	1 (0%)	39	37
4	R	231/260 (89%)	230 (100%)	0	1 (0%)	39	37
5	E	229/234 (98%)	218 (95%)	11 (5%)	0	100	100
5	S	229/234 (98%)	218 (95%)	11 (5%)	0	100	100
6	F	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
6	T	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
9	W	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
10	J	193/198 (98%)	187 (97%)	5 (3%)	1 (0%)	34	30
10	X	193/198 (98%)	187 (97%)	5 (3%)	1 (0%)	34	30
11	K	209/212 (99%)	206 (99%)	3 (1%)	0	100	100
11	Y	209/212 (99%)	206 (99%)	3 (1%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	220 (95%)	11 (5%)	0	100	100
13	a	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6280/6614 (95%)	6105 (97%)	159 (2%)	16 (0%)	46	45

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	202	GLN
3	C	205	ALA
3	Q	202	GLN
3	Q	205	ALA
2	B	51	VAL
4	D	2	ARG
2	P	51	VAL
4	R	2	ARG
3	C	239	GLN
3	Q	239	GLN
1	A	166	LYS
1	O	166	LYS
10	J	24	GLY
10	X	24	GLY
3	C	183	PRO
3	Q	183	PRO

### 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	208/209 (100%)	199 (96%)	9 (4%)	35	34
1	O	208/209 (100%)	199 (96%)	9 (4%)	35	34
2	B	203/216 (94%)	188 (93%)	15 (7%)	17	13
2	P	203/216 (94%)	187 (92%)	16 (8%)	15	11
3	C	212/226 (94%)	189 (89%)	23 (11%)	8	4
3	Q	212/226 (94%)	189 (89%)	23 (11%)	8	4
4	D	194/215 (90%)	175 (90%)	19 (10%)	10	6
4	R	194/215 (90%)	174 (90%)	20 (10%)	9	5
5	E	190/193 (98%)	171 (90%)	19 (10%)	9	6
5	S	190/193 (98%)	171 (90%)	19 (10%)	9	6
6	F	201/239 (84%)	185 (92%)	16 (8%)	15	11
6	T	201/239 (84%)	185 (92%)	16 (8%)	15	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	206/210 (98%)	192 (93%)	14 (7%)	20	16
7	U	206/210 (98%)	192 (93%)	14 (7%)	20	16
8	H	185/190 (97%)	176 (95%)	9 (5%)	31	28
8	V	185/190 (97%)	175 (95%)	10 (5%)	27	24
9	I	172/173 (99%)	165 (96%)	7 (4%)	37	36
9	W	172/173 (99%)	165 (96%)	7 (4%)	37	36
10	J	173/175 (99%)	165 (95%)	8 (5%)	33	31
10	X	173/175 (99%)	165 (95%)	8 (5%)	33	31
11	K	168/169 (99%)	159 (95%)	9 (5%)	27	24
11	Y	168/169 (99%)	159 (95%)	9 (5%)	27	24
12	L	185/185 (100%)	173 (94%)	12 (6%)	21	17
12	Z	185/185 (100%)	172 (93%)	13 (7%)	19	15
13	M	199/208 (96%)	189 (95%)	10 (5%)	30	27
13	a	199/208 (96%)	188 (94%)	11 (6%)	27	23
14	N	162/162 (100%)	152 (94%)	10 (6%)	23	19
14	b	162/162 (100%)	152 (94%)	10 (6%)	23	19
All	All	5316/5540 (96%)	4951 (93%)	365 (7%)	19	15

All (365) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	59	GLU
1	A	122	THR
1	A	157	PHE
1	A	172	LYS
1	A	201	GLU
1	A	231	LYS
1	A	248	GLU
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	63	GLU
2	B	65	LEU
2	B	79	LEU
2	B	102	ASN

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Mol	Chain	Res	Type
2	B	113	ARG
2	B	114	LEU
2	B	119	GLN
2	B	191	LEU
2	B	203	SER
2	B	217	LYS
2	B	221	ASP
2	B	237	ILE
2	B	238	LEU
3	C	4	ARG
3	C	35	LYS
3	C	38	ASN
3	C	48	SER
3	C	51	LYS
3	C	52	LEU
3	C	53	GLN
3	C	58	THR
3	C	61	LYS
3	C	116	GLN
3	C	147	GLN
3	C	160	GLN
3	C	167	LYS
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	201	VAL
3	C	203	THR
3	C	206	LYS
3	C	213	VAL
3	C	222	LEU
3	C	238	LYS
3	C	240	GLU
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	60	VAL
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	169	GLU
4	D	174	GLU
4	D	176	LEU

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Mol	Chain	Res	Type
4	D	190	LEU
4	D	193	LEU
4	D	202	GLU
4	D	203	LYS
4	D	214	ILE
4	D	233	LYS
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	3	ASN
5	E	8	ASP
5	E	9	THR
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	55	LEU
5	E	59	GLN
5	E	71	LEU
5	E	99	ASN
5	E	106	ARG
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	207	VAL
5	E	208	ASP
5	E	211	SER
5	E	217	LYS
5	E	222	THR
6	F	94	SER
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	165	ARG
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	207	ASP
6	F	214	TRP
6	F	215	CYS
6	F	221	ASN

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Mol	Chain	Res	Type
6	F	240	GLN
6	F	241	LYS
7	G	13	GLU
7	G	26	THR
7	G	34	LEU
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	166	GLN
7	G	179	LYS
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	63	ILE
8	H	106	THR
8	H	127	LEU
8	H	144	GLN
8	H	153	LYS
8	H	196	ARG
9	I	37	ASN
9	I	96	GLU
9	I	114	LYS
9	I	126	ILE
9	I	133	LYS
9	I	171	LEU
9	I	182	TRP
10	J	2	ASP
10	J	3	ILE
10	J	23	ARG
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
10	J	110	LYS
10	J	172	MET
11	K	4	LEU
11	K	9	GLN

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Mol	Chain	Res	Type
11	K	35	ILE
11	K	57	THR
11	K	104	TYR
11	K	116	ASP
11	K	128	CYS
11	K	140	LEU
11	K	148	LEU
12	L	3	ASN
12	L	18	GLU
12	L	23	LEU
12	L	31	THR
12	L	42	LYS
12	L	49	ASN
12	L	71	SER
12	L	108	HIS
12	L	136	CYS
12	L	161	GLU
12	L	172	LEU
12	L	173	LYS
13	M	2	GLN
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	138	SER
13	M	161	ARG
13	M	187	ARG
13	M	192	SER
13	M	212	LEU
14	N	9	LYS
14	N	20	THR
14	N	36	ARG
14	N	44	CYS
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
14	N	115	LEU
14	N	160	SER
14	N	178	LEU
1	O	29	LYS
1	O	59	GLU
1	O	122	THR

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Mol	Chain	Res	Type
1	O	157	PHE
1	O	172	LYS
1	O	201	GLU
1	O	231	LYS
1	O	248	GLU
1	O	250	LEU
2	P	50	LYS
2	P	51	VAL
2	P	55	LEU
2	P	63	GLU
2	P	65	LEU
2	P	79	LEU
2	P	102	ASN
2	P	113	ARG
2	P	114	LEU
2	P	119	GLN
2	P	191	LEU
2	P	203	SER
2	P	217	LYS
2	P	221	ASP
2	P	237	ILE
2	P	238	LEU
3	Q	4	ARG
3	Q	35	LYS
3	Q	38	ASN
3	Q	48	SER
3	Q	51	LYS
3	Q	52	LEU
3	Q	53	GLN
3	Q	58	THR
3	Q	61	LYS
3	Q	116	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	167	LYS
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	201	VAL
3	Q	203	THR
3	Q	206	LYS
3	Q	213	VAL

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Mol	Chain	Res	Type
3	Q	222	LEU
3	Q	238	LYS
3	Q	240	GLU
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	60	VAL
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	169	GLU
4	R	174	GLU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	202	GLU
4	R	203	LYS
4	R	214	ILE
4	R	217	GLN
4	R	233	LYS
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	3	ASN
5	S	8	ASP
5	S	9	THR
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	55	LEU
5	S	59	GLN
5	S	71	LEU
5	S	99	ASN
5	S	106	ARG
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	207	VAL
5	S	208	ASP
5	S	211	SER
5	S	217	LYS
5	S	222	THR

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Mol	Chain	Res	Type
6	T	94	SER
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	165	ARG
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	207	ASP
6	T	214	TRP
6	T	215	CYS
6	T	221	ASN
6	T	240	GLN
6	T	241	LYS
7	U	13	GLU
7	U	26	THR
7	U	34	LEU
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	166	GLN
7	U	179	LYS
7	U	208	GLU
7	U	221	LYS
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	63	ILE
8	V	68	LEU
8	V	106	THR
8	V	127	LEU
8	V	144	GLN
8	V	153	LYS
8	V	196	ARG
9	W	37	ASN
9	W	96	GLU

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Mol	Chain	Res	Type
9	W	114	LYS
9	W	126	ILE
9	W	133	LYS
9	W	171	LEU
9	W	182	TRP
10	X	2	ASP
10	X	3	ILE
10	X	23	ARG
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
10	X	110	LYS
10	X	172	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	57	THR
11	Y	104	TYR
11	Y	116	ASP
11	Y	128	CYS
11	Y	140	LEU
11	Y	148	LEU
12	Z	3	ASN
12	Z	18	GLU
12	Z	23	LEU
12	Z	31	THR
12	Z	42	LYS
12	Z	49	ASN
12	Z	71	SER
12	Z	108	HIS
12	Z	136	CYS
12	Z	150	LEU
12	Z	161	GLU
12	Z	172	LEU
12	Z	173	LYS
13	a	2	GLN
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	106	LYS
13	a	138	SER

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Mol	Chain	Res	Type
13	a	161	ARG
13	a	187	ARG
13	a	192	SER
13	a	212	LEU
14	b	9	LYS
14	b	20	THR
14	b	36	ARG
14	b	44	CYS
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS
14	b	115	LEU
14	b	160	SER
14	b	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	100	ASN
4	D	146	GLN
4	D	210	GLN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN

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Mol	Chain	Res	Type
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
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	86	HIS
8	H	114	HIS
8	H	116	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
10	J	55	GLN
10	J	63	ASN
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	80	ASN
12	L	159	GLN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	179	ASN

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Mol	Chain	Res	Type
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
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	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	100	ASN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
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	166	GLN
7	U	167	GLN
7	U	175	ASN

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Mol	Chain	Res	Type
8	V	30	ASN
8	V	66	HIS
8	V	86	HIS
8	V	114	HIS
8	V	116	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	37	ASN
10	X	55	GLN
10	X	63	ASN
10	X	86	GLN
10	X	191	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	80	ASN
12	Z	159	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
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

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
16	3K4	K	301	11	4,6,7	4.75	3 (75%)	2,8,10	2.36	1 (50%)
16	3K4	Y	301	11	4,6,7	4.47	3 (75%)	2,8,10	2.14	1 (50%)

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
16	3K4	K	301	11	-	0/0/7/9	0/0/1/1
16	3K4	Y	301	11	-	0/0/7/9	0/0/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	301	3K4	C5-N6	-7.68	1.42	1.47
16	Y	301	3K4	C5-N6	-6.98	1.42	1.47
16	Y	301	3K4	C2-C5	-4.12	1.40	1.48
16	K	301	3K4	C2-C5	-4.07	1.40	1.48
16	K	301	3K4	C7-C5	-3.74	1.45	1.52
16	Y	301	3K4	C7-C5	-3.68	1.45	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	301	3K4	C2-C5-N6	2.60	60.79	59.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	301	3K4	C2-C5-N6	2.95	60.93	59.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	249/250 (99%)	-0.19	10 (4%)	42 51	28, 38, 67, 111	0
1	O	249/250 (99%)	-0.03	11 (4%)	38 47	31, 44, 82, 118	0
2	B	244/258 (94%)	0.04	14 (5%)	27 35	26, 43, 80, 140	0
2	P	244/258 (94%)	0.10	14 (5%)	27 35	31, 46, 84, 131	0
3	C	240/254 (94%)	0.16	20 (8%)	14 19	27, 46, 102, 122	0
3	Q	240/254 (94%)	0.45	33 (13%)	4 5	31, 53, 120, 146	0
4	D	235/260 (90%)	-0.08	4 (1%)	73 78	31, 46, 75, 110	0
4	R	235/260 (90%)	-0.00	12 (5%)	32 40	32, 49, 79, 110	0
5	E	231/234 (98%)	0.02	12 (5%)	31 39	35, 48, 80, 126	0
5	S	231/234 (98%)	0.27	18 (7%)	16 22	35, 57, 90, 137	0
6	F	243/288 (84%)	-0.08	8 (3%)	50 59	29, 45, 85, 113	0
6	T	243/288 (84%)	0.02	15 (6%)	24 32	30, 50, 94, 118	0
7	G	241/252 (95%)	-0.20	6 (2%)	61 67	24, 38, 68, 115	0
7	U	241/252 (95%)	-0.06	16 (6%)	22 29	31, 43, 69, 102	0
8	H	226/232 (97%)	-0.20	8 (3%)	48 57	26, 38, 64, 116	0
8	V	226/232 (97%)	-0.12	8 (3%)	48 57	30, 42, 66, 124	0
9	I	204/205 (99%)	-0.42	4 (1%)	68 73	25, 35, 60, 82	0
9	W	204/205 (99%)	-0.42	3 (1%)	76 81	26, 36, 63, 92	0
10	J	195/198 (98%)	-0.30	6 (3%)	52 61	25, 38, 62, 129	0
10	X	195/198 (98%)	-0.32	4 (2%)	67 72	25, 39, 63, 125	0
11	K	211/212 (99%)	-0.40	1 (0%)	91 93	26, 36, 55, 71	0
11	Y	211/212 (99%)	-0.37	1 (0%)	91 93	29, 38, 57, 74	0
12	L	222/222 (100%)	-0.36	2 (0%)	85 88	27, 39, 61, 95	0
12	Z	222/222 (100%)	-0.39	3 (1%)	78 82	27, 38, 61, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.45	4 (1%)	73	78	25, 39, 59, 77	0
13	a	233/246 (94%)	-0.42	4 (1%)	73	78	25, 37, 54, 72	0
14	N	196/196 (100%)	-0.42	2 (1%)	84	87	26, 36, 62, 88	0
14	b	196/196 (100%)	-0.34	3 (1%)	76	81	28, 37, 61, 95	0
All	All	6340/6614 (95%)	-0.15	246 (3%)	43	52	24, 42, 78, 146	0

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	50	LEU	11.1
2	B	218	GLY	9.0
2	B	219	ALA	8.9
2	P	51	VAL	7.8
1	O	249	ALA	7.6
3	Q	49	THR	7.5
2	B	51	VAL	7.1
5	S	202	ASP	7.0
2	P	219	ALA	7.0
5	E	202	ASP	6.9
2	P	222	GLY	6.8
3	C	49	THR	6.4
10	X	1	MET	6.4
2	B	221	ASP	6.3
3	Q	240	GLU	6.3
8	V	224	GLN	6.2
3	C	239	GLN	6.2
2	P	218	GLY	6.1
7	U	242	GLN	6.1
8	V	223	ILE	5.8
12	L	174	TYR	5.8
8	V	226	GLU	5.6
9	W	1	SER	5.6
9	I	1	SER	5.5
1	O	53	SER	5.4
6	T	243	ILE	5.4
2	P	221	ASP	5.4
6	F	244	ASN	5.4
10	X	194	ASP	5.3
3	Q	202	GLN	5.1
3	C	238	LYS	5.1
10	J	1	MET	5.0

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Mol	Chain	Res	Type	RSRZ
3	Q	55	THR	5.0
8	V	221	CYS	4.9
1	A	250	LEU	4.9
2	B	222	GLY	4.9
8	V	222	ASP	4.8
10	J	194	ASP	4.8
5	S	233	ILE	4.8
3	Q	239	GLN	4.7
3	Q	206	LYS	4.7
4	D	242	GLU	4.7
6	F	205	GLU	4.7
1	O	250	LEU	4.7
3	C	206	LYS	4.6
5	E	122	TYR	4.6
7	G	240	ALA	4.6
2	P	52	THR	4.6
6	T	2	THR	4.5
10	X	193	ASP	4.4
7	G	242	GLN	4.4
9	W	133	LYS	4.4
3	Q	236	GLN	4.4
3	C	203	THR	4.3
5	S	122	TYR	4.3
8	H	223	ILE	4.2
8	H	224	GLN	4.2
3	Q	48	SER	4.2
1	A	248	GLU	4.2
1	O	2	THR	4.2
1	A	249	ALA	4.1
1	A	2	THR	4.1
5	E	123	GLY	4.1
14	b	195	GLN	4.1
5	E	201	ARG	4.0
3	Q	187	GLU	4.0
8	H	221	CYS	4.0
6	T	244	ASN	3.9
1	O	52	SER	3.9
3	Q	204	GLY	3.9
8	H	222	ASP	3.9
14	N	195	GLN	3.9
8	H	226	GLU	3.8
3	C	205	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
2	P	59	ASP	3.8
3	C	240	GLU	3.7
5	S	210	LEU	3.6
4	D	1	ASP	3.6
12	Z	174	TYR	3.6
13	M	1	THR	3.6
2	P	220	ASN	3.6
4	R	125	LEU	3.5
6	F	2	THR	3.5
10	J	193	ASP	3.5
6	F	181	GLU	3.5
1	A	203	GLU	3.5
5	E	210	LEU	3.4
3	Q	51	LYS	3.4
2	B	217	LYS	3.4
7	G	3	TYR	3.4
3	C	50	LEU	3.4
6	F	202	ASP	3.3
6	T	206	LYS	3.3
4	R	241	ALA	3.3
1	A	229	THR	3.3
9	I	192	ASP	3.3
3	Q	237	GLU	3.3
3	Q	234	ILE	3.2
3	Q	47	ARG	3.2
4	R	1	ASP	3.2
3	Q	238	LYS	3.2
5	S	173	ARG	3.2
3	Q	201	VAL	3.2
9	W	192	ASP	3.2
5	E	203	GLU	3.2
3	C	202	GLN	3.2
6	T	204	LYS	3.1
1	O	201	GLU	3.1
5	S	201	ARG	3.1
3	Q	60	SER	3.1
6	F	204	LYS	3.1
6	T	180	PRO	3.1
3	C	216	ASP	3.1
2	P	182	ASP	3.1
3	C	51	LYS	3.1
7	U	181	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	236	GLN	3.0
7	U	51	PRO	3.0
7	U	183	ASP	3.0
6	F	215	CYS	3.0
14	b	105	LYS	3.0
7	U	241	GLU	3.0
6	T	205	GLU	2.9
7	U	2	GLY	2.9
13	a	1	THR	2.9
5	E	233	ILE	2.9
2	P	60	THR	2.9
5	S	165	GLN	2.9
6	T	201	GLU	2.9
8	H	225	GLU	2.9
4	R	201	GLU	2.9
2	B	220	ASN	2.9
3	C	181	GLU	2.9
2	B	52	THR	2.9
4	R	242	GLU	2.9
7	U	188	GLU	2.9
3	C	60	SER	2.8
3	Q	223	SER	2.8
6	T	181	GLU	2.8
10	J	24	GLY	2.8
3	C	225	GLU	2.7
7	U	206	GLY	2.7
3	Q	180	LYS	2.7
5	S	52	ALA	2.7
3	Q	59	PRO	2.7
1	A	54	PRO	2.7
5	S	207	VAL	2.7
3	Q	205	ALA	2.7
4	R	217	GLN	2.7
3	C	48	SER	2.7
4	R	117	GLU	2.7
9	I	133	LYS	2.7
3	Q	225	GLU	2.7
5	S	3	ASN	2.6
1	A	62	SER	2.6
7	U	3	TYR	2.6
6	T	178	HIS	2.6
8	V	145	ASP	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	R	240	ALA	2.6
6	T	166	GLN	2.6
6	T	215	CYS	2.6
3	C	180	LYS	2.6
4	D	2	ARG	2.6
10	X	195	PHE	2.5
4	R	113	LEU	2.5
3	Q	216	ASP	2.5
1	A	231	LYS	2.5
3	Q	58	THR	2.5
5	S	180	LYS	2.5
3	C	47	ARG	2.5
2	B	203	SER	2.5
5	S	203	GLU	2.5
7	G	241	GLU	2.5
7	U	58	THR	2.5
1	O	203	GLU	2.5
3	C	175	LYS	2.4
4	D	241	ALA	2.4
7	U	219	ALA	2.4
3	Q	229	GLN	2.4
3	Q	203	THR	2.4
3	Q	175	LYS	2.4
13	a	47	ASP	2.3
2	P	244	THR	2.3
5	S	171	LEU	2.3
8	V	219	ASN	2.3
5	E	173	ARG	2.3
3	Q	57	ILE	2.3
14	N	105	LYS	2.3
2	B	59	ASP	2.3
6	T	230	ASP	2.3
7	U	222	ASP	2.3
3	C	229	GLN	2.3
3	Q	232	THR	2.3
5	E	217	LYS	2.3
3	Q	52	LEU	2.3
3	Q	221	ALA	2.3
7	G	2	GLY	2.3
3	Q	181	GLU	2.3
1	A	201	GLU	2.3
4	R	54	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	169	SER	2.3
2	B	244	THR	2.3
5	S	30	GLN	2.3
7	U	68	ARG	2.3
2	P	50	LYS	2.3
8	H	219	ASN	2.3
5	E	3	ASN	2.2
5	S	51	ASN	2.2
6	T	193	ALA	2.2
13	M	82	ASP	2.2
1	O	248	GLU	2.2
9	I	131	GLU	2.2
6	F	51	THR	2.2
12	Z	173	LYS	2.2
2	P	203	SER	2.2
5	E	54	GLU	2.2
7	U	230	GLU	2.2
5	E	218	ASP	2.2
14	b	9	LYS	2.2
7	U	53	LYS	2.1
1	O	229	THR	2.1
13	a	216	ASN	2.1
10	J	195	PHE	2.1
11	Y	212	GLY	2.1
10	J	135	TYR	2.1
5	S	194	GLU	2.1
4	R	177	ASN	2.1
5	S	54	GLU	2.1
8	V	198	GLU	2.1
2	B	240	LYS	2.1
2	P	240	LYS	2.1
12	Z	172	LEU	2.1
1	O	231	LYS	2.1
8	H	22	GLN	2.1
4	R	230	GLU	2.0
5	S	163	ARG	2.0
6	T	54	LEU	2.0
13	a	121	SER	2.0
13	M	47	ASP	2.0
7	U	207	THR	2.0
12	L	173	LYS	2.0
7	G	51	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
13	M	121	SER	2.0
1	O	50	LYS	2.0
11	K	106	ARG	2.0
2	B	93	HIS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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(Å <sup>2</sup> )	Q<0.9
15	MG	J	201	1/1	0.97	0.22	15.46	37,37,37,37	0
15	MG	I	302	1/1	0.89	0.37	13.96	59,59,59,59	0
15	MG	K	303	1/1	0.97	0.18	3.32	41,41,41,41	0
16	3K4	K	301	6/7	0.94	0.15	2.53	36,41,45,48	0
16	3K4	Y	301	6/7	0.95	0.13	1.81	41,47,50,54	0
15	MG	Y	302	1/1	0.97	0.08	-0.86	31,31,31,31	0
15	MG	G	301	1/1	0.98	0.04	-1.45	31,31,31,31	0
15	MG	V	301	1/1	0.98	0.04	-1.91	38,38,38,38	0
15	MG	K	302	1/1	0.99	0.05	-2.01	29,29,29,29	0
15	MG	I	301	1/1	0.99	0.03	-2.27	34,34,34,34	0
15	MG	Z	301	1/1	0.99	0.07	-2.44	40,40,40,40	0
15	MG	N	201	1/1	0.96	0.04	-2.46	40,40,40,40	0
15	MG	H	301	1/1	0.72	0.13	-	53,53,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.