



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:03 PM GMT

PDB ID : 4QLV  
Title : yCP in complex with tripeptidic epoxyketone inhibitor 17  
Authors : de Bruin, G.; Huber, E.; Xin, B.; van Rooden, E.; Al-Ayed, K.; Kim, K.; Kisselev, A.; Driessen, C.; van der Marel, G.; Groll, M.; Overkleeft, H.  
Deposited on : 2014-06-13  
Resolution : 2.90 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

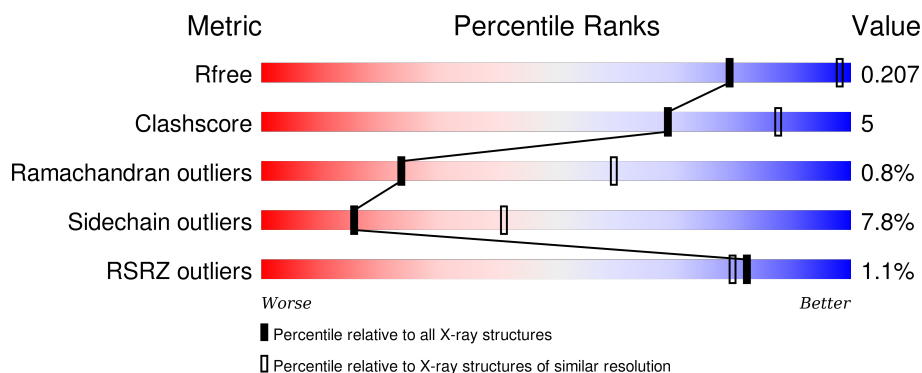
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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>2%</div> <div>87% 12% •</div> </div>
1	O	250	<div> <div>%</div> <div>85% 14% •</div> </div>
2	B	258	<div> <div>2%</div> <div>72% 21% • 5%</div> </div>
2	P	258	<div> <div>3%</div> <div>74% 18% • 5%</div> </div>
3	C	254	<div> <div>2%</div> <div>74% 17% • 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	N	201	-	-	-	X
15	MG	Z	301	-	-	-	X
16	MES	Y	302	-	-	-	X

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49622 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	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 Probable 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	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
			1683	1061	293	322	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	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	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).

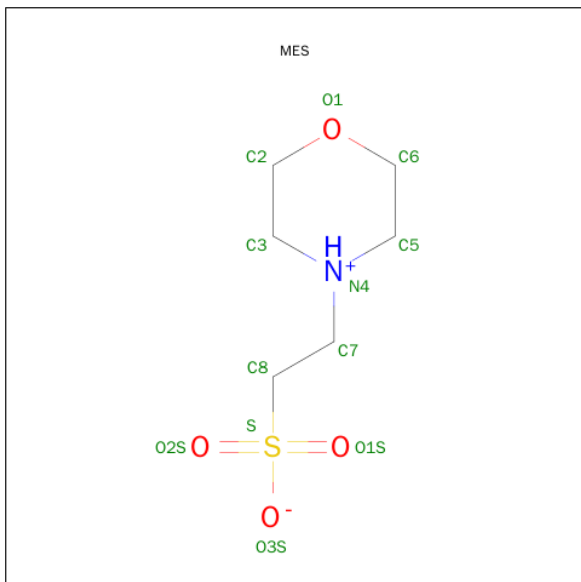
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	K	1	Total	Mg	0	0
			1	1		

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

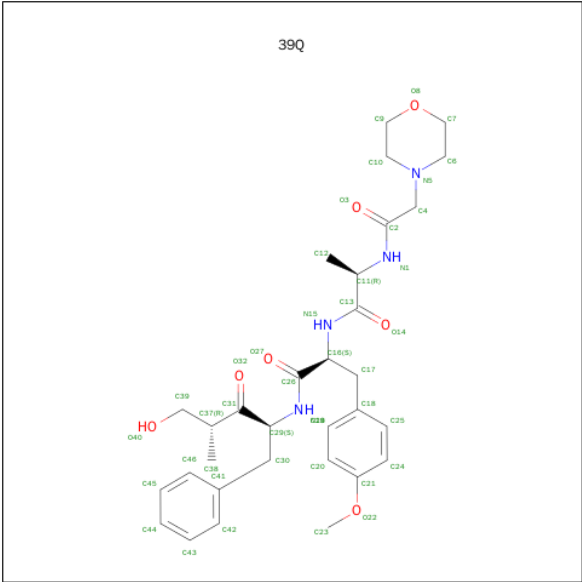
- Molecule 16 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
16	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 17 is N-(MORPHOLIN-4-YLACETYL)-D-ALANYL-N-[(2S,4R)-5-HYDROXY-4-METHYL-3-OXO-1-PHENYLPENTAN-2-YL]-O-METHYL-L-TYROSINAMIDE (three-letter code: 39Q) (formula: C<sub>31</sub>H<sub>42</sub>N<sub>4</sub>O<sub>7</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	K	1	Total	C	N	O	0	0
			42	31	4	7		
17	Y	1	Total	C	N	O	0	0
			42	31	4	7		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	5	Total	O	0	0
			5	5		
18	B	10	Total	O	0	0
			10	10		
18	C	9	Total	O	0	0
			9	9		
18	D	4	Total	O	0	0
			4	4		
18	E	5	Total	O	0	0
			5	5		
18	F	6	Total	O	0	0
			6	6		
18	G	6	Total	O	0	0
			6	6		
18	H	9	Total	O	0	0
			9	9		
18	I	6	Total	O	0	0
			6	6		
18	J	7	Total	O	0	0
			7	7		

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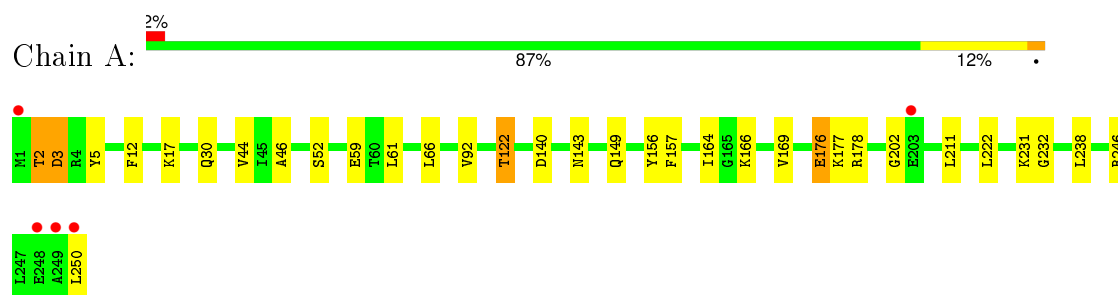
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	K	13	Total 13	O 13	0	0
18	L	8	Total 8	O 8	0	0
18	M	15	Total 15	O 15	0	0
18	N	7	Total 7	O 7	0	0
18	O	2	Total 2	O 2	0	0
18	P	6	Total 6	O 6	0	0
18	Q	9	Total 9	O 9	0	0
18	R	3	Total 3	O 3	0	0
18	S	5	Total 5	O 5	0	0
18	T	5	Total 5	O 5	0	0
18	U	9	Total 9	O 9	0	0
18	V	11	Total 11	O 11	0	0
18	W	4	Total 4	O 4	0	0
18	X	8	Total 8	O 8	0	0
18	Y	10	Total 10	O 10	0	0
18	Z	7	Total 7	O 7	0	0
18	a	13	Total 13	O 13	0	0
18	b	9	Total 9	O 9	0	0

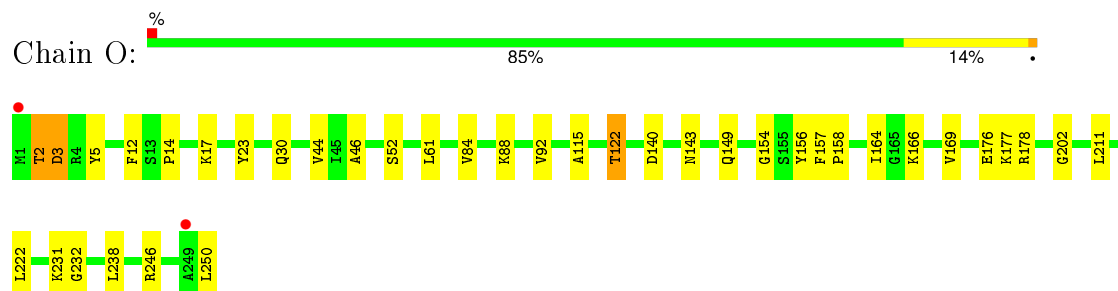
### 3 Residue-property plots [i](#)

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.

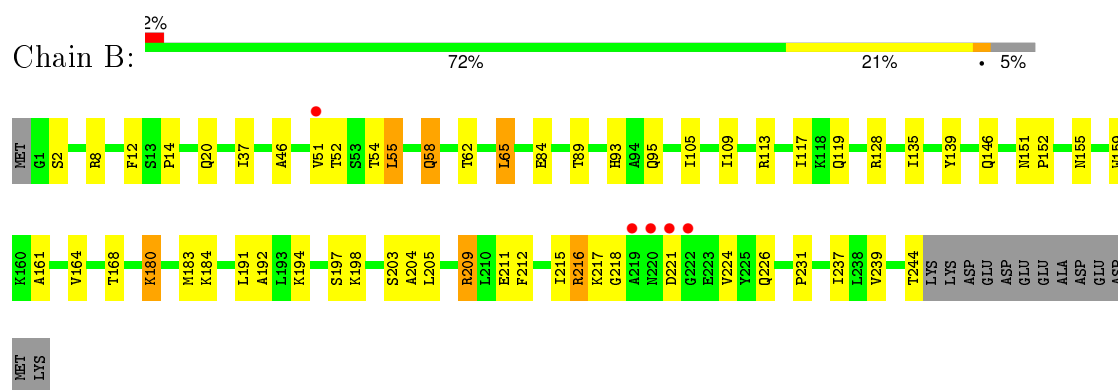
- Molecule 1: Proteasome subunit alpha type-2



- Molecule 1: Proteasome subunit alpha type-2

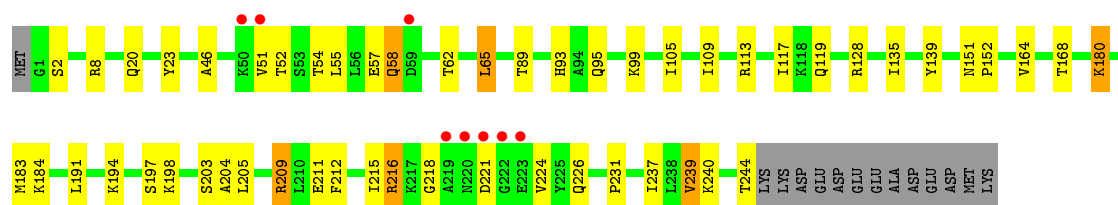


- Molecule 2: Proteasome subunit alpha type-3

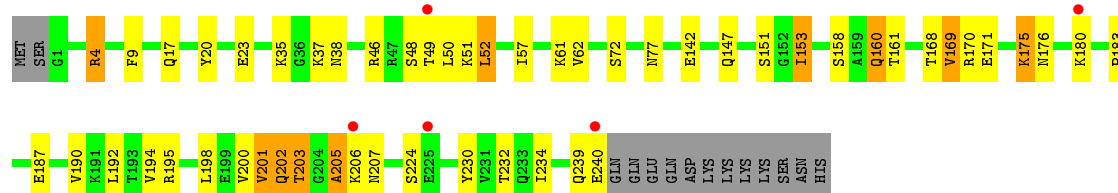
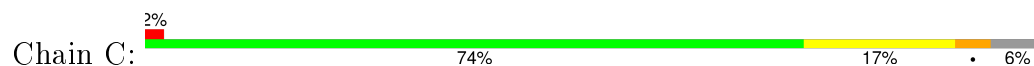


- Molecule 2: Proteasome subunit alpha type-3

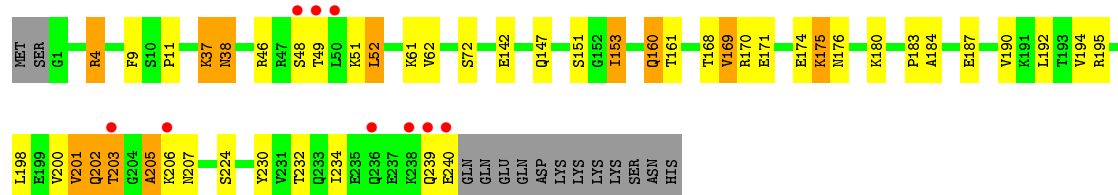
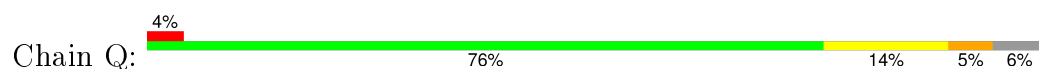




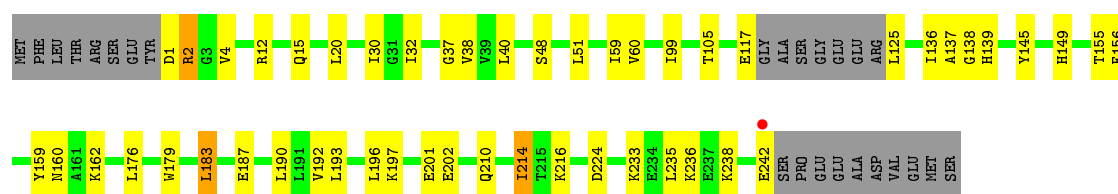
• Molecule 3: Proteasome subunit alpha type-4



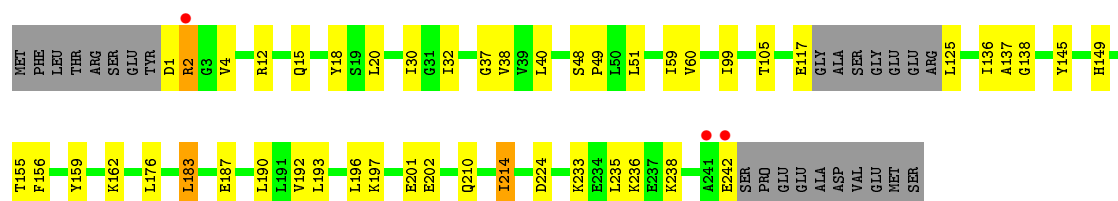
• Molecule 3: Proteasome subunit alpha type-4



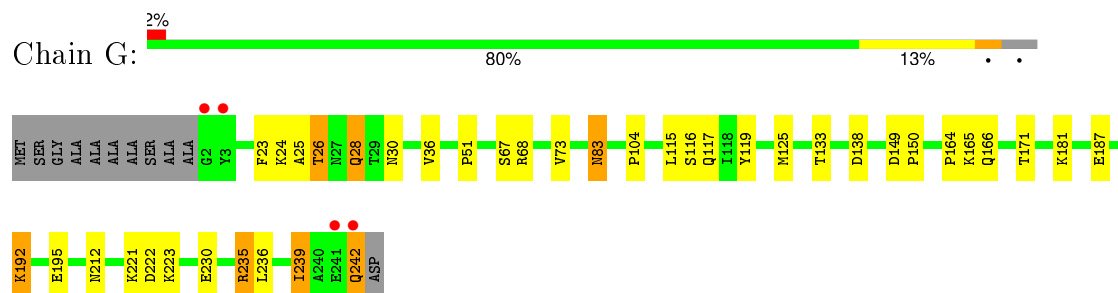
• Molecule 4: Proteasome subunit alpha type-5



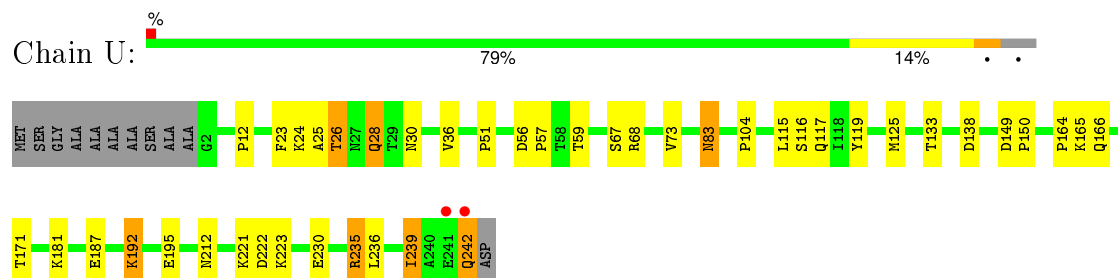
• Molecule 4: Proteasome subunit alpha type-5



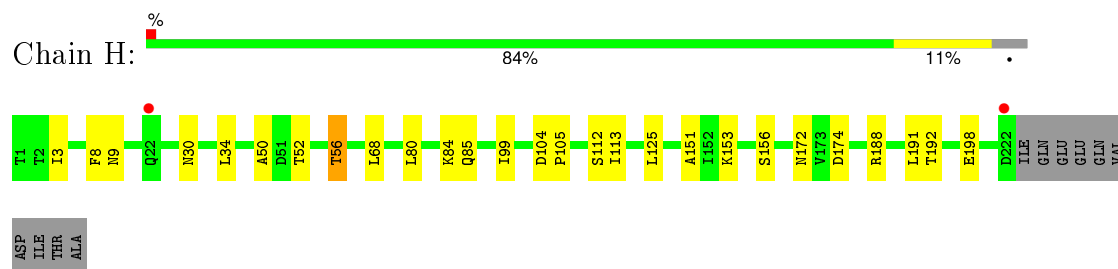
• Molecule 5: Proteasome subunit alpha type-6



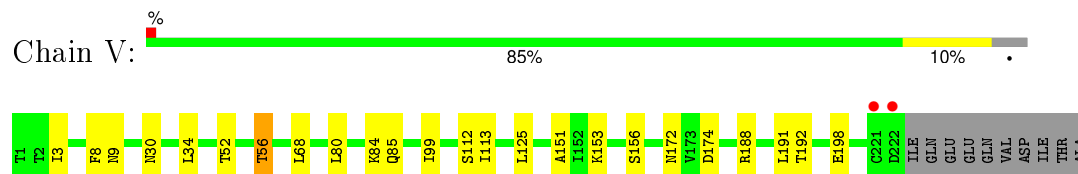
- Molecule 7: Proteasome subunit alpha type-1



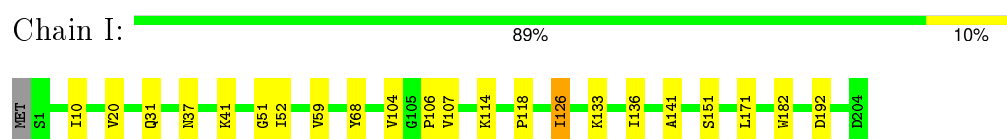
- Molecule 8: Proteasome subunit beta type-2



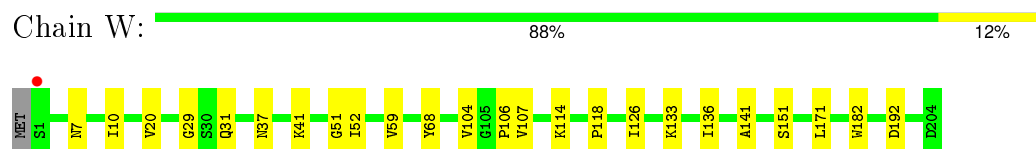
- Molecule 8: Proteasome subunit beta type-2



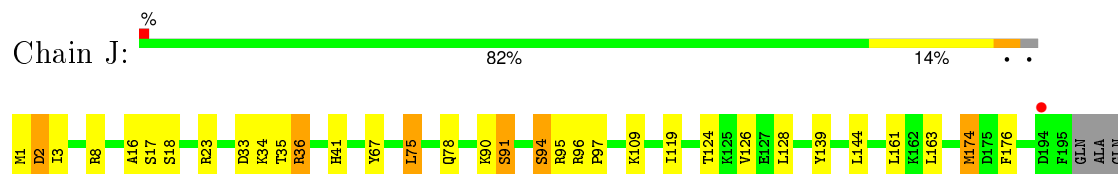
- Molecule 9: Proteasome subunit beta type-3



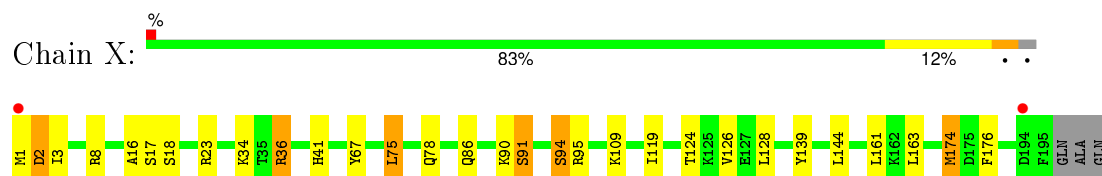
- Molecule 9: Proteasome subunit beta type-3



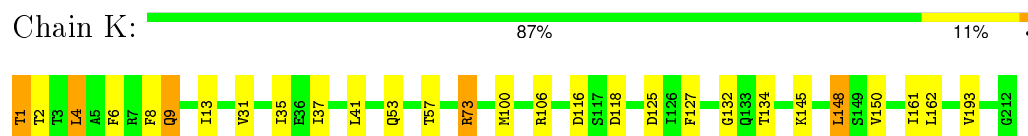
- Molecule 10: Proteasome subunit beta type-4



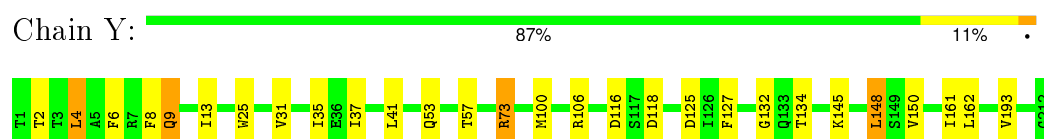
- Molecule 10: Proteasome subunit beta type-4



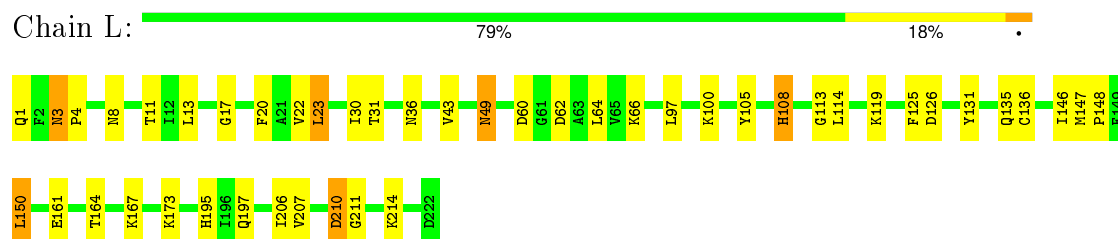
- Molecule 11: Proteasome subunit beta type-5



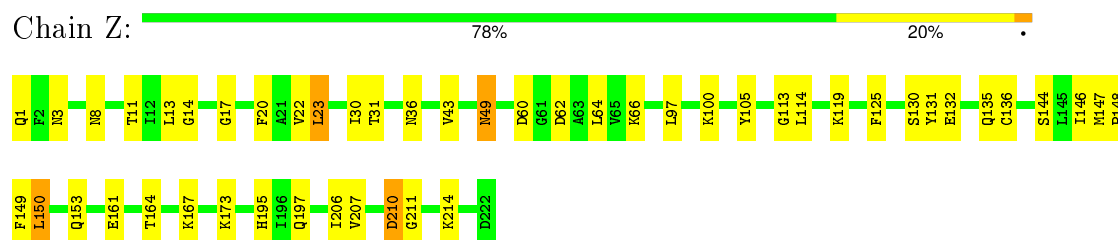
- Molecule 11: Proteasome subunit beta type-5



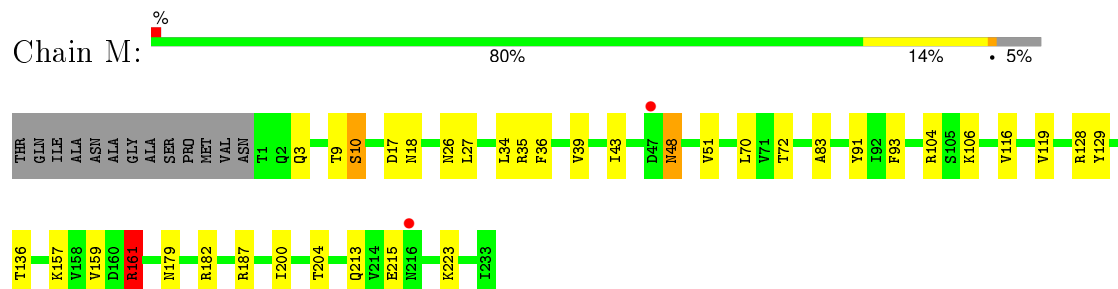
- Molecule 12: Proteasome subunit beta type-6



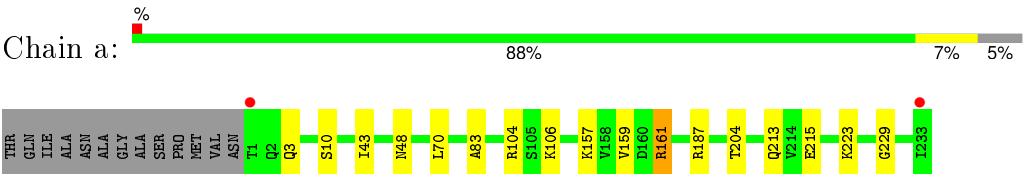
- Molecule 12: Proteasome subunit beta type-6



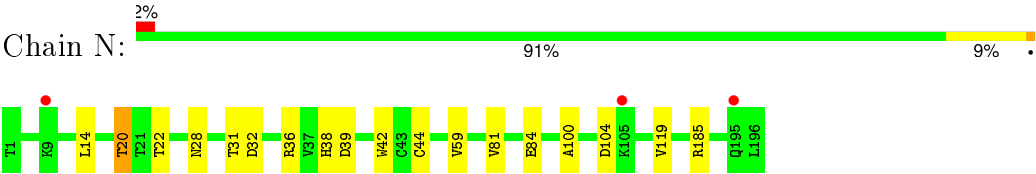
- Molecule 13: Proteasome subunit beta type-7



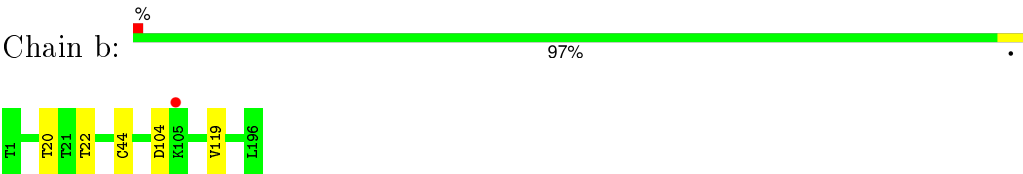
- Molecule 13: Proteasome subunit beta type-7



• Molecule 14: Proteasome subunit beta type-1



• 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, $\alpha$ , $\beta$ , $\gamma$	136.04Å 300.38Å 146.52Å 90.00° 112.97° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.5 (15.00-2.90) 95.6 (15.00-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.184 , 0.209 0.185 , 0.207	Depositor DCC
$R_{free}$ test set	11308 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.8	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 226162 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	49622	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: MG, 39Q, MES

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	0/1952	0.56	0/2642
1	O	0.29	0/1952	0.56	0/2642
2	B	0.30	0/1934	0.62	0/2618
2	P	0.30	0/1934	0.62	0/2618
3	C	0.30	0/1910	0.61	0/2586
3	Q	0.30	0/1910	0.61	0/2586
4	D	0.30	0/1837	0.59	0/2475
4	R	0.31	0/1837	0.59	0/2475
5	E	0.30	0/1800	0.58	0/2433
5	S	0.30	0/1800	0.58	0/2433
6	F	0.30	0/1932	0.57	0/2609
6	T	0.30	0/1932	0.57	0/2609
7	G	0.31	0/1945	0.58	0/2634
7	U	0.30	0/1945	0.58	0/2634
8	H	0.27	0/1715	0.55	0/2326
8	V	0.27	0/1714	0.55	0/2325
9	I	0.30	0/1611	0.57	0/2174
9	W	0.30	0/1611	0.57	0/2174
10	J	0.29	0/1589	0.57	0/2142
10	X	0.29	0/1589	0.57	0/2142
11	K	0.30	0/1681	0.58	0/2274
11	Y	0.31	0/1681	0.58	0/2274
12	L	0.30	0/1795	0.56	0/2420
12	Z	0.30	0/1795	0.56	0/2420
13	M	0.30	0/1855	0.60	1/2514 (0.0%)
13	a	0.30	0/1855	0.60	1/2514 (0.0%)
14	N	0.27	0/1541	0.54	0/2087
14	b	0.27	0/1541	0.54	0/2087
All	All	0.30	0/50193	0.58	2/67867 (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
6	F	0	1
6	T	0	1
11	K	0	1
12	L	0	1
12	Z	0	1
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	161	ARG	NE-CZ-NH1	5.21	122.91	120.30
13	M	161	ARG	NE-CZ-NH1	5.20	122.90	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	203	ASN	Peptide
11	K	1	THR	Peptide
12	L	135	GLN	Peptide
6	T	203	ASN	Peptide
12	Z	135	GLN	Peptide

## 5.2 Too-close contacts [i](#)

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	14	0
1	O	1915	0	1929	17	0
2	B	1904	0	1904	32	0
2	P	1904	0	1904	25	0
3	C	1881	0	1895	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	1881	0	1895	27	0
4	D	1813	0	1797	16	0
4	R	1813	0	1797	16	0
5	E	1773	0	1775	17	0
5	S	1773	0	1775	18	0
6	F	1892	0	1883	16	0
6	T	1892	0	1883	16	0
7	G	1907	0	1901	14	0
7	U	1907	0	1901	18	0
8	H	1684	0	1688	10	0
8	V	1683	0	1688	8	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	8	0
10	J	1561	0	1569	17	0
10	X	1561	0	1569	16	0
11	K	1644	0	1593	18	0
11	Y	1644	0	1593	17	0
12	L	1757	0	1711	26	0
12	Z	1757	0	1711	27	0
13	M	1824	0	1832	15	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	9	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	2	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	12	0	13	1	0
16	Y	12	0	13	0	0
17	K	42	0	41	5	0
17	Y	42	0	41	7	0
18	A	5	0	0	0	0
18	B	10	0	0	0	0
18	C	9	0	0	0	0
18	D	4	0	0	0	0
18	E	5	0	0	0	0
18	F	6	0	0	0	0
18	G	6	0	0	0	0
18	H	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	I	6	0	0	0	0
18	J	7	0	0	0	0
18	K	13	0	0	0	0
18	L	8	0	0	0	0
18	M	15	0	0	0	0
18	N	7	0	0	0	0
18	O	2	0	0	0	0
18	P	6	0	0	0	0
18	Q	9	0	0	0	0
18	R	3	0	0	0	0
18	S	5	0	0	0	0
18	T	5	0	0	0	0
18	U	9	0	0	0	0
18	V	11	0	0	0	0
18	W	4	0	0	0	0
18	X	8	0	0	0	0
18	Y	10	0	0	0	0
18	Z	7	0	0	0	0
18	a	13	0	0	0	0
18	b	9	0	0	0	0
All	All	49622	0	49172	424	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 5.

All (424) 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:P:93:HIS:HB3	2:P:113:ARG:HH21	1.34	0.90
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.33	0.90
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.54	0.87
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.57	0.85
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.44	0.83
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.43	0.83
11:Y:100:MET:HE3	11:Y:127:PHE:CB	2.09	0.82
6:T:34:ILE:HG22	6:T:160:ALA:HB2	1.61	0.82
11:K:100:MET:HE3	11:K:127:PHE:CB	2.11	0.81
6:F:34:ILE:HG22	6:F:160:ALA:HB2	1.61	0.80
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.18	0.74
7:G:23:PHE:O	7:G:26:THR:HB	1.89	0.73
11:K:100:MET:CE	11:K:127:PHE:HB2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:303:39Q:H3	12:L:126:ASP:HB3	1.71	0.72
7:U:23:PHE:O	7:U:26:THR:HB	1.88	0.72
3:C:51:LYS:O	3:C:52:LEU:HB2	1.90	0.72
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.72	0.70
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.72	0.70
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.90	0.70
17:Y:303:39Q:H36	17:Y:303:39Q:O27	1.91	0.70
2:B:93:HIS:HB3	2:B:113:ARG:NH2	2.05	0.70
2:P:93:HIS:HB3	2:P:113:ARG:NH2	2.06	0.69
7:G:25:ALA:O	7:G:28:GLN:HB2	1.92	0.68
5:E:35:VAL:HG22	5:E:159:ALA:HB2	1.74	0.68
5:S:35:VAL:HG22	5:S:159:ALA:HB2	1.73	0.68
7:U:25:ALA:O	7:U:28:GLN:HB2	1.94	0.68
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.76	0.67
3:Q:230:TYR:O	3:Q:234:ILE:HG13	1.95	0.66
4:R:38:VAL:HG11	4:R:137:ALA:HB1	1.78	0.66
13:M:161:ARG:HH11	13:M:161:ARG:HG3	1.61	0.66
4:D:38:VAL:HG11	4:D:137:ALA:HB1	1.78	0.65
16:K:302:MES:O3S	17:K:303:39Q:O40	2.13	0.65
3:C:230:TYR:O	3:C:234:ILE:HG13	1.95	0.65
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.12	0.65
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.12	0.65
3:C:201:VAL:HG13	3:C:202:GLN:N	2.12	0.64
17:K:303:39Q:O40	17:K:303:39Q:O32	2.14	0.64
3:C:201:VAL:HG13	3:C:202:GLN:H	1.64	0.63
5:S:9:THR:HG21	5:S:119:THR:HA	1.81	0.62
14:N:20:THR:CG2	14:N:31:THR:OG1	2.47	0.62
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.82	0.62
7:G:83:ASN:C	7:G:83:ASN:HD22	2.03	0.62
3:Q:190:VAL:O	3:Q:194:VAL:HG23	1.99	0.62
3:Q:201:VAL:HG13	3:Q:202:GLN:H	1.63	0.61
3:C:190:VAL:O	3:C:194:VAL:HG23	2.00	0.61
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.82	0.61
5:S:136:TYR:CE1	5:S:217:LYS:HA	2.36	0.61
7:G:73:VAL:HG12	7:G:133:THR:HB	1.82	0.61
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.00	0.61
7:U:83:ASN:C	7:U:83:ASN:HD22	2.03	0.61
5:E:9:THR:HG21	5:E:119:THR:HA	1.82	0.61
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.83	0.60
5:E:136:TYR:CE1	5:E:217:LYS:HA	2.36	0.60
2:P:8:ARG:HD2	3:Q:4:ARG:NH2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:73:VAL:HG12	7:U:133:THR:HB	1.83	0.60
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.83	0.59
3:Q:168:THR:O	3:Q:171:GLU:HB3	2.02	0.59
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.84	0.59
11:Y:73:ARG:HB2	11:Y:73:ARG:NH1	2.18	0.59
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.85	0.58
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.85	0.58
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.34	0.58
11:K:53:GLN:O	11:K:57:THR:HG23	2.03	0.58
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.84	0.58
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.34	0.58
7:G:195:GLU:HG3	7:G:235:ARG:HG3	1.85	0.58
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.52	0.58
3:C:168:THR:O	3:C:171:GLU:HB3	2.03	0.57
11:K:73:ARG:HB2	11:K:73:ARG:NH1	2.18	0.57
17:Y:303:39Q:O3	17:Y:303:39Q:H8	2.04	0.57
3:C:198:LEU:HA	3:C:201:VAL:HG12	1.87	0.56
9:W:107:VAL:HG13	9:W:136:ILE:HG21	1.87	0.56
2:B:12:PHE:H	3:C:17:GLN:HE22	1.52	0.56
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.87	0.56
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.86	0.56
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.70	0.56
2:P:95:GLN:HB3	9:W:68:TYR:CD2	2.41	0.56
1:O:12:PHE:H	2:P:20:GLN:HE22	1.52	0.56
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.88	0.56
2:P:89:THR:HG21	2:P:117:ILE:CD1	2.36	0.56
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.88	0.56
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.18	0.56
3:Q:62:VAL:HG22	3:Q:72:SER:HB3	1.88	0.56
17:Y:303:39Q:H3	12:Z:130:SER:HB3	1.87	0.56
2:B:89:THR:HG21	2:B:117:ILE:CD1	2.37	0.55
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.72	0.55
9:I:107:VAL:HG13	9:I:136:ILE:HG21	1.88	0.55
3:Q:195:ARG:HG2	3:Q:234:ILE:HG21	1.89	0.55
3:C:195:ARG:HG2	3:C:234:ILE:HG21	1.89	0.54
3:C:62:VAL:HG22	3:C:72:SER:HB3	1.89	0.54
7:G:83:ASN:ND2	7:G:83:ASN:C	2.61	0.54
7:G:73:VAL:CG1	7:G:133:THR:HB	2.37	0.54
6:T:201:GLU:O	6:T:204:LYS:HG2	2.07	0.54
6:F:201:GLU:O	6:F:204:LYS:HG2	2.07	0.54
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:303:39Q:HB9	17:K:303:39Q:O3	2.08	0.54
1:A:46:ALA:HB2	1:A:211:LEU:HG	1.90	0.54
2:P:65:LEU:HD22	2:P:211:GLU:HB3	1.90	0.53
7:U:83:ASN:C	7:U:83:ASN:ND2	2.61	0.53
7:U:73:VAL:CG1	7:U:133:THR:HB	2.37	0.53
2:P:105:ILE:HD11	2:P:109:ILE:HG22	1.91	0.53
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.90	0.53
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.74	0.53
6:T:50:ILE:HG13	6:T:208:PHE:HA	1.90	0.53
6:F:50:ILE:HG13	6:F:208:PHE:HA	1.90	0.53
12:Z:161:GLU:HB3	12:Z:164:THR:CG2	2.39	0.53
12:L:161:GLU:HB3	12:L:164:THR:CG2	2.39	0.53
10:J:1:MET:HA	10:J:34:LYS:HE3	1.91	0.53
6:F:240:GLN:NE2	6:F:240:GLN:HA	2.24	0.53
10:J:91:SER:HA	10:J:94:SER:HG	1.73	0.53
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.90	0.53
10:X:91:SER:HA	10:X:94:SER:HG	1.74	0.52
2:B:105:ILE:HD11	2:B:109:ILE:HG22	1.91	0.52
12:L:8:ASN:HA	12:L:30:ILE:O	2.10	0.52
2:B:155:ASN:ND2	3:C:77:ASN:HB2	2.24	0.52
17:Y:303:39Q:O40	17:Y:303:39Q:O32	2.23	0.52
11:Y:100:MET:HE3	11:Y:127:PHE:HB3	1.89	0.52
2:B:65:LEU:HD22	2:B:211:GLU:HB3	1.90	0.52
10:J:3:ILE:HB	10:J:18:SER:HB3	1.92	0.52
4:R:1:ASP:O	4:R:2:ARG:HB2	2.08	0.52
1:A:140:ASP:OD1	1:A:143:ASN:HB2	2.09	0.52
1:O:46:ALA:HB2	1:O:211:LEU:HG	1.90	0.51
10:X:1:MET:HA	10:X:34:LYS:HE3	1.92	0.51
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.45	0.51
3:C:151:SER:OG	3:C:153:ILE:HG12	2.11	0.51
4:D:1:ASP:O	4:D:2:ARG:HB2	2.09	0.51
1:O:140:ASP:OD1	1:O:143:ASN:HB2	2.10	0.51
6:T:240:GLN:HA	6:T:240:GLN:NE2	2.24	0.51
14:N:20:THR:HG22	14:N:31:THR:OG1	2.10	0.51
4:D:4:VAL:HG13	4:D:15:GLN:HG3	1.92	0.51
4:R:159:TYR:CZ	4:R:162:LYS:HD3	2.46	0.51
10:X:3:ILE:HB	10:X:18:SER:HB3	1.92	0.51
3:Q:151:SER:OG	3:Q:153:ILE:HG12	2.11	0.51
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.47	0.50
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.10	0.50
12:L:62:ASP:O	12:L:66:LYS:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:PHE:H	2:B:20:GLN:HE22	1.60	0.50
4:D:159:TYR:CZ	4:D:162:LYS:HD3	2.47	0.50
12:Z:114:LEU:HA	12:Z:119:LYS:O	2.12	0.50
11:K:100:MET:HE3	11:K:127:PHE:HB3	1.90	0.50
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.46	0.50
2:B:95:GLN:HB3	9:I:68:TYR:CD2	2.47	0.50
4:R:4:VAL:HG13	4:R:15:GLN:HG3	1.94	0.50
11:K:1:THR:HG22	11:K:2:THR:N	2.26	0.49
3:C:160:GLN:NE2	3:C:161:THR:H	2.10	0.49
10:J:91:SER:HA	10:J:94:SER:OG	2.12	0.49
8:V:84:LYS:HG3	8:V:85:GLN:N	2.27	0.49
6:F:202:ASP:OD1	6:F:202:ASP:N	2.44	0.49
5:E:170:TYR:HB2	5:E:198:GLN:HG3	1.95	0.49
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.94	0.49
12:L:113:GLY:HA2	12:L:207:VAL:HG11	1.94	0.49
5:E:118:ASN:N	5:E:118:ASN:HD22	2.11	0.49
5:S:118:ASN:N	5:S:118:ASN:HD22	2.11	0.49
1:A:149:GLN:O	1:A:156:TYR:HA	2.13	0.49
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.47	0.49
3:C:9:PHE:H	4:D:15:GLN:HE22	1.61	0.49
5:S:170:TYR:C	5:S:170:TYR:CD1	2.86	0.49
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.95	0.49
8:H:84:LYS:HG3	8:H:85:GLN:N	2.26	0.49
2:B:84:GLU:OE1	6:T:97:LYS:NZ	92.84	0.49
10:X:91:SER:HA	10:X:94:SER:OG	2.13	0.49
5:S:170:TYR:HB2	5:S:198:GLN:HG3	1.94	0.49
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.59	0.48
12:Z:113:GLY:HA2	12:Z:207:VAL:HG11	1.95	0.48
12:L:114:LEU:HA	12:L:119:LYS:O	2.13	0.48
12:Z:62:ASP:O	12:Z:66:LYS:HB2	2.13	0.48
2:B:159:TRP:HH2	3:C:50:LEU:HD22	1.78	0.48
2:B:14:PRO:HA	3:C:20:TYR:CG	2.48	0.48
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.77	0.48
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.48	0.48
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.96	0.48
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.60	0.48
5:E:170:TYR:C	5:E:170:TYR:CD1	2.87	0.48
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.78	0.48
14:N:14:LEU:HD11	14:N:100:ALA:HB3	1.94	0.48
3:Q:160:GLN:NE2	3:Q:161:THR:H	2.11	0.48
10:J:1:MET:HA	10:J:34:LYS:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:1:MET:HA	10:X:34:LYS:CE	2.43	0.48
2:B:58:GLN:NE2	2:B:231:PRO:HB3	2.29	0.48
3:Q:175:LYS:HG3	3:Q:176:ASN:HD22	1.79	0.48
12:Z:161:GLU:HB3	12:Z:164:THR:HG21	1.96	0.48
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.96	0.48
12:Z:64:LEU:HD22	12:Z:97:LEU:HD21	1.95	0.48
14:N:59:VAL:HG22	14:N:81:VAL:HG12	1.95	0.48
2:P:58:GLN:NE2	2:P:231:PRO:HB3	2.29	0.48
12:Z:22:VAL:HG12	12:Z:206:ILE:HG13	1.96	0.47
1:O:149:GLN:O	1:O:156:TYR:HA	2.13	0.47
11:K:2:THR:OG1	11:K:132:GLY:HA3	2.15	0.47
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.49	0.47
14:N:20:THR:HG23	14:N:28:ASN:HB3	1.95	0.47
1:O:44:VAL:CG2	1:O:211:LEU:HD21	2.45	0.47
12:L:22:VAL:HG12	12:L:206:ILE:HG13	1.96	0.47
3:C:175:LYS:HG3	3:C:176:ASN:HD22	1.80	0.47
13:M:51:VAL:HG22	13:M:116:VAL:HG22	1.94	0.47
4:R:149:HIS:O	4:R:156:PHE:HA	2.14	0.47
12:L:161:GLU:HB3	12:L:164:THR:HG21	1.97	0.47
11:Y:2:THR:OG1	11:Y:132:GLY:HA3	2.14	0.47
4:D:149:HIS:O	4:D:156:PHE:HA	2.15	0.47
2:B:180:LYS:O	2:B:183:MET:HB2	2.15	0.47
17:Y:303:39Q:O3	17:Y:303:39Q:H5	2.14	0.47
10:J:3:ILE:HD12	10:J:176:PHE:CG	2.50	0.47
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.97	0.47
3:Q:205:ALA:C	3:Q:207:ASN:H	2.18	0.47
5:E:14:PRO:HA	6:F:22:TYR:CD2	2.50	0.47
8:H:172:ASN:HD22	8:H:192:THR:HA	1.79	0.47
6:F:123:ASN:C	6:F:123:ASN:HD22	2.18	0.47
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.50	0.47
12:Z:17:GLY:HA3	12:Z:20:PHE:CE1	2.50	0.47
12:L:17:GLY:HA3	12:L:20:PHE:CE1	2.50	0.47
10:J:139:TYR:CZ	11:Y:134:THR:HG22	2.50	0.46
1:O:3:ASP:OD1	1:O:5:TYR:HB2	2.15	0.46
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.14	0.46
4:D:32:ILE:CD1	4:D:192:VAL:HG23	2.45	0.46
8:V:172:ASN:HD22	8:V:192:THR:HA	1.80	0.46
4:R:32:ILE:CD1	4:R:192:VAL:HG23	2.45	0.46
4:R:183:LEU:HD23	4:R:187:GLU:HB3	1.98	0.46
2:B:204:ALA:O	2:B:209:ARG:NH2	2.49	0.46
3:C:201:VAL:O	3:C:202:GLN:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.50	0.46
12:L:64:LEU:HD22	12:L:97:LEU:HD21	1.96	0.46
9:I:52:ILE:HB	9:I:59:VAL:HG13	1.98	0.46
1:A:3:ASP:OD1	1:A:5:TYR:HB2	2.15	0.46
10:J:174:MET:HA	10:X:174:MET:HA	1.97	0.46
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.98	0.46
9:I:104:VAL:HG23	9:I:106:PRO:HD3	1.97	0.46
1:A:44:VAL:CG2	1:A:211:LEU:HD21	2.46	0.46
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.51	0.46
3:C:205:ALA:C	3:C:207:ASN:H	2.18	0.46
2:P:180:LYS:O	2:P:183:MET:HB2	2.16	0.45
5:E:71:LEU:HD23	5:E:71:LEU:C	2.36	0.45
5:S:71:LEU:HD23	5:S:71:LEU:C	2.36	0.45
2:P:46:ALA:HB2	2:P:212:PHE:CE1	2.51	0.45
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.50	0.45
2:B:161:ALA:HB3	3:C:52:LEU:HD23	1.99	0.45
12:L:146:ILE:HG22	12:L:150:LEU:HD22	1.98	0.45
11:K:73:ARG:HH11	11:K:73:ARG:HB2	1.81	0.45
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.98	0.45
4:D:183:LEU:HD23	4:D:187:GLU:HB3	1.98	0.45
2:B:46:ALA:HB2	2:B:212:PHE:CE1	2.51	0.45
5:S:178:PHE:HA	5:S:181:ILE:HG13	1.98	0.45
2:P:99:LYS:HE3	10:X:86:GLN:NE2	2.31	0.45
6:T:33:SER:HB3	6:T:46:VAL:HG23	1.98	0.45
5:E:178:PHE:HA	5:E:181:ILE:HG13	1.98	0.45
7:U:239:ILE:O	7:U:242:GLN:HB3	2.17	0.45
6:T:123:ASN:C	6:T:123:ASN:HD22	2.19	0.45
9:W:104:VAL:HG23	9:W:106:PRO:HD3	1.98	0.45
6:F:33:SER:HB3	6:F:46:VAL:HG23	1.98	0.45
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.52	0.45
2:P:135:ILE:HD11	2:P:164:VAL:HG22	1.99	0.45
6:T:41:GLY:HA3	6:T:215:CYS:O	2.17	0.45
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	1.98	0.45
12:Z:64:LEU:CD2	12:Z:97:LEU:HD21	2.46	0.45
3:C:176:ASN:HB3	3:C:192:LEU:HD11	1.99	0.45
2:P:204:ALA:O	2:P:209:ARG:NH2	2.50	0.45
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.99	0.45
1:A:211:LEU:HD22	1:A:238:LEU:HD12	1.98	0.45
2:B:14:PRO:O	3:C:23:GLU:HG3	2.17	0.45
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.51	0.45
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.82	0.45
8:H:50:ALA:HB3	9:I:126:ILE:CG2	2.46	0.45
11:Y:73:ARG:HB2	11:Y:73:ARG:HH11	1.81	0.44
2:B:135:ILE:HD11	2:B:164:VAL:HG22	1.99	0.44
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.65	0.44
6:T:202:ASP:OD1	6:T:202:ASP:N	2.50	0.44
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.52	0.44
5:S:212:ILE:HD12	5:S:229:VAL:HG12	2.00	0.44
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.52	0.44
12:L:64:LEU:CD2	12:L:97:LEU:HD21	2.47	0.44
5:E:109:HIS:HB3	6:F:82:ARG:NH2	2.33	0.44
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.83	0.44
12:L:195:HIS:HD2	12:L:197:GLN:H	1.66	0.44
13:M:35:ARG:HG3	13:M:36:PHE:CZ	2.52	0.44
4:R:105:THR:HG23	4:R:136:ILE:HD12	1.99	0.44
7:G:239:ILE:O	7:G:242:GLN:HB3	2.17	0.44
13:M:27:LEU:HD11	13:M:34:LEU:HB3	2.00	0.44
11:K:134:THR:HG22	10:X:139:TYR:CZ	2.53	0.44
3:C:160:GLN:HE21	3:C:161:THR:H	1.64	0.44
8:V:174:ASP:OD2	8:V:188:ARG:NH1	2.50	0.44
2:B:216:ARG:C	2:B:218:GLY:H	2.21	0.44
10:J:41:HIS:CE1	10:J:109:LYS:HE2	2.53	0.44
8:H:3:ILE:HG22	8:H:99:ILE:HD12	2.00	0.44
7:U:221:LYS:O	7:U:222:ASP:HB2	2.17	0.44
10:X:119:ILE:HA	10:X:124:THR:O	2.18	0.44
3:C:202:GLN:HG3	3:C:203:THR:H	1.83	0.44
1:O:211:LEU:HD22	1:O:238:LEU:HD12	1.99	0.44
3:Q:176:ASN:HB3	3:Q:192:LEU:HD11	1.99	0.44
10:X:41:HIS:CE1	10:X:109:LYS:HE2	2.53	0.43
13:M:119:VAL:HG23	13:M:200:ILE:HG22	2.00	0.43
1:O:158:PRO:HB2	2:P:57:GLU:HB3	1.99	0.43
1:O:44:VAL:HG23	1:O:211:LEU:HD21	1.99	0.43
6:F:41:GLY:HA3	6:F:215:CYS:O	2.17	0.43
4:R:59:ILE:HD12	4:R:210:GLN:HG2	2.00	0.43
8:H:174:ASP:OD2	8:H:188:ARG:NH1	2.52	0.43
3:Q:160:GLN:HE21	3:Q:161:THR:H	1.65	0.43
11:K:1:THR:CG2	11:K:2:THR:N	2.81	0.43
4:D:59:ILE:HD12	4:D:210:GLN:HG2	1.99	0.43
4:D:105:THR:HG23	4:D:136:ILE:HD12	1.99	0.43
7:G:221:LYS:O	7:G:222:ASP:HB2	2.18	0.43
2:B:58:GLN:HE22	2:B:231:PRO:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:23:LEU:HD13	12:L:43:VAL:HG13	2.00	0.43
5:E:68:HIS:HE1	5:E:102:LEU:O	2.02	0.43
12:L:210:ASP:OD1	12:L:210:ASP:N	2.52	0.43
2:P:58:GLN:HE22	2:P:231:PRO:HB3	1.84	0.43
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.48	0.43
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.54	0.43
8:V:3:ILE:HG22	8:V:99:ILE:HD12	2.01	0.43
3:Q:174:GLU:HG2	4:R:49:PRO:HG2	2.00	0.43
1:A:44:VAL:HG23	1:A:211:LEU:HD21	2.00	0.42
5:S:109:HIS:HB3	6:T:82:ARG:NH2	2.34	0.42
10:J:36:ARG:HD3	10:J:36:ARG:HA	1.83	0.42
9:I:41:LYS:O	9:I:51:GLY:HA2	2.18	0.42
5:S:68:HIS:HE1	5:S:102:LEU:O	2.02	0.42
7:U:116:SER:HA	7:U:119:TYR:CD2	2.54	0.42
11:Y:8:PHE:CE1	11:Y:13:ILE:HG12	2.54	0.42
11:K:37:ILE:HB	11:K:41:LEU:HB3	2.01	0.42
2:P:216:ARG:C	2:P:218:GLY:H	2.23	0.42
12:L:147:MET:N	12:L:148:PRO:HD2	2.35	0.42
11:K:116:ASP:C	11:K:116:ASP:OD1	2.58	0.42
3:Q:201:VAL:CG1	3:Q:202:GLN:N	2.81	0.42
5:E:9:THR:CG2	5:E:119:THR:HA	2.49	0.42
11:K:8:PHE:CE1	11:K:13:ILE:HG12	2.55	0.42
4:R:30:ILE:HD12	4:R:196:LEU:HG	2.01	0.42
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	2.00	0.42
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	2.01	0.42
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.54	0.42
7:U:187:GLU:CG	7:U:192:LYS:HB2	2.50	0.42
11:Y:25:TRP:CH2	12:Z:144:SER:HA	2.54	0.42
10:J:119:ILE:HA	10:J:124:THR:O	2.20	0.42
7:G:187:GLU:CG	7:G:192:LYS:HB2	2.49	0.42
5:E:212:ILE:HD12	5:E:229:VAL:HG12	2.00	0.42
13:M:93:PHE:CE2	13:M:128:ARG:HD3	2.54	0.42
1:O:115:ALA:HB1	1:O:154:GLY:O	2.19	0.42
9:W:41:LYS:O	9:W:51:GLY:HA2	2.19	0.42
2:P:215:ILE:HG12	2:P:226:GLN:HG3	2.02	0.42
6:F:183:LEU:HD11	6:F:187:GLU:HB3	2.01	0.42
7:G:116:SER:HA	7:G:119:TYR:CD2	2.54	0.42
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.49	0.42
11:Y:4:LEU:HD13	11:Y:161:ILE:HD11	2.02	0.42
14:N:32:ASP:OD2	14:N:185:ARG:NH2	2.52	0.42
14:N:38:HIS:O	14:N:39:ASP:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:52:THR:O	8:V:56:THR:HB	2.20	0.42
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.48	0.42
11:Y:162:LEU:CD1	11:Y:193:VAL:HG13	2.50	0.42
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.02	0.42
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.66	0.42
4:D:30:ILE:HD12	4:D:196:LEU:HG	2.01	0.42
12:Z:210:ASP:OD1	12:Z:210:ASP:N	2.53	0.41
2:P:198:LYS:HE2	2:P:198:LYS:HB3	1.89	0.41
12:L:108:HIS:ND1	12:L:108:HIS:C	2.73	0.41
5:E:98:PHE:O	13:M:91:TYR:HA	2.20	0.41
12:Z:60:ASP:OD2	12:Z:105:TYR:HA	2.20	0.41
5:S:112:CYS:SG	6:T:82:ARG:HD3	2.60	0.41
11:K:162:LEU:CD1	11:K:193:VAL:HG13	2.50	0.41
6:T:183:LEU:HD11	6:T:187:GLU:HB3	2.01	0.41
6:T:185:ALA:O	6:T:189:VAL:HG23	2.20	0.41
6:F:97:LYS:NZ	14:N:84:GLU:OE1	2.52	0.41
12:L:60:ASP:OD2	12:L:105:TYR:HA	2.19	0.41
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.35	0.41
13:M:26:ASN:HA	13:M:39:VAL:O	2.18	0.41
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.41
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.03	0.41
11:K:6:PHE:HA	11:K:125:ASP:O	2.20	0.41
5:S:9:THR:CG2	5:S:119:THR:HA	2.48	0.41
5:E:70:GLY:HA3	5:E:221:PHE:CE2	2.55	0.41
2:P:239:VAL:HG12	2:P:240:LYS:N	2.36	0.41
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.03	0.41
3:C:169:VAL:HG12	3:C:200:VAL:HG21	2.03	0.41
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.55	0.41
7:G:30:ASN:HD22	7:G:164:PRO:HG2	1.85	0.41
8:H:52:THR:O	8:H:56:THR:HB	2.21	0.41
10:J:96:ARG:HA	10:J:97:PRO:HD3	1.89	0.41
7:U:56:ASP:HA	7:U:57:PRO:HD2	1.89	0.41
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.20	0.41
3:C:35:LYS:HG2	3:C:158:SER:O	2.21	0.41
6:F:68:ARG:NH1	13:M:72:THR:OG1	2.50	0.41
10:X:36:ARG:HD3	10:X:36:ARG:HA	1.84	0.41
1:A:66:LEU:C	1:A:66:LEU:HD23	2.41	0.41
10:J:18:SER:O	10:J:34:LYS:HD2	2.21	0.41
1:O:84:VAL:O	1:O:88:LYS:HG3	2.21	0.41
12:Z:149:PHE:CE1	12:Z:153:GLN:HG3	2.56	0.41
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:49:LYS:HB3	5:S:58:TYR:HB3	2.02	0.41
10:J:33:ASP:OD1	10:J:35:THR:HG22	2.21	0.41
1:A:59:GLU:CD	1:A:59:GLU:H	2.24	0.41
3:Q:37:LYS:HB2	3:Q:184:ALA:HA	2.02	0.41
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.56	0.41
6:F:185:ALA:O	6:F:189:VAL:HG23	2.20	0.41
4:D:139:HIS:ND1	4:D:216:LYS:HB2	2.36	0.41
6:T:146:MET:CE	6:T:161:THR:HB	2.51	0.41
5:S:12:PHE:CE1	5:S:18:LEU:HD21	2.56	0.41
13:M:17:ASP:OD1	13:M:18:ASN:N	2.53	0.41
3:Q:169:VAL:HG12	3:Q:200:VAL:HG21	2.03	0.41
7:G:104:PRO:HB3	7:G:138:ASP:OD1	2.21	0.41
11:Y:116:ASP:C	11:Y:116:ASP:OD1	2.59	0.41
12:Z:100:LYS:HD3	12:Z:105:TYR:CZ	2.56	0.41
5:E:197:SER:HA	5:E:200:LEU:HG	2.03	0.41
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.03	0.41
5:S:77:ALA:HB3	5:S:78:PRO:HD3	2.03	0.41
13:M:48:ASN:HD22	13:M:48:ASN:N	2.18	0.41
6:F:146:MET:CE	6:F:161:THR:HB	2.51	0.41
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.03	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.51	0.40
3:Q:38:ASN:N	3:Q:38:ASN:HD22	2.19	0.40
17:K:303:39Q:N15	17:K:303:39Q:C19	2.83	0.40
1:O:23:TYR:CE1	7:U:12:PRO:HA	2.56	0.40
11:K:4:LEU:HD13	11:K:161:ILE:HD11	2.03	0.40
13:M:9:THR:OG1	13:M:10:SER:N	2.53	0.40
7:U:104:PRO:HB3	7:U:138:ASP:OD1	2.21	0.40
9:W:7:ASN:HA	9:W:29:GLY:O	2.21	0.40
2:B:215:ILE:HG12	2:B:226:GLN:HG3	2.02	0.40
13:M:161:ARG:CG	13:M:161:ARG:HH11	2.33	0.40
12:Z:13:LEU:HD12	12:Z:14:GLY:N	2.36	0.40
10:X:18:SER:O	10:X:34:LYS:HD2	2.22	0.40
5:E:77:ALA:HB3	5:E:78:PRO:HD3	2.04	0.40
2:B:37:ILE:HD12	2:B:192:ALA:HB2	2.03	0.40
2:B:198:LYS:HE2	2:B:198:LYS:HB3	1.89	0.40
17:Y:303:39Q:H29	17:Y:303:39Q:H42	1.78	0.40
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.51	0.40
5:S:53:ASP:OD1	5:S:53:ASP:C	2.60	0.40
17:Y:303:39Q:C26	17:Y:303:39Q:H36	2.49	0.40
7:U:30:ASN:HD22	7:U:164:PRO:HG2	1.86	0.40
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:129:TYR:O	13:M:136:THR:HA	2.22	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	248/250 (99%)	235 (95%)	9 (4%)	4 (2%)	12	40
1	O	248/250 (99%)	235 (95%)	9 (4%)	4 (2%)	12	40
2	B	242/258 (94%)	227 (94%)	11 (4%)	4 (2%)	11	38
2	P	242/258 (94%)	227 (94%)	12 (5%)	3 (1%)	16	48
3	C	238/254 (94%)	223 (94%)	8 (3%)	7 (3%)	6	23
3	Q	238/254 (94%)	223 (94%)	8 (3%)	7 (3%)	6	23
4	D	231/260 (89%)	223 (96%)	6 (3%)	2 (1%)	21	57
4	R	231/260 (89%)	223 (96%)	6 (3%)	2 (1%)	21	57
5	E	229/234 (98%)	214 (93%)	12 (5%)	3 (1%)	15	46
5	S	229/234 (98%)	213 (93%)	13 (6%)	3 (1%)	15	46
6	F	241/288 (84%)	231 (96%)	10 (4%)	0	100	100
6	T	241/288 (84%)	231 (96%)	10 (4%)	0	100	100
7	G	239/252 (95%)	228 (95%)	10 (4%)	1 (0%)	39	74
7	U	239/252 (95%)	228 (95%)	10 (4%)	1 (0%)	39	74
8	H	220/232 (95%)	211 (96%)	8 (4%)	1 (0%)	34	71
8	V	220/232 (95%)	211 (96%)	8 (4%)	1 (0%)	34	71
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	186 (96%)	6 (3%)	1 (0%)	34	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	X	193/198 (98%)	186 (96%)	6 (3%)	1 (0%)	34	71
11	K	210/212 (99%)	202 (96%)	6 (3%)	2 (1%)	19	54
11	Y	210/212 (99%)	201 (96%)	7 (3%)	2 (1%)	19	54
12	L	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
12	Z	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
13	M	231/246 (94%)	221 (96%)	9 (4%)	1 (0%)	39	74
13	a	231/246 (94%)	221 (96%)	8 (4%)	2 (1%)	21	57
14	N	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
14	b	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
All	All	6276/6614 (95%)	5982 (95%)	242 (4%)	52 (1%)	24	60

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	52	THR
3	C	202	GLN
3	C	206	LYS
5	E	231	LYS
1	O	2	THR
2	P	52	THR
3	Q	202	GLN
3	Q	206	LYS
5	S	231	LYS
1	A	3	ASP
1	A	166	LYS
2	B	51	VAL
3	C	201	VAL
3	C	205	ALA
4	D	2	ARG
5	E	217	LYS
8	H	9	ASN
10	J	2	ASP
1	O	3	ASP
1	O	166	LYS
2	P	51	VAL
3	Q	201	VAL
3	Q	205	ALA
4	R	2	ARG

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Mol	Chain	Res	Type
5	S	217	LYS
8	V	9	ASN
10	X	2	ASP
5	E	209	ASN
7	G	51	PRO
5	S	209	ASN
7	U	51	PRO
3	C	183	PRO
3	Q	183	PRO
3	C	52	LEU
3	C	224	SER
4	D	201	GLU
13	M	83	ALA
3	Q	52	LEU
3	Q	224	SER
4	R	201	GLU
13	a	83	ALA
2	B	217	LYS
2	B	221	ASP
11	K	9	GLN
2	P	221	ASP
11	Y	9	GLN
1	A	202	GLY
1	O	202	GLY
11	K	150	VAL
11	Y	150	VAL
13	a	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%)	193 (92%)	16 (8%)	16	42
1	O	209/209 (100%)	193 (92%)	16 (8%)	16	42
2	B	203/216 (94%)	183 (90%)	20 (10%)	10	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	203/216 (94%)	183 (90%)	20 (10%)	10	29
3	C	212/226 (94%)	193 (91%)	19 (9%)	12	34
3	Q	212/226 (94%)	193 (91%)	19 (9%)	12	34
4	D	194/215 (90%)	171 (88%)	23 (12%)	6	19
4	R	194/215 (90%)	171 (88%)	23 (12%)	6	19
5	E	190/193 (98%)	172 (90%)	18 (10%)	11	31
5	S	190/193 (98%)	172 (90%)	18 (10%)	11	31
6	F	201/239 (84%)	183 (91%)	18 (9%)	12	34
6	T	201/239 (84%)	182 (90%)	19 (10%)	11	31
7	G	206/210 (98%)	184 (89%)	22 (11%)	8	24
7	U	206/210 (98%)	184 (89%)	22 (11%)	8	24
8	H	181/190 (95%)	173 (96%)	8 (4%)	35	70
8	V	181/190 (95%)	173 (96%)	8 (4%)	35	70
9	I	172/173 (99%)	163 (95%)	9 (5%)	29	64
9	W	172/173 (99%)	163 (95%)	9 (5%)	29	64
10	J	173/175 (99%)	159 (92%)	14 (8%)	15	39
10	X	173/175 (99%)	159 (92%)	14 (8%)	15	39
11	K	169/169 (100%)	161 (95%)	8 (5%)	32	68
11	Y	169/169 (100%)	161 (95%)	8 (5%)	32	68
12	L	185/185 (100%)	173 (94%)	12 (6%)	21	52
12	Z	185/185 (100%)	173 (94%)	12 (6%)	21	52
13	M	199/208 (96%)	184 (92%)	15 (8%)	17	44
13	a	199/208 (96%)	184 (92%)	15 (8%)	17	44
14	N	162/162 (100%)	157 (97%)	5 (3%)	47	82
14	b	162/162 (100%)	157 (97%)	5 (3%)	47	82
All	All	5312/5540 (96%)	4897 (92%)	415 (8%)	16	41

All (415) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	17	LYS
1	A	30	GLN

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Mol	Chain	Res	Type
1	A	52	SER
1	A	61	LEU
1	A	92	VAL
1	A	122	THR
1	A	157	PHE
1	A	164	ILE
1	A	169	VAL
1	A	176	GLU
1	A	177	LYS
1	A	178	ARG
1	A	231	LYS
1	A	246	ARG
1	A	250	LEU
2	B	2	SER
2	B	54	THR
2	B	55	LEU
2	B	58	GLN
2	B	62	THR
2	B	65	LEU
2	B	119	GLN
2	B	168	THR
2	B	180	LYS
2	B	184	LYS
2	B	191	LEU
2	B	194	LYS
2	B	197	SER
2	B	203	SER
2	B	205	LEU
2	B	209	ARG
2	B	216	ARG
2	B	237	ILE
2	B	239	VAL
2	B	244	THR
3	C	4	ARG
3	C	37	LYS
3	C	38	ASN
3	C	46	ARG
3	C	48	SER
3	C	49	THR
3	C	61	LYS
3	C	142	GLU
3	C	147	GLN

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Mol	Chain	Res	Type
3	C	153	ILE
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	187	GLU
3	C	203	THR
3	C	232	THR
3	C	239	GLN
3	C	240	GLU
4	D	12	ARG
4	D	20	LEU
4	D	40	LEU
4	D	48	SER
4	D	51	LEU
4	D	60	VAL
4	D	99	ILE
4	D	117	GLU
4	D	125	LEU
4	D	155	THR
4	D	176	LEU
4	D	183	LEU
4	D	190	LEU
4	D	193	LEU
4	D	197	LYS
4	D	202	GLU
4	D	214	ILE
4	D	224	ASP
4	D	233	LYS
4	D	235	LEU
4	D	236	LYS
4	D	238	LYS
4	D	242	GLU
5	E	4	ASN
5	E	8	ASP
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	55	LEU
5	E	60	LYS
5	E	71	LEU

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Mol	Chain	Res	Type
5	E	87	LEU
5	E	116	GLN
5	E	118	ASN
5	E	169	THR
5	E	184	ASN
5	E	188	LEU
5	E	204	SER
5	E	207	VAL
5	E	219	THR
6	F	14	ASP
6	F	31	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	174	LYS
6	F	181	GLU
6	F	186	ARG
6	F	202	ASP
6	F	203	ASN
6	F	204	LYS
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
6	F	228	LYS
7	G	24	LYS
7	G	26	THR
7	G	28	GLN
7	G	36	VAL
7	G	67	SER
7	G	68	ARG
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	125	MET
7	G	165	LYS
7	G	166	GLN
7	G	171	THR
7	G	181	LYS
7	G	192	LYS

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Mol	Chain	Res	Type
7	G	212	ASN
7	G	223	LYS
7	G	230	GLU
7	G	235	ARG
7	G	236	LEU
7	G	239	ILE
7	G	242	GLN
8	H	30	ASN
8	H	34	LEU
8	H	56	THR
8	H	68	LEU
8	H	153	LYS
8	H	156	SER
8	H	191	LEU
8	H	198	GLU
9	I	31	GLN
9	I	37	ASN
9	I	114	LYS
9	I	126	ILE
9	I	133	LYS
9	I	151	SER
9	I	171	LEU
9	I	182	TRP
9	I	192	ASP
10	J	2	ASP
10	J	8	ARG
10	J	17	SER
10	J	23	ARG
10	J	36	ARG
10	J	75	LEU
10	J	78	GLN
10	J	90	LYS
10	J	91	SER
10	J	94	SER
10	J	95	ARG
10	J	144	LEU
10	J	163	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	31	VAL
11	K	35	ILE

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Mol	Chain	Res	Type
11	K	73	ARG
11	K	106	ARG
11	K	118	ASP
11	K	148	LEU
12	L	1	GLN
12	L	3	ASN
12	L	11	THR
12	L	23	LEU
12	L	49	ASN
12	L	108	HIS
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
12	L	173	LYS
12	L	210	ASP
12	L	214	LYS
13	M	3	GLN
13	M	10	SER
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	106	LYS
13	M	157	LYS
13	M	159	VAL
13	M	161	ARG
13	M	187	ARG
13	M	204	THR
13	M	213	GLN
13	M	215	GLU
13	M	223	LYS
14	N	20	THR
14	N	22	THR
14	N	44	CYS
14	N	104	ASP
14	N	119	VAL
1	O	2	THR
1	O	17	LYS
1	O	30	GLN
1	O	52	SER
1	O	61	LEU
1	O	92	VAL

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Mol	Chain	Res	Type
1	O	122	THR
1	O	157	PHE
1	O	164	ILE
1	O	169	VAL
1	O	176	GLU
1	O	177	LYS
1	O	178	ARG
1	O	231	LYS
1	O	246	ARG
1	O	250	LEU
2	P	2	SER
2	P	54	THR
2	P	55	LEU
2	P	58	GLN
2	P	62	THR
2	P	65	LEU
2	P	119	GLN
2	P	168	THR
2	P	180	LYS
2	P	184	LYS
2	P	191	LEU
2	P	194	LYS
2	P	197	SER
2	P	203	SER
2	P	205	LEU
2	P	209	ARG
2	P	216	ARG
2	P	237	ILE
2	P	239	VAL
2	P	244	THR
3	Q	4	ARG
3	Q	37	LYS
3	Q	38	ASN
3	Q	46	ARG
3	Q	48	SER
3	Q	49	THR
3	Q	61	LYS
3	Q	142	GLU
3	Q	147	GLN
3	Q	153	ILE
3	Q	160	GLN
3	Q	169	VAL

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Mol	Chain	Res	Type
3	Q	175	LYS
3	Q	180	LYS
3	Q	187	GLU
3	Q	203	THR
3	Q	232	THR
3	Q	239	GLN
3	Q	240	GLU
4	R	12	ARG
4	R	20	LEU
4	R	40	LEU
4	R	48	SER
4	R	51	LEU
4	R	60	VAL
4	R	99	ILE
4	R	117	GLU
4	R	125	LEU
4	R	155	THR
4	R	176	LEU
4	R	183	LEU
4	R	190	LEU
4	R	193	LEU
4	R	197	LYS
4	R	202	GLU
4	R	214	ILE
4	R	224	ASP
4	R	233	LYS
4	R	235	LEU
4	R	236	LYS
4	R	238	LYS
4	R	242	GLU
5	S	4	ASN
5	S	8	ASP
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	55	LEU
5	S	60	LYS
5	S	71	LEU
5	S	87	LEU
5	S	116	GLN
5	S	118	ASN

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Mol	Chain	Res	Type
5	S	169	THR
5	S	184	ASN
5	S	188	LEU
5	S	204	SER
5	S	207	VAL
5	S	219	THR
6	T	14	ASP
6	T	31	THR
6	T	68	ARG
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	174	LYS
6	T	181	GLU
6	T	186	ARG
6	T	202	ASP
6	T	203	ASN
6	T	204	LYS
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
6	T	228	LYS
7	U	24	LYS
7	U	26	THR
7	U	28	GLN
7	U	36	VAL
7	U	67	SER
7	U	68	ARG
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	125	MET
7	U	165	LYS
7	U	166	GLN
7	U	171	THR
7	U	181	LYS
7	U	192	LYS
7	U	212	ASN
7	U	223	LYS

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Mol	Chain	Res	Type
7	U	230	GLU
7	U	235	ARG
7	U	236	LEU
7	U	239	ILE
7	U	242	GLN
8	V	30	ASN
8	V	34	LEU
8	V	56	THR
8	V	68	LEU
8	V	153	LYS
8	V	156	SER
8	V	191	LEU
8	V	198	GLU
9	W	31	GLN
9	W	37	ASN
9	W	114	LYS
9	W	126	ILE
9	W	133	LYS
9	W	151	SER
9	W	171	LEU
9	W	182	TRP
9	W	192	ASP
10	X	2	ASP
10	X	8	ARG
10	X	17	SER
10	X	23	ARG
10	X	36	ARG
10	X	75	LEU
10	X	78	GLN
10	X	90	LYS
10	X	91	SER
10	X	94	SER
10	X	95	ARG
10	X	144	LEU
10	X	163	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	31	VAL
11	Y	35	ILE
11	Y	73	ARG
11	Y	106	ARG

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Mol	Chain	Res	Type
11	Y	118	ASP
11	Y	148	LEU
12	Z	1	GLN
12	Z	3	ASN
12	Z	11	THR
12	Z	23	LEU
12	Z	49	ASN
12	Z	132	GLU
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
12	Z	173	LYS
12	Z	210	ASP
12	Z	214	LYS
13	a	3	GLN
13	a	10	SER
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	106	LYS
13	a	157	LYS
13	a	159	VAL
13	a	161	ARG
13	a	187	ARG
13	a	204	THR
13	a	213	GLN
13	a	215	GLU
13	a	223	LYS
14	b	20	THR
14	b	22	THR
14	b	44	CYS
14	b	104	ASP
14	b	119	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (150) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	102	ASN

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Mol	Chain	Res	Type
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	147	GLN
3	C	160	GLN
3	C	233	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	139	HIS
4	D	146	GLN
4	D	225	ASN
5	E	30	GLN
5	E	59	GLN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	147	GLN
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	167	GLN
7	G	175	ASN
7	G	184	HIS
7	G	186	ASN
8	H	30	ASN

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Mol	Chain	Res	Type
8	H	66	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
9	I	63	ASN
10	J	55	GLN
10	J	78	GLN
10	J	86	GLN
10	J	118	GLN
10	J	191	GLN
11	K	66	HIS
11	K	85	ASN
11	K	176	ASN
12	L	1	GLN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	195	HIS
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	69	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	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	147	GLN
3	Q	160	GLN
3	Q	233	GLN

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Mol	Chain	Res	Type
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	139	HIS
4	R	146	GLN
4	R	225	ASN
5	S	30	GLN
5	S	59	GLN
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	147	GLN
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	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	63	ASN
10	X	55	GLN
10	X	78	GLN
10	X	86	GLN
10	X	118	GLN

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Mol	Chain	Res	Type
10	X	191	GLN
11	Y	66	HIS
11	Y	85	ASN
11	Y	176	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	108	HIS
12	Z	195	HIS
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	69	GLN
14	b	161	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	MES	K	302	-	11,12,12	0.62	0	14,16,16	1.33	1 (7%)
17	39Q	K	303	-	42,44,44	1.84	3 (7%)	52,58,58	1.47	9 (17%)
16	MES	Y	302	-	11,12,12	0.63	0	14,16,16	1.14	1 (7%)
17	39Q	Y	303	-	42,44,44	1.69	3 (7%)	52,58,58	1.69	7 (13%)

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	MES	K	302	-	-	0/6/14/14	0/1/1/1
17	39Q	K	303	-	-	0/43/52/52	0/3/3/3
16	MES	Y	302	-	-	0/6/14/14	0/1/1/1
17	39Q	Y	303	-	-	0/43/52/52	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	303	39Q	C17-C18	-5.41	1.38	1.51
17	Y	303	39Q	C30-C41	-5.38	1.38	1.51
17	Y	303	39Q	C17-C18	-5.30	1.38	1.51
17	K	303	39Q	C30-C41	-4.88	1.39	1.51
17	Y	303	39Q	O32-C31	7.13	1.34	1.21
17	K	303	39Q	O32-C31	8.35	1.36	1.21

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	303	39Q	O32-C31-C37	-6.82	106.60	120.95
17	K	303	39Q	O32-C31-C37	-5.21	109.99	120.95
17	Y	303	39Q	C13-C11-N1	-4.14	101.33	111.67
17	K	303	39Q	C4-N5-C6	-3.90	105.31	111.07
17	Y	303	39Q	C30-C29-N28	-3.75	102.96	110.80
17	K	303	39Q	C12-C11-N1	-2.93	104.78	110.31
17	Y	303	39Q	O8-C7-C6	-2.61	105.85	111.84
17	K	303	39Q	O8-C9-C10	-2.56	105.96	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	303	39Q	C13-C11-N1	-2.54	105.33	111.67
17	K	303	39Q	O8-C7-C6	-2.42	106.28	111.84
17	K	303	39Q	C30-C29-N28	-2.39	105.80	110.80
17	K	303	39Q	C17-C16-N15	-2.29	106.00	110.80
17	Y	303	39Q	C4-N5-C6	-2.00	108.11	111.07
16	Y	302	MES	O2S-S-C8	2.82	109.31	106.91
17	K	303	39Q	C6-N5-C10	2.93	115.24	108.90
17	Y	303	39Q	C11-N1-C2	3.64	127.01	121.44
16	K	302	MES	O2S-S-C8	3.78	110.13	106.91
17	Y	303	39Q	C6-N5-C10	3.78	117.09	108.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	302	MES	1	0
17	K	303	39Q	5	0
17	Y	303	39Q	7	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%)	-0.56	5 (2%) 68 64	47, 67, 100, 134	0
1	O	250/250 (100%)	-0.53	2 (0%) 87 86	48, 72, 114, 143	0
2	B	244/258 (94%)	-0.45	5 (2%) 68 64	49, 73, 114, 161	0
2	P	244/258 (94%)	-0.42	8 (3%) 50 42	54, 75, 123, 162	0
3	C	240/254 (94%)	-0.36	5 (2%) 67 62	49, 77, 127, 148	0
3	Q	240/254 (94%)	-0.26	9 (3%) 44 37	54, 82, 142, 156	0
4	D	235/260 (90%)	-0.49	1 (0%) 93 92	54, 80, 110, 149	0
4	R	235/260 (90%)	-0.47	3 (1%) 79 78	55, 78, 109, 145	0
5	E	231/234 (98%)	-0.42	2 (0%) 85 84	53, 84, 112, 149	0
5	S	231/234 (98%)	-0.37	3 (1%) 79 78	51, 83, 119, 150	0
6	F	243/288 (84%)	-0.48	5 (2%) 67 62	52, 74, 115, 153	0
6	T	243/288 (84%)	-0.51	2 (0%) 87 86	51, 74, 117, 136	0
7	G	241/252 (95%)	-0.59	4 (1%) 73 70	43, 68, 105, 139	0
7	U	241/252 (95%)	-0.57	2 (0%) 87 86	47, 68, 98, 124	0
8	H	222/232 (95%)	-0.53	2 (0%) 85 84	46, 66, 90, 135	0
8	V	222/232 (95%)	-0.54	2 (0%) 85 84	51, 70, 95, 139	0
9	I	204/205 (99%)	-0.77	0 100 100	47, 62, 88, 117	0
9	W	204/205 (99%)	-0.71	1 (0%) 91 90	46, 66, 89, 127	0
10	J	195/198 (98%)	-0.67	1 (0%) 91 90	46, 64, 93, 144	0
10	X	195/198 (98%)	-0.57	2 (1%) 84 82	45, 67, 93, 156	0
11	K	212/212 (100%)	-0.68	0 100 100	47, 67, 90, 116	0
11	Y	212/212 (100%)	-0.69	0 100 100	43, 65, 88, 116	0
12	L	222/222 (100%)	-0.64	0 100 100	48, 69, 96, 114	0
12	Z	222/222 (100%)	-0.65	0 100 100	45, 66, 89, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.62	2 (0%) 85 84	45, 66, 91, 119	0
13	a	233/246 (94%)	-0.64	2 (0%) 85 84	47, 65, 93, 109	0
14	N	196/196 (100%)	-0.66	3 (1%) 76 74	47, 64, 91, 110	0
14	b	196/196 (100%)	-0.69	1 (0%) 91 90	47, 63, 88, 118	0
All	All	6336/6614 (95%)	-0.55	72 (1%) 82 80	43, 70, 109, 162	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	222	ASP	5.5
3	Q	49	THR	5.2
2	B	220	ASN	5.1
1	A	1	MET	4.6
10	X	194	ASP	4.5
2	P	219	ALA	4.4
2	B	221	ASP	4.3
5	S	202	ASP	4.3
2	P	220	ASN	4.2
8	H	222	ASP	4.1
2	B	219	ALA	4.1
3	C	206	LYS	3.9
3	Q	50	LEU	3.9
2	P	222	GLY	3.8
3	C	49	THR	3.6
6	F	181	GLU	3.6
2	B	222	GLY	3.6
1	O	1	MET	3.5
8	V	221	CYS	3.5
3	Q	238	LYS	3.5
4	D	242	GLU	3.3
3	Q	206	LYS	3.2
3	C	240	GLU	3.2
2	P	59	ASP	3.2
3	Q	236	GLN	3.1
2	B	51	VAL	3.0
7	G	2	GLY	3.0
3	Q	240	GLU	2.9
4	R	241	ALA	2.9
2	P	221	ASP	2.9
2	P	50	LYS	2.9
3	Q	239	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	249	ALA	2.8
9	W	1	SER	2.8
3	Q	203	THR	2.8
5	E	202	ASP	2.7
8	H	22	GLN	2.7
3	Q	48	SER	2.7
7	G	241	GLU	2.7
1	O	249	ALA	2.5
3	C	225	GLU	2.5
7	G	3	TYR	2.5
7	U	241	GLU	2.5
6	F	202	ASP	2.4
14	b	105	LYS	2.4
2	P	223	GLU	2.4
6	F	205	GLU	2.3
14	N	195	GLN	2.3
10	J	194	ASP	2.3
4	R	2	ARG	2.3
10	X	1	MET	2.3
7	U	242	GLN	2.3
1	A	248	GLU	2.2
13	M	47	ASP	2.2
5	E	201	ARG	2.2
5	S	52	ALA	2.2
13	a	233	ILE	2.2
4	R	242	GLU	2.2
2	P	51	VAL	2.2
1	A	250	LEU	2.2
1	A	203	GLU	2.1
6	T	2	THR	2.1
14	N	9	LYS	2.1
13	M	216	ASN	2.1
6	T	243	ILE	2.1
3	C	180	LYS	2.1
14	N	105	LYS	2.1
6	F	203	ASN	2.1
13	a	1	THR	2.1
7	G	242	GLN	2.1
6	F	180	PRO	2.0
5	S	173	ARG	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	Z	301	1/1	0.96	0.27	6.90	69,69,69,69	0
16	MES	Y	302	12/12	0.97	0.21	3.54	64,76,80,80	0
15	MG	N	201	1/1	0.88	0.18	2.01	68,68,68,68	0
16	MES	K	302	12/12	0.97	0.17	1.92	69,75,87,93	0
15	MG	V	301	1/1	0.98	0.18	1.75	68,68,68,68	0
17	39Q	Y	303	42/42	0.92	0.18	1.56	47,63,90,97	0
17	39Q	K	303	42/42	0.91	0.20	1.24	36,65,95,101	0
15	MG	I	301	1/1	0.99	0.14	0.50	51,51,51,51	0
15	MG	K	301	1/1	0.97	0.11	-0.51	78,78,78,78	0
15	MG	G	301	1/1	0.97	0.04	-1.85	63,63,63,63	0
15	MG	Y	301	1/1	0.98	0.06	-2.34	57,57,57,57	0
15	MG	N	202	1/1	0.66	0.24	-	78,78,78,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.