



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:45 PM GMT

PDB ID : 3UN8  
Title : Yeast 20S proteasome in complex with PR-957 (epoxide)  
Authors : Huber, E.; Basler, M.; Schwab, R.; Heinemeyer, W.; Kirk, C.; Groettrup, M.; Groll, M.  
Deposited on : 2011-11-15  
Resolution : 2.70 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

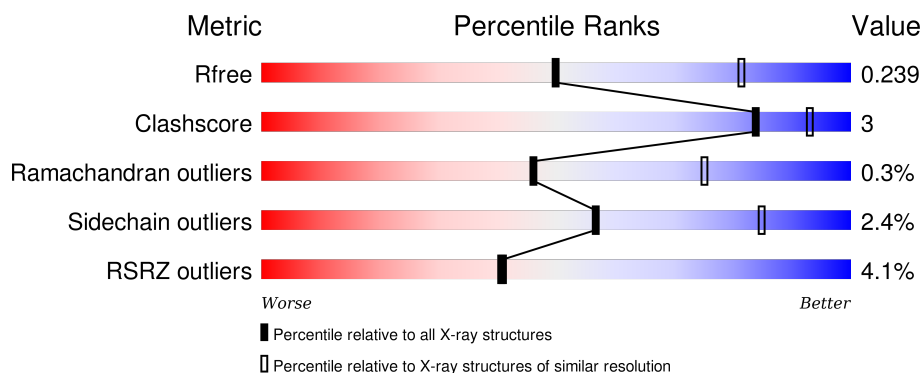
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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>90%</div> <div>10%</div> </div>
1	O	250	<div> <div>4%</div> <div>91%</div> <div>9%</div> </div>
2	B	258	<div> <div>6%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
2	P	258	<div> <div>8%</div> <div>82%</div> <div>11%</div> <div>5%</div> </div>
3	C	254	<div> <div>9%</div> <div>86%</div> <div>8%</div> <div>5%</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	233	
13	a	233	
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	049	K	213	-	-	-	X
15	049	Y	213	-	-	-	X

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50914 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 component Y7.

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 component Y13.

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 component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

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

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

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

- Molecule 7 is a protein called Proteasome component C7-alpha.

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

- Molecule 8 is a protein called Proteasome component PUP1.

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

- Molecule 9 is a protein called Proteasome component PUP3.

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 component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

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 component C5.

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			

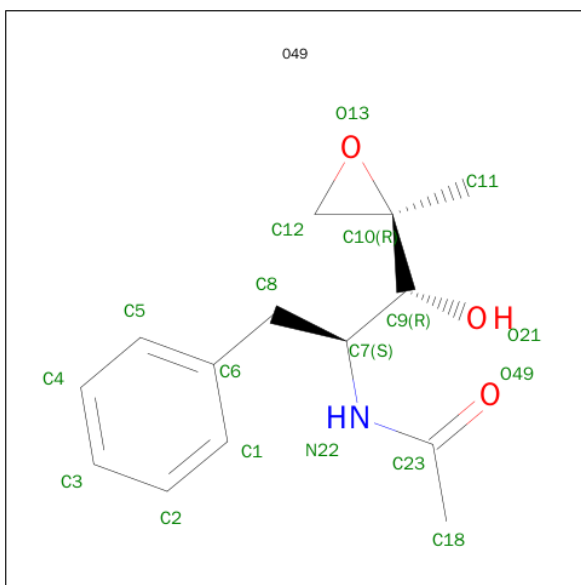
- Molecule 13 is a protein called Proteasome component PRE4.

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 component PRE3.

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 2-(ACETYLAMINO)-4,5-ANHYDRO-1,2-DIDEOXY-4-METHYL-1-PHENYL-D-XYLITOL (three-letter code: 049) (formula: C<sub>14</sub>H<sub>19</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	K	1	Total	C	N	O	0	0
			18	14	1	3		
15	Y	1	Total	C	N	O	0	0
			18	14	1	3		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	61	Total	O	0	0
			61	61		
16	B	37	Total	O	0	0
			37	37		
16	C	42	Total	O	0	0
			42	42		
16	D	37	Total	O	0	0
			37	37		
16	E	21	Total	O	0	0
			21	21		
16	F	48	Total	O	0	0
			48	48		
16	G	60	Total	O	0	0
			60	60		
16	H	54	Total	O	0	0
			54	54		
16	I	65	Total	O	0	0
			65	65		
16	J	52	Total	O	0	0
			52	52		

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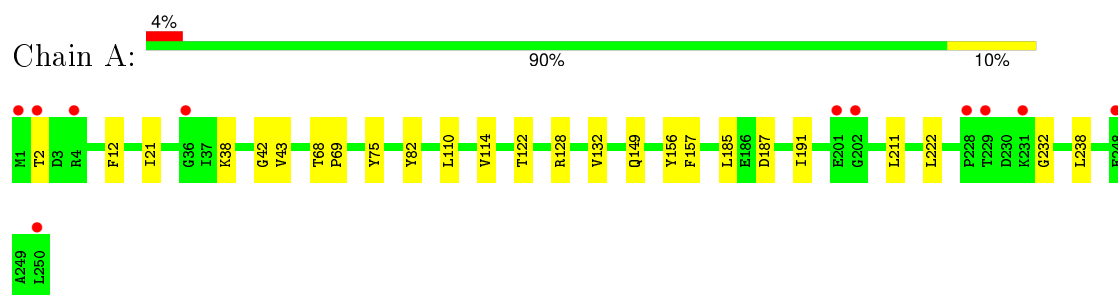
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	K	46	Total 46	O 46	0	0
16	L	56	Total 56	O 56	0	0
16	M	73	Total 73	O 73	0	0
16	N	58	Total 58	O 58	0	0
16	O	34	Total 34	O 34	0	0
16	P	29	Total 29	O 29	0	0
16	Q	28	Total 28	O 28	0	0
16	R	29	Total 29	O 29	0	0
16	S	20	Total 20	O 20	0	0
16	T	41	Total 41	O 41	0	0
16	U	61	Total 61	O 61	0	0
16	V	53	Total 53	O 53	0	0
16	W	60	Total 60	O 60	0	0
16	X	45	Total 45	O 45	0	0
16	Y	53	Total 53	O 53	0	0
16	Z	47	Total 47	O 47	0	0
16	a	73	Total 73	O 73	0	0
16	b	57	Total 57	O 57	0	0

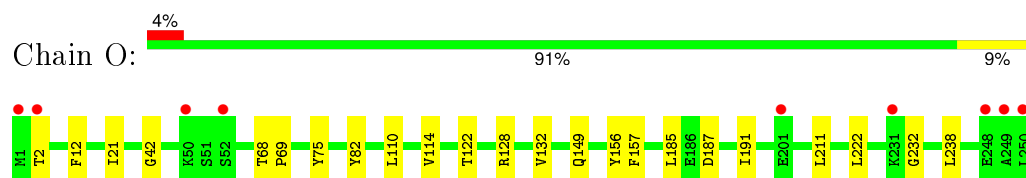
### 3 Residue-property plots

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.

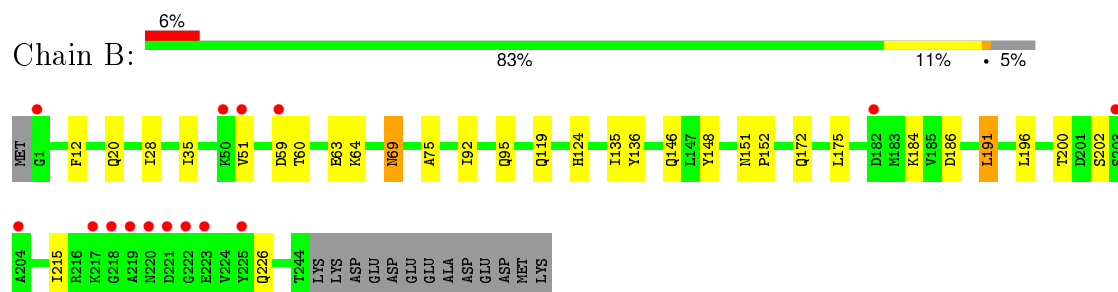
#### • Molecule 1: Proteasome component Y7



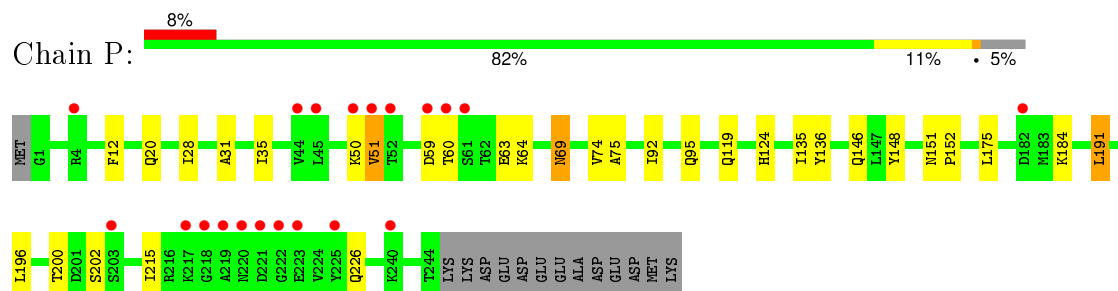
#### • Molecule 1: Proteasome component Y7



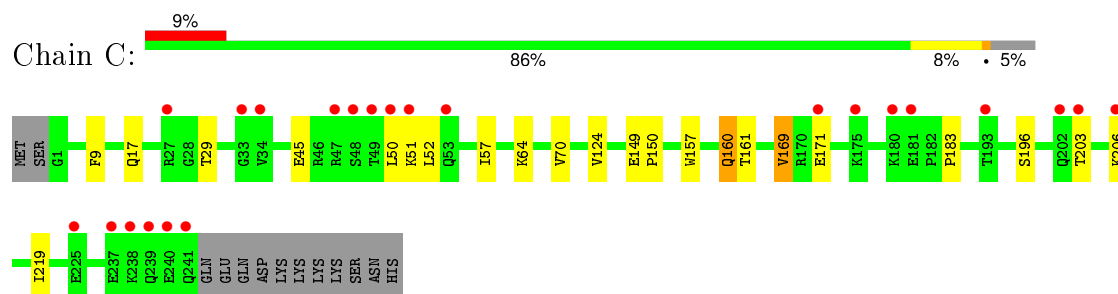
#### • Molecule 2: Proteasome component Y13



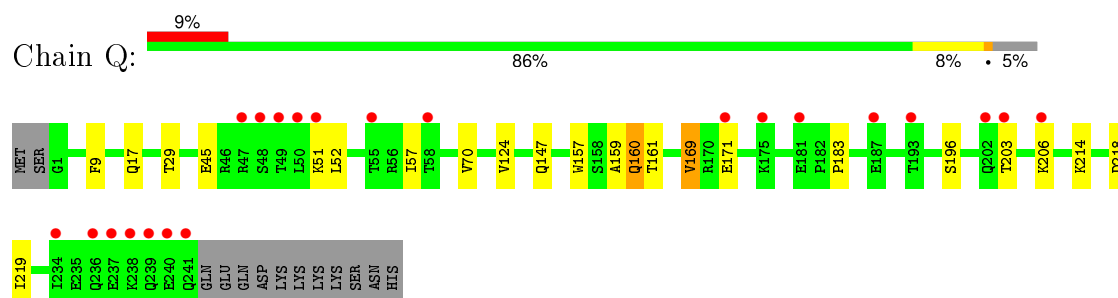
#### • Molecule 2: Proteasome component Y13



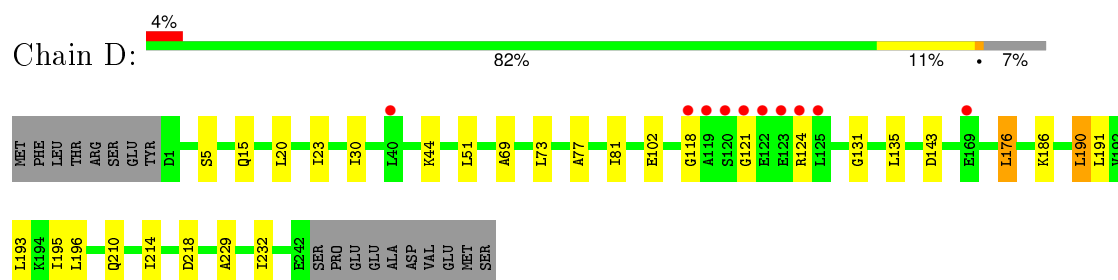
- Molecule 3: Proteasome component PRE6



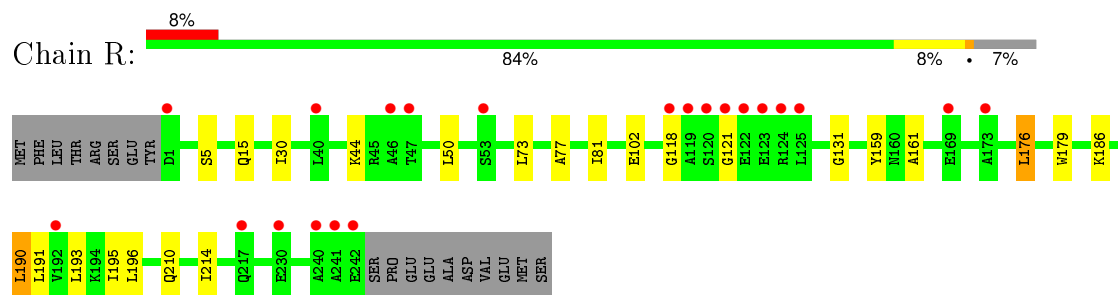
- Molecule 3: Proteasome component PRE6



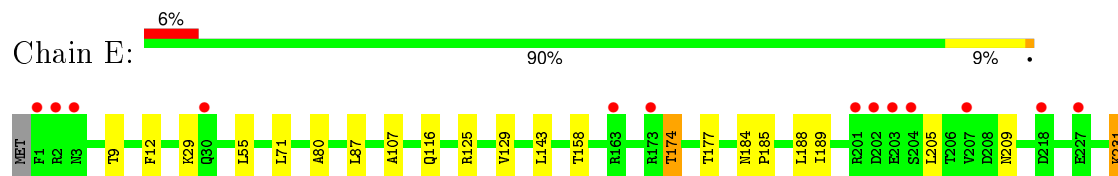
- Molecule 4: Proteasome component PUP2

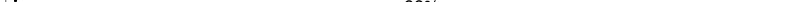


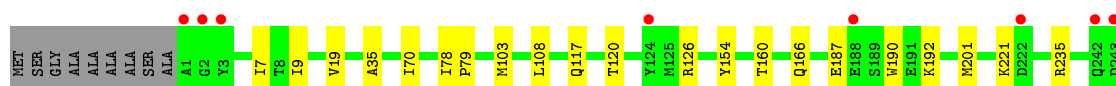
- Molecule 4: Proteasome component PUP2



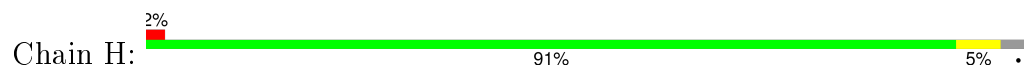
- Molecule 5: Proteasome component PRE5



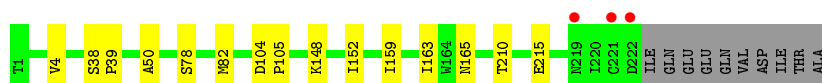
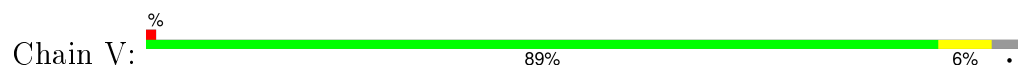
Chain U:  3% 88% 8%



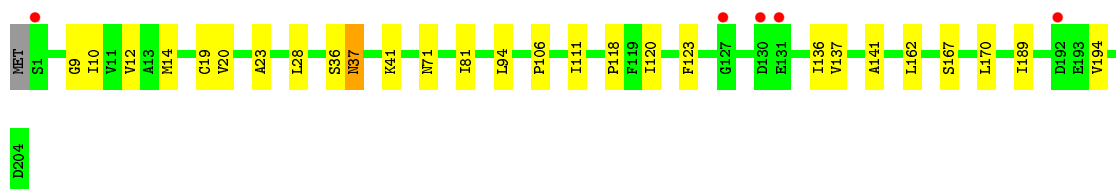
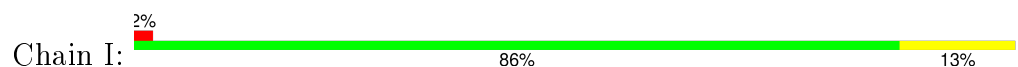
- Molecule 8: Proteasome component PUP1



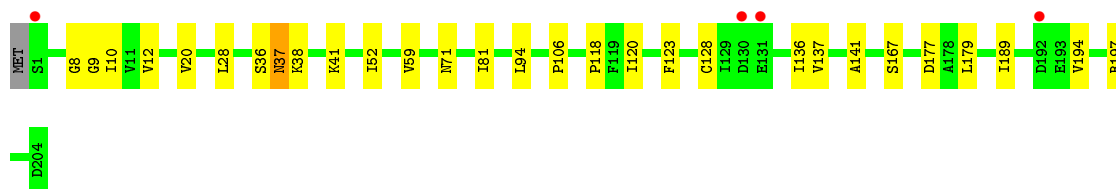
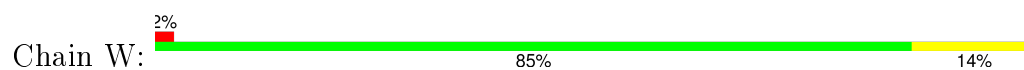
- Molecule 8: Proteasome component PUP1



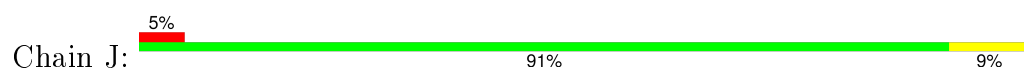
- Molecule 9: Proteasome component PUP3



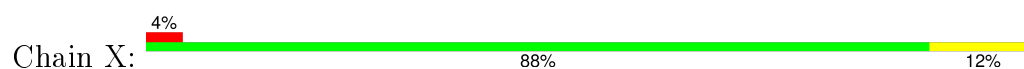
- Molecule 9: Proteasome component PUP3

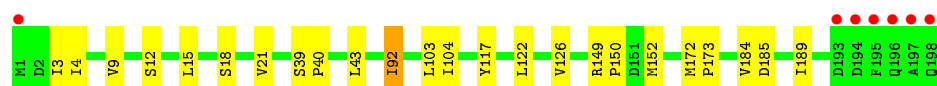


- Molecule 10: Proteasome component C11

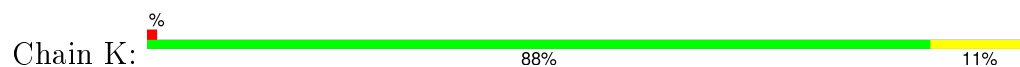


- Molecule 10: Proteasome component C11





- Molecule 11: Proteasome component PRE2



- Molecule 11: Proteasome component PRE2



- Molecule 12: Proteasome component C5



- Molecule 12: Proteasome component C5



- Molecule 13: Proteasome component PRE4

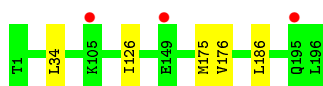


- Molecule 13: Proteasome component PRE4

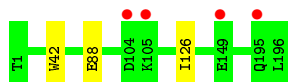


- Molecule 14: Proteasome component PRE3





- Molecule 14: Proteasome component PRE3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.42Å 300.42Å 143.93Å 90.00° 112.83° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 24.94 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (15.00-2.70) 99.4 (24.94-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.217 , 0.240 0.217 , 0.239	Depositor DCC
$R_{free}$ test set	14279 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	0.809	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.0	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 286910 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	50914	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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:  
049

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	0.37	0/1952	0.46	0/2642
1	O	0.36	0/1952	0.46	0/2642
2	B	0.33	0/1934	0.46	0/2618
2	P	0.33	0/1934	0.46	0/2618
3	C	0.34	0/1919	0.46	0/2598
3	Q	0.34	1/1919 (0.1%)	0.46	0/2598
4	D	0.36	0/1886	0.47	0/2541
4	R	0.36	1/1886 (0.1%)	0.47	0/2541
5	E	0.31	0/1823	0.45	0/2463
5	S	0.31	0/1823	0.44	0/2463
6	F	0.41	1/1936 (0.1%)	0.44	0/2614
6	T	0.41	1/1936 (0.1%)	0.44	0/2614
7	G	0.34	0/1959	0.46	0/2652
7	U	0.34	1/1959 (0.1%)	0.46	0/2652
8	H	0.44	1/1715 (0.1%)	0.46	0/2326
8	V	0.44	0/1715	0.46	0/2326
9	I	0.34	0/1611	0.47	0/2174
9	W	0.34	0/1611	0.47	0/2174
10	J	0.32	0/1613	0.45	0/2173
10	X	0.31	0/1613	0.45	0/2173
11	K	0.50	1/1681 (0.1%)	0.49	1/2274 (0.0%)
11	Y	0.51	2/1681 (0.1%)	0.50	1/2274 (0.0%)
12	L	0.36	0/1795	0.45	0/2420
12	Z	0.36	0/1795	0.45	0/2420
13	M	0.36	0/1855	0.47	0/2514
13	a	0.36	1/1855 (0.1%)	0.48	0/2514
14	N	0.39	0/1541	0.44	0/2087
14	b	0.39	1/1541 (0.1%)	0.45	0/2087
All	All	0.37	11/50440 (0.0%)	0.46	2/68192 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	42	TRP	CD2-CE2	5.05	1.47	1.41
11	Y	146	TRP	CD2-CE2	5.04	1.47	1.41
4	R	179	TRP	CD2-CE2	5.04	1.47	1.41
6	F	214	TRP	CD2-CE2	5.03	1.47	1.41
3	Q	157	TRP	CD2-CE2	5.03	1.47	1.41
7	U	190	TRP	CD2-CE2	5.02	1.47	1.41
11	Y	198	TRP	CD2-CE2	5.02	1.47	1.41
6	T	214	TRP	CD2-CE2	5.01	1.47	1.41
13	a	219	TRP	CD2-CE2	5.01	1.47	1.41
8	H	164	TRP	CD2-CE2	5.00	1.47	1.41
11	K	146	TRP	CD2-CE2	5.00	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	4	LEU	CA-CB-CG	5.62	128.24	115.30
11	K	4	LEU	CA-CB-CG	5.59	128.15	115.30

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	1915	0	1929	12	0
1	O	1915	0	1929	11	0
2	B	1904	0	1904	17	0
2	P	1904	0	1904	16	0
3	C	1890	0	1903	14	0
3	Q	1890	0	1903	11	0
4	D	1861	0	1839	13	0
4	R	1861	0	1839	12	0
5	E	1795	0	1800	10	0
5	S	1795	0	1800	14	0
6	F	1896	0	1889	14	0
6	T	1896	0	1889	13	0
7	G	1921	0	1913	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	U	1921	0	1913	9	0
8	H	1684	0	1688	6	0
8	V	1684	0	1688	10	0
9	I	1581	0	1574	17	0
9	W	1581	0	1574	19	0
10	J	1585	0	1590	10	0
10	X	1585	0	1590	14	0
11	K	1644	0	1594	16	0
11	Y	1644	0	1594	12	0
12	L	1757	0	1711	6	0
12	Z	1757	0	1711	11	0
13	M	1824	0	1832	12	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	2	0
14	b	1512	0	1481	0	0
15	K	18	0	17	3	0
15	Y	18	0	17	4	0
16	A	61	0	0	0	0
16	B	37	0	0	0	0
16	C	42	0	0	0	0
16	D	37	0	0	0	0
16	E	21	0	0	0	0
16	F	48	0	0	0	0
16	G	60	0	0	0	0
16	H	54	0	0	0	0
16	I	65	0	0	0	0
16	J	52	0	0	0	0
16	K	46	0	0	0	0
16	L	56	0	0	0	0
16	M	73	0	0	0	0
16	N	58	0	0	0	0
16	O	34	0	0	0	0
16	P	29	0	0	0	0
16	Q	28	0	0	0	0
16	R	29	0	0	0	0
16	S	20	0	0	0	0
16	T	41	0	0	0	0
16	U	61	0	0	0	0
16	V	53	0	0	0	0
16	W	60	0	0	0	0
16	X	45	0	0	0	0
16	Y	53	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Z	47	0	0	0	0
16	a	73	0	0	0	0
16	b	57	0	0	0	0
All	All	50914	0	49328	275	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 3.

All (275) 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)
11:Y:170:TYR:HB3	15:Y:213:049:H12A	1.53	0.89
11:K:1:THR:CB	15:K:213:049:C9	2.51	0.87
12:L:109:THR:HG23	12:L:125:PHE:HB2	1.66	0.78
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.50	0.76
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.53	0.73
3:C:9:PHE:H	4:D:15:GLN:HE22	1.38	0.69
2:B:12:PHE:H	3:C:17:GLN:HE22	1.42	0.68
2:P:200:THR:HG22	2:P:202:SER:H	1.59	0.66
12:Z:109:THR:HG23	12:Z:125:PHE:HB2	1.77	0.65
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.79	0.65
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.79	0.65
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.43	0.65
11:Y:170:TYR:CB	15:Y:213:049:H12A	2.26	0.65
1:A:12:PHE:H	2:B:20:GLN:HE22	1.44	0.63
1:O:12:PHE:H	2:P:20:GLN:HE22	1.44	0.63
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.80	0.63
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.81	0.61
5:E:12:PHE:H	6:F:19:GLN:HE22	1.47	0.60
4:D:44:LYS:HE3	4:D:210:GLN:HB2	1.83	0.60
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.83	0.60
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.49	0.59
5:S:12:PHE:H	6:T:19:GLN:HE22	1.49	0.59
10:J:150:PRO:HG3	11:Y:208:ASN:HD21	1.68	0.59
2:B:200:THR:HG22	2:B:202:SER:H	1.68	0.59
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.85	0.59
4:R:44:LYS:HE3	4:R:210:GLN:HB2	1.85	0.58
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.51	0.58
7:U:103:MET:HE3	7:U:108:LEU:HD13	1.84	0.58
13:M:48:ASN:H	13:M:48:ASN:HD22	1.50	0.58
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.51	0.58
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.52	0.58
1:O:21:ILE:HD11	1:O:122:THR:HG21	1.86	0.58
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.86	0.57
13:M:27:LEU:HB2	13:M:192:SER:HB2	1.86	0.57
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.84	0.57
11:K:38:ASN:HB2	11:K:39:PRO:HD2	1.85	0.57
11:K:45:MET:HB3	15:K:213:049:H3	1.86	0.57
1:O:211:LEU:HD22	1:O:238:LEU:HD12	1.86	0.57
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	1.87	0.56
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.87	0.56
6:F:31:THR:HG23	6:F:47:GLU:HB3	1.87	0.56
11:K:208:ASN:HD21	10:X:150:PRO:HG3	1.71	0.56
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.87	0.56
2:B:215:ILE:HG12	2:B:226:GLN:HG2	1.88	0.56
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.88	0.56
6:T:191:GLN:O	6:T:195:ILE:HG12	2.06	0.55
1:A:21:ILE:HD11	1:A:122:THR:HG21	1.88	0.55
1:A:211:LEU:HD22	1:A:238:LEU:HD12	1.87	0.55
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.89	0.55
4:R:5:SER:HB2	5:S:125:ARG:HD3	1.89	0.55
10:X:104:ILE:HB	10:X:117:TYR:HB2	1.89	0.55
2:P:215:ILE:HG12	2:P:226:GLN:HG2	1.89	0.55
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.88	0.55
11:K:83:LEU:HD23	11:K:101:ILE:HD11	1.89	0.55
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.89	0.54
7:G:78:ILE:N	7:G:79:PRO:HD2	2.22	0.54
6:F:191:GLN:O	6:F:195:ILE:HG12	2.07	0.54
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.90	0.54
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.89	0.54
11:K:1:THR:HB	15:K:213:049:C9	2.35	0.54
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.90	0.54
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.90	0.53
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.55	0.53
7:G:103:MET:HE3	7:G:108:LEU:HD13	1.89	0.53
7:U:78:ILE:N	7:U:79:PRO:HD2	2.23	0.53
5:E:80:ALA:HB2	5:E:129:VAL:HG21	1.91	0.53
15:Y:213:049:H11A	16:Y:1202:HOH:O	2.09	0.53
6:F:91:GLU:HG3	6:F:111:ARG:HH11	1.73	0.53
5:S:80:ALA:HB2	5:S:129:VAL:HG21	1.90	0.53
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:94:LEU:HD11	9:W:106:PRO:HG2	1.90	0.52
2:B:63:GLU:HG3	2:B:64:LYS:HG3	1.92	0.52
13:M:129:TYR:HE1	13:M:144:THR:HG22	1.74	0.52
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.91	0.52
10:J:104:ILE:HB	10:J:117:TYR:HB2	1.91	0.52
9:W:28:LEU:HB3	9:W:36:SER:HB3	1.91	0.52
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.92	0.51
2:B:136:TYR:HB2	2:B:148:TYR:HB2	1.93	0.51
6:T:31:THR:HG21	6:T:47:GLU:O	2.11	0.51
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.93	0.51
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.93	0.50
4:D:5:SER:HB2	5:E:125:ARG:HD3	1.92	0.50
6:T:91:GLU:HG3	6:T:111:ARG:HH11	1.77	0.50
11:K:14:VAL:HB	11:K:178:TYR:HB2	1.93	0.50
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.94	0.50
9:W:106:PRO:HD2	9:W:123:PHE:HB2	1.92	0.50
3:C:161:THR:HG21	3:C:169:VAL:HG13	1.94	0.50
8:H:148:LYS:O	8:H:152:ILE:HG12	2.11	0.50
8:V:148:LYS:O	8:V:152:ILE:HG12	2.12	0.50
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.93	0.50
2:P:75:ALA:HB3	2:P:135:ILE:HB	1.93	0.50
13:M:15:LYS:HG3	13:M:165:ILE:HD12	1.94	0.50
4:D:73:LEU:HD12	4:D:131:GLY:HA3	1.94	0.49
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.94	0.49
4:R:73:LEU:HD12	4:R:131:GLY:HA3	1.94	0.49
7:U:19:VAL:HG21	7:U:120:THR:HG23	1.94	0.49
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.95	0.49
11:K:107:LYS:H	11:K:107:LYS:HD2	1.77	0.49
12:L:195:HIS:HD2	12:L:197:GLN:H	1.61	0.49
11:Y:14:VAL:HB	11:Y:178:TYR:HB2	1.95	0.49
4:R:77:ALA:O	4:R:81:ILE:HG12	2.13	0.49
6:T:31:THR:HG23	6:T:47:GLU:HB3	1.93	0.49
2:P:146:GLN:HG2	3:Q:57:ILE:HG21	1.95	0.49
8:H:38:SER:HB2	8:H:39:PRO:HD2	1.95	0.48
2:B:75:ALA:HB3	2:B:135:ILE:HB	1.94	0.48
11:Y:107:LYS:H	11:Y:107:LYS:HD2	1.78	0.48
2:P:63:GLU:HG3	2:P:64:LYS:HG3	1.95	0.48
2:B:35:ILE:HD12	2:B:196:LEU:HG	1.94	0.48
8:V:38:SER:HB2	8:V:39:PRO:HD2	1.95	0.48
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.96	0.48
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:191:LEU:O	4:R:195:ILE:HD12	2.14	0.48
9:I:106:PRO:HD2	9:I:123:PHE:HB2	1.94	0.48
8:V:210:THR:HG21	9:W:167:SER:HB3	1.93	0.48
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.95	0.48
10:X:4:ILE:HG22	10:X:103:LEU:HD12	1.96	0.48
12:Z:126:ASP:HB2	12:Z:130:SER:HB3	1.95	0.48
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.95	0.48
2:P:136:TYR:HB2	2:P:148:TYR:HB2	1.95	0.47
4:D:191:LEU:O	4:D:195:ILE:HD12	2.15	0.47
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.96	0.47
10:X:39:SER:HB2	10:X:40:PRO:HD2	1.97	0.47
5:S:185:PRO:O	5:S:189:ILE:HG12	2.15	0.47
9:W:120:ILE:HD12	9:W:136:ILE:HG12	1.97	0.47
10:J:149:ARG:HB2	10:J:152:MET:HG3	1.96	0.47
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.97	0.47
6:F:31:THR:HG21	6:F:47:GLU:O	2.15	0.46
11:K:7:ARG:HD2	11:K:110:PRO:O	2.15	0.46
13:M:48:ASN:HD22	13:M:48:ASN:N	2.10	0.46
4:D:69:ALA:HB3	4:D:135:LEU:HB2	1.97	0.46
1:O:110:LEU:O	1:O:114:VAL:HG23	2.16	0.46
9:W:36:SER:HB2	10:X:126:VAL:HG21	1.98	0.46
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.46	0.46
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.98	0.46
12:Z:111:ILE:HG12	12:Z:125:PHE:HE1	1.81	0.46
15:Y:213:049:HN22	15:Y:213:049:H1	1.81	0.46
12:Z:17:GLY:HA2	12:Z:174:TYR:HE1	1.81	0.46
1:A:42:GLY:HA3	1:A:185:LEU:HD13	1.98	0.46
9:I:36:SER:HB2	10:J:126:VAL:HG21	1.98	0.46
5:S:143:LEU:HD21	5:S:158:THR:HG22	1.97	0.46
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.26	0.46
13:M:27:LEU:HD11	13:M:34:LEU:HB3	1.98	0.46
8:V:78:SER:O	8:V:82:MET:HG3	2.16	0.46
3:Q:214:LYS:HB2	3:Q:218:ASP:HB3	1.97	0.46
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.46
10:J:3:ILE:HB	10:J:18:SER:HB3	1.97	0.46
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.81	0.46
2:P:35:ILE:HD12	2:P:196:LEU:HG	1.97	0.45
7:U:35:ALA:HB3	7:U:160:THR:HG22	1.99	0.45
8:H:210:THR:HG21	9:I:167:SER:HB3	1.97	0.45
6:T:9:SER:HB2	7:U:126:ARG:HB3	1.98	0.45
5:E:185:PRO:O	5:E:189:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:7:ARG:HD2	11:Y:110:PRO:O	2.16	0.45
1:O:42:GLY:HA3	1:O:185:LEU:HD13	1.98	0.45
4:R:176:LEU:HD22	5:S:55:LEU:HD13	1.99	0.45
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.47	0.45
9:I:120:ILE:HD12	9:I:136:ILE:HG12	1.98	0.45
3:C:149:GLU:HB2	3:C:150:PRO:HD2	1.99	0.45
1:A:38:LYS:HG3	1:A:43:VAL:HG22	1.99	0.45
1:A:187:ASP:O	1:A:191:ILE:HD12	2.17	0.45
6:T:50:ILE:HD11	6:T:209:GLU:HB2	1.98	0.45
4:D:176:LEU:HD22	5:E:55:LEU:HD13	1.99	0.45
10:J:4:ILE:HG22	10:J:103:LEU:HD12	1.99	0.45
3:C:29:THR:HB	3:C:45:GLU:HG3	1.98	0.44
5:E:174:THR:HG22	5:E:177:THR:HB	1.99	0.44
12:L:111:ILE:HG12	12:L:125:PHE:HE1	1.81	0.44
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.45	0.44
12:L:126:ASP:HB2	12:L:130:SER:HB3	1.99	0.44
7:G:19:VAL:HG21	7:G:120:THR:HG23	1.99	0.44
4:R:161:ALA:HB3	5:S:55:LEU:HD23	1.99	0.44
11:K:97:MET:HG2	11:K:117:SER:HB3	2.00	0.44
2:B:172:GLN:HG2	3:C:50:LEU:HD12	1.98	0.44
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.44	0.44
10:J:92:ILE:HG13	10:J:122:LEU:HA	2.00	0.44
1:A:110:LEU:O	1:A:114:VAL:HG23	2.18	0.44
6:F:123:ASN:HD22	6:F:123:ASN:C	2.21	0.44
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.99	0.44
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.00	0.44
10:X:149:ARG:HB2	10:X:152:MET:HG3	1.98	0.44
1:O:149:GLN:O	1:O:156:TYR:HA	2.17	0.44
11:K:158:LYS:HD3	11:K:196:LEU:HD11	2.00	0.44
9:I:189:ILE:HA	9:I:194:VAL:HG22	2.00	0.43
1:O:68:THR:HB	1:O:69:PRO:HD2	2.00	0.43
9:I:28:LEU:HB3	9:I:36:SER:HB3	2.00	0.43
2:B:69:ASN:HD22	2:B:69:ASN:HA	1.69	0.43
1:A:149:GLN:O	1:A:156:TYR:HA	2.18	0.43
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.00	0.43
5:E:205:LEU:HA	5:E:209:ASN:HD22	1.83	0.43
9:I:12:VAL:HG23	9:I:137:VAL:HG12	2.00	0.43
6:F:205:GLU:HG3	6:F:206:LYS:HG3	2.00	0.43
10:X:184:VAL:HG22	10:X:189:ILE:HG12	1.99	0.43
6:F:9:SER:HB2	7:G:126:ARG:HB3	1.99	0.43
6:F:122:TYR:HB2	6:F:125:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:77:ALA:O	4:D:81:ILE:HG12	2.19	0.43
3:Q:70:VAL:HG13	3:Q:219:ILE:HD13	2.00	0.43
9:I:23:ALA:HB1	9:I:170:LEU:HD22	2.01	0.43
8:V:215:GLU:HG3	9:W:197:ARG:HG2	1.99	0.43
13:M:140:PRO:HB3	13:M:165:ILE:HD11	2.00	0.43
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.84	0.43
7:U:7:ILE:HG13	7:U:9:ILE:HG12	2.01	0.42
6:F:46:VAL:HB	6:F:73:VAL:HG21	2.01	0.42
2:P:69:ASN:HA	2:P:69:ASN:HD22	1.67	0.42
11:K:12:ILE:HB	11:K:180:VAL:HB	2.00	0.42
5:S:174:THR:HG22	5:S:177:THR:HB	2.00	0.42
10:X:3:ILE:HB	10:X:18:SER:HB3	2.01	0.42
1:A:68:THR:HB	1:A:69:PRO:HD2	2.00	0.42
12:Z:207:VAL:HG22	12:Z:212:VAL:HG22	2.00	0.42
12:L:161:GLU:HA	12:L:162:PRO:HD3	1.94	0.42
6:F:50:ILE:HD11	6:F:209:GLU:HB2	2.01	0.42
12:Z:100:LYS:O	12:Z:104:PRO:HA	2.20	0.42
5:E:231:LYS:H	5:E:231:LYS:HD2	1.84	0.42
9:I:37:ASN:HD22	9:I:37:ASN:C	2.23	0.42
9:W:37:ASN:HD22	9:W:38:LYS:HG3	1.85	0.42
5:S:205:LEU:HA	5:S:209:ASN:HD22	1.84	0.42
11:Y:97:MET:HG2	11:Y:117:SER:HB3	2.02	0.42
9:W:12:VAL:HG23	9:W:137:VAL:HG12	2.01	0.42
13:M:96:LEU:O	13:M:100:MET:HG2	2.19	0.42
9:W:189:ILE:HA	9:W:194:VAL:HG22	2.01	0.42
9:W:141:ALA:HB2	9:W:177:ASP:HB2	2.02	0.42
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.02	0.42
3:C:70:VAL:HG13	3:C:219:ILE:HD13	2.00	0.42
8:V:50:ALA:HB2	9:W:128:CYS:HB2	2.02	0.42
6:T:123:ASN:HD22	6:T:124:SER:N	2.18	0.42
10:X:15:LEU:HD12	10:X:43:LEU:HD23	2.01	0.42
5:S:131:LEU:HB2	5:S:146:PHE:HB3	2.02	0.41
1:O:187:ASP:O	1:O:191:ILE:HD12	2.20	0.41
12:Z:90:ALA:HA	12:Z:125:PHE:HZ	1.85	0.41
11:K:80:SER:HA	11:K:101:ILE:HD13	2.02	0.41
10:X:92:ILE:HG13	10:X:122:LEU:HA	2.02	0.41
6:T:46:VAL:HB	6:T:73:VAL:HG21	2.02	0.41
5:S:134:ILE:HD12	5:S:215:VAL:HG12	2.02	0.41
7:G:7:ILE:HG13	7:G:9:ILE:HG12	2.02	0.41
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.50	0.41
10:J:15:LEU:HD12	10:J:43:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:8:GLY:HA3	9:W:179:LEU:HB3	2.02	0.41
7:G:52:ASP:HB3	7:G:55:LEU:HG	2.03	0.41
4:D:20:LEU:HA	4:D:23:ILE:HD12	2.03	0.41
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.02	0.41
6:F:36:ILE:HG13	6:F:172:LEU:HD11	2.02	0.41
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	2.02	0.41
8:V:4:VAL:HG22	8:V:159:ILE:HD11	2.03	0.41
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.55	0.41
7:G:35:ALA:HB3	7:G:160:THR:HG22	2.02	0.41
2:P:50:LYS:HG2	2:P:51:VAL:HG23	2.02	0.41
9:I:14:MET:HB3	9:I:162:LEU:HD11	2.03	0.41
11:Y:80:SER:HA	11:Y:101:ILE:HD13	2.03	0.41
7:U:70:ILE:HD11	7:U:103:MET:O	2.20	0.41
11:K:208:ASN:ND2	10:X:150:PRO:HG3	2.36	0.41
2:P:31:ALA:HA	2:P:50:LYS:HD2	2.03	0.41
10:J:96:ARG:HA	10:J:97:PRO:HD3	1.89	0.41
8:H:159:ILE:O	8:H:163:ILE:HD12	2.21	0.41
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.55	0.41
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.56	0.41
4:R:186:LYS:O	4:R:190:LEU:HD22	2.21	0.41
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.55	0.41
5:E:143:LEU:HD21	5:E:158:THR:HG22	2.02	0.41
3:Q:29:THR:HB	3:Q:45:GLU:HG3	2.03	0.41
10:X:12:SER:HB3	10:X:185:ASP:HB3	2.03	0.41
4:D:186:LYS:O	4:D:190:LEU:HD22	2.21	0.40
2:B:175:LEU:HD23	2:B:191:LEU:HD22	2.03	0.40
3:Q:159:ALA:HB3	4:R:50:LEU:HD22	2.02	0.40
5:S:76:LEU:HD12	5:S:128:GLY:HA3	2.03	0.40
10:X:172:MET:HA	10:X:173:PRO:HD3	1.86	0.40
2:B:196:LEU:O	2:B:200:THR:OG1	2.38	0.40
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.57	0.40
2:P:175:LEU:HD23	2:P:191:LEU:HD22	2.03	0.40
6:T:205:GLU:HG3	6:T:206:LYS:HG3	2.02	0.40
14:N:34:LEU:HD13	14:N:176:VAL:HG23	2.03	0.40
6:T:117:GLN:HB3	6:T:117:GLN:HE21	1.78	0.40
9:I:19:CYS:HA	9:I:111:ILE:HD11	2.04	0.40
3:C:64:LYS:HE3	3:C:219:ILE:HD12	2.04	0.40
4:D:229:ALA:HA	4:D:232:ILE:HD12	2.04	0.40
12:Z:205:LEU:HG	12:Z:214:LYS:HG2	2.04	0.40
7:G:149:ASP:HB2	7:G:150:PRO:HD2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	242 (98%)	5 (2%)	1 (0%)	39	69
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	39	69
2	B	242/258 (94%)	236 (98%)	5 (2%)	1 (0%)	39	69
2	P	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	39	69
3	C	239/254 (94%)	233 (98%)	3 (1%)	3 (1%)	15	37
3	Q	239/254 (94%)	232 (97%)	4 (2%)	3 (1%)	15	37
4	D	240/260 (92%)	235 (98%)	3 (1%)	2 (1%)	24	51
4	R	240/260 (92%)	234 (98%)	4 (2%)	2 (1%)	24	51
5	E	231/234 (99%)	227 (98%)	4 (2%)	0	100	100
5	S	231/234 (99%)	226 (98%)	5 (2%)	0	100	100
6	F	242/288 (84%)	235 (97%)	7 (3%)	0	100	100
6	T	242/288 (84%)	235 (97%)	7 (3%)	0	100	100
7	G	241/252 (96%)	233 (97%)	8 (3%)	0	100	100
7	U	241/252 (96%)	235 (98%)	6 (2%)	0	100	100
8	H	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
8	V	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	196/198 (99%)	186 (95%)	9 (5%)	1 (0%)	34	63
10	X	196/198 (99%)	188 (96%)	7 (4%)	1 (0%)	34	63
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/233 (99%)	221 (96%)	9 (4%)	1 (0%)	39	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/233 (99%)	221 (96%)	9 (4%)	1 (0%)	39	69
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	6312/6588 (96%)	6130 (97%)	164 (3%)	18 (0%)	46	75

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	118	GLY
1	A	2	THR
3	C	52	LEU
3	C	203	THR
1	O	2	THR
3	Q	52	LEU
3	Q	203	THR
4	R	118	GLY
2	B	51	VAL
2	P	51	VAL
10	J	9	VAL
3	C	183	PRO
3	Q	183	PRO
10	X	9	VAL
13	M	229	GLY
13	a	229	GLY
4	D	121	GLY
4	R	121	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%)	207 (99%)	2 (1%)	82	94
1	O	209/209 (100%)	207 (99%)	2 (1%)	82	94
2	B	203/216 (94%)	194 (96%)	9 (4%)	35	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	203/216 (94%)	194 (96%)	9 (4%)	35	65
3	C	213/226 (94%)	208 (98%)	5 (2%)	58	85
3	Q	213/226 (94%)	207 (97%)	6 (3%)	51	81
4	D	198/215 (92%)	190 (96%)	8 (4%)	38	69
4	R	198/215 (92%)	193 (98%)	5 (2%)	55	84
5	E	192/193 (100%)	184 (96%)	8 (4%)	36	68
5	S	192/193 (100%)	183 (95%)	9 (5%)	32	63
6	F	201/239 (84%)	191 (95%)	10 (5%)	30	60
6	T	201/239 (84%)	191 (95%)	10 (5%)	30	60
7	G	207/210 (99%)	201 (97%)	6 (3%)	50	80
7	U	207/210 (99%)	201 (97%)	6 (3%)	50	80
8	H	181/190 (95%)	180 (99%)	1 (1%)	90	97
8	V	181/190 (95%)	180 (99%)	1 (1%)	90	97
9	I	172/173 (99%)	170 (99%)	2 (1%)	78	93
9	W	172/173 (99%)	170 (99%)	2 (1%)	78	93
10	J	175/175 (100%)	174 (99%)	1 (1%)	90	97
10	X	175/175 (100%)	174 (99%)	1 (1%)	90	97
11	K	169/169 (100%)	165 (98%)	4 (2%)	57	85
11	Y	169/169 (100%)	166 (98%)	3 (2%)	66	89
12	L	185/185 (100%)	183 (99%)	2 (1%)	80	94
12	Z	185/185 (100%)	183 (99%)	2 (1%)	80	94
13	M	199/199 (100%)	192 (96%)	7 (4%)	43	74
13	a	199/199 (100%)	193 (97%)	6 (3%)	48	79
14	N	162/162 (100%)	161 (99%)	1 (1%)	90	97
14	b	162/162 (100%)	160 (99%)	2 (1%)	78	93
All	All	5332/5522 (97%)	5202 (98%)	130 (2%)	57	85

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	VAL
1	A	157	PHE
2	B	28	ILE

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Mol	Chain	Res	Type
2	B	59	ASP
2	B	60	THR
2	B	69	ASN
2	B	92	ILE
2	B	119	GLN
2	B	184	LYS
2	B	186	ASP
2	B	191	LEU
3	C	51	LYS
3	C	160	GLN
3	C	169	VAL
3	C	171	GLU
3	C	206	LYS
4	D	102	GLU
4	D	124	ARG
4	D	143	ASP
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	214	ILE
4	D	218	ASP
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	116	GLN
5	E	174	THR
5	E	184	ASN
5	E	188	LEU
5	E	231	LYS
6	F	39	ASN
6	F	91	GLU
6	F	117	GLN
6	F	123	ASN
6	F	130	VAL
6	F	181	GLU
6	F	186	ARG
6	F	201	GLU
6	F	203	ASN
6	F	214	TRP
7	G	44	VAL
7	G	117	GLN
7	G	166	GLN

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Mol	Chain	Res	Type
7	G	201	MET
7	G	221	LYS
7	G	235	ARG
8	H	34	LEU
9	I	37	ASN
9	I	81	ILE
10	J	92	ILE
11	K	4	LEU
11	K	9	GLN
11	K	65	LEU
11	K	104	TYR
12	L	49	ASN
12	L	109	THR
13	M	12	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	159	VAL
13	M	161	ARG
13	M	226	LYS
14	N	126	ILE
1	O	132	VAL
1	O	157	PHE
2	P	28	ILE
2	P	59	ASP
2	P	60	THR
2	P	69	ASN
2	P	74	VAL
2	P	92	ILE
2	P	119	GLN
2	P	184	LYS
2	P	191	LEU
3	Q	51	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	171	GLU
3	Q	206	LYS
4	R	102	GLU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU

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Mol	Chain	Res	Type
4	R	214	ILE
5	S	8	ASP
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	116	GLN
5	S	174	THR
5	S	184	ASN
5	S	188	LEU
5	S	231	LYS
6	T	39	ASN
6	T	91	GLU
6	T	117	GLN
6	T	123	ASN
6	T	130	VAL
6	T	181	GLU
6	T	186	ARG
6	T	201	GLU
6	T	203	ASN
6	T	214	TRP
7	U	117	GLN
7	U	154	TYR
7	U	166	GLN
7	U	201	MET
7	U	221	LYS
7	U	235	ARG
8	V	163	ILE
9	W	37	ASN
9	W	81	ILE
10	X	92	ILE
11	Y	4	LEU
11	Y	9	GLN
11	Y	104	TYR
12	Z	49	ASN
12	Z	128	VAL
13	a	12	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	226	LYS
14	b	88	GLU

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Mol	Chain	Res	Type
14	b	126	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	69	ASN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	17	GLN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	241	GLN
4	D	15	GLN
4	D	100	ASN
4	D	210	GLN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
5	E	209	ASN
6	F	19	GLN
6	F	39	ASN
6	F	86	ASN
6	F	117	GLN
7	G	6	HIS
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	22	GLN

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Mol	Chain	Res	Type
8	H	30	ASN
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
10	J	55	GLN
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	152	ASN
12	L	153	GLN
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	171	GLN
13	M	179	ASN
13	M	213	GLN
14	N	60	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	69	ASN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	146	GLN
2	P	155	ASN
3	Q	17	GLN
3	Q	92	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	241	GLN
4	R	15	GLN

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Mol	Chain	Res	Type
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
5	S	209	ASN
6	T	19	GLN
6	T	39	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
7	U	6	HIS
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	175	ASN
8	V	22	GLN
8	V	30	ASN
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	37	ASN
9	W	88	GLN
10	X	55	GLN
10	X	118	GLN
11	Y	9	GLN
11	Y	62	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	80	ASN
12	Z	158	ASN
12	Z	195	HIS
13	a	18	ASN
13	a	48	ASN

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Mol	Chain	Res	Type
13	a	102	GLN
13	a	171	GLN
13	a	179	ASN
13	a	213	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
15	049	K	213	11	18,19,19	2.72	6 (33%)	24,27,27	5.19	10 (41%)
15	049	Y	213	11	18,19,19	2.82	6 (33%)	24,27,27	5.72	8 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	049	K	213	11	-	0/18/22/22	0/1/2/2
15	049	Y	213	11	-	0/18/22/22	0/1/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	213	049	C8-C7	-8.25	1.35	1.53
15	K	213	049	C8-C7	-8.22	1.35	1.53
15	Y	213	049	C8-C6	-4.24	1.40	1.51
15	K	213	049	C8-C6	-3.94	1.41	1.51
15	Y	213	049	O13-C10	-3.08	1.40	1.45
15	K	213	049	O13-C10	-3.02	1.40	1.45
15	K	213	049	C1-C6	2.23	1.43	1.38
15	Y	213	049	C1-C6	2.26	1.43	1.38
15	K	213	049	C10-C9	2.83	1.59	1.54
15	Y	213	049	C10-C9	3.66	1.60	1.54
15	Y	213	049	C12-C10	4.12	1.59	1.46
15	K	213	049	C12-C10	4.13	1.59	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	213	049	C10-C9-C7	-21.14	92.36	115.32
15	K	213	049	C10-C9-C7	-16.55	97.35	115.32
15	K	213	049	O13-C12-C10	-3.49	55.26	59.83
15	Y	213	049	O13-C12-C10	-3.45	55.31	59.83
15	Y	213	049	O13-C10-C12	-3.03	55.38	59.55
15	K	213	049	O13-C10-C12	-2.88	55.59	59.55
15	K	213	049	C11-C10-C12	-2.51	114.35	119.83
15	Y	213	049	O49-C23-C18	-2.44	117.58	122.06
15	K	213	049	O49-C23-C18	-2.17	118.08	122.06
15	K	213	049	O13-C10-C9	3.00	119.53	113.48
15	Y	213	049	O21-C9-C10	5.70	122.62	108.82
15	Y	213	049	C6-C8-C7	7.75	125.82	113.48
15	K	213	049	C12-O13-C10	8.19	69.15	60.62
15	Y	213	049	C12-O13-C10	8.34	69.31	60.62
15	K	213	049	O21-C9-C10	8.41	129.18	108.82
15	K	213	049	C6-C8-C7	8.46	126.94	113.48
15	K	213	049	C8-C7-C9	10.93	131.81	111.69
15	Y	213	049	C8-C7-C9	11.46	132.80	111.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	K	213	049	3	0
15	Y	213	049	4	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%)	0.08	11 (4%) 38 37	34, 48, 77, 99	0
1	O	250/250 (100%)	0.18	9 (3%) 46 46	38, 54, 87, 111	0
2	B	244/258 (94%)	0.26	15 (6%) 25 23	34, 52, 81, 112	0
2	P	244/258 (94%)	0.39	20 (8%) 14 11	38, 54, 87, 116	0
3	C	241/254 (94%)	0.40	23 (9%) 10 8	36, 56, 105, 147	0
3	Q	241/254 (94%)	0.44	22 (9%) 11 9	40, 63, 119, 160	0
4	D	242/260 (93%)	0.31	10 (4%) 41 41	41, 55, 83, 110	0
4	R	242/260 (93%)	0.43	21 (8%) 13 10	42, 60, 94, 115	0
5	E	233/234 (99%)	0.23	13 (5%) 28 26	41, 58, 86, 101	0
5	S	233/234 (99%)	0.40	18 (7%) 16 14	45, 62, 91, 104	0
6	F	244/288 (84%)	0.19	12 (4%) 33 32	38, 55, 89, 113	0
6	T	244/288 (84%)	0.27	13 (5%) 30 28	37, 57, 92, 119	0
7	G	243/252 (96%)	-0.04	8 (3%) 50 50	35, 50, 79, 120	0
7	U	243/252 (96%)	0.06	8 (3%) 50 50	38, 50, 75, 115	0
8	H	222/232 (95%)	0.06	4 (1%) 71 72	38, 48, 68, 100	0
8	V	222/232 (95%)	0.01	3 (1%) 78 77	37, 49, 68, 101	0
9	I	204/205 (99%)	-0.14	5 (2%) 61 61	34, 45, 66, 75	0
9	W	204/205 (99%)	-0.07	4 (1%) 68 69	36, 47, 68, 83	0
10	J	198/198 (100%)	0.01	9 (4%) 37 36	35, 47, 66, 116	0
10	X	198/198 (100%)	0.03	7 (3%) 48 48	39, 49, 65, 111	0
11	K	212/212 (100%)	-0.10	2 (0%) 85 86	33, 43, 63, 70	0
11	Y	212/212 (100%)	-0.03	2 (0%) 85 86	35, 46, 66, 75	0
12	L	222/222 (100%)	-0.12	5 (2%) 64 64	34, 46, 73, 85	0
12	Z	222/222 (100%)	-0.06	4 (1%) 71 72	35, 47, 72, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/233 (100%)	-0.14	3 (1%) 79 79	33, 47, 69, 85	0
13	a	233/233 (100%)	-0.15	2 (0%) 85 86	32, 46, 64, 77	0
14	N	196/196 (100%)	-0.17	3 (1%) 76 76	33, 43, 64, 79	0
14	b	196/196 (100%)	-0.14	4 (2%) 68 69	34, 45, 64, 75	0
All	All	6368/6588 (96%)	0.10	260 (4%) 41 41	32, 50, 85, 160	0

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	121	GLY	11.9
4	R	119	ALA	10.2
3	C	49	THR	9.5
3	C	50	LEU	9.4
2	B	220	ASN	9.2
4	D	119	ALA	9.0
4	R	120	SER	8.6
2	P	220	ASN	8.4
2	P	219	ALA	8.3
10	J	197	ALA	7.7
7	G	1	ALA	7.5
1	O	2	THR	7.5
7	U	1	ALA	7.5
10	X	197	ALA	7.3
5	S	1	PHE	7.3
4	D	121	GLY	7.1
4	D	120	SER	7.0
5	E	1	PHE	7.0
10	J	198	GLN	6.9
2	B	51	VAL	6.9
2	B	219	ALA	6.6
4	D	124	ARG	6.6
3	Q	50	LEU	6.6
3	Q	203	THR	6.6
10	X	198	GLN	6.5
4	D	118	GLY	6.5
1	O	1	MET	6.4
1	A	1	MET	6.4
7	U	243	ASP	6.3
5	E	202	ASP	6.1
1	A	2	THR	6.1
4	R	124	ARG	5.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	S	2	ARG	5.9
2	P	51	VAL	5.8
6	F	202	ASP	5.8
8	H	221	CYS	5.6
4	R	118	GLY	5.6
8	H	222	ASP	5.5
4	D	125	LEU	5.5
8	V	221	CYS	5.5
5	S	202	ASP	5.3
6	T	2	THR	5.3
8	V	222	ASP	5.2
4	D	122	GLU	5.2
3	C	203	THR	5.1
3	Q	48	SER	5.1
2	B	221	ASP	5.1
2	P	223	GLU	5.1
6	F	1	GLY	5.1
3	Q	239	GLN	5.0
12	Z	173	LYS	5.0
2	P	221	ASP	4.9
4	R	125	LEU	4.9
3	Q	49	THR	4.9
10	X	196	GLN	4.9
9	W	1	SER	4.8
7	G	243	ASP	4.8
1	O	249	ALA	4.7
5	E	2	ARG	4.6
5	S	207	VAL	4.6
5	S	3	ASN	4.6
10	J	196	GLN	4.5
6	T	243	ILE	4.4
4	R	122	GLU	4.4
12	Z	174	TYR	4.4
6	T	244	ASN	4.4
9	I	1	SER	4.3
2	P	59	ASP	4.2
5	S	173	ARG	4.2
13	a	1	THR	4.1
3	Q	51	LYS	4.1
6	T	181	GLU	4.1
5	E	207	VAL	4.1
1	O	250	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
6	T	1	GLY	4.1
13	M	233	ILE	4.0
13	M	1	THR	4.0
12	L	174	TYR	3.8
1	A	250	LEU	3.7
1	O	231	LYS	3.7
1	O	52	SER	3.7
3	Q	241	GLN	3.7
3	Q	187	GLU	3.7
3	C	241	GLN	3.6
3	Q	193	THR	3.6
3	C	48	SER	3.6
5	E	3	ASN	3.6
2	P	240	LYS	3.5
3	Q	240	GLU	3.5
12	Z	1	GLN	3.5
6	F	181	GLU	3.5
6	F	203	ASN	3.4
14	N	105	LYS	3.4
3	C	202	GLN	3.4
3	C	238	LYS	3.4
6	F	204	LYS	3.4
2	P	218	GLY	3.4
9	I	131	GLU	3.4
3	Q	202	GLN	3.3
2	B	218	GLY	3.3
4	R	46	ALA	3.3
3	Q	206	LYS	3.3
10	X	194	ASP	3.3
2	P	225	TYR	3.3
1	A	201	GLU	3.3
3	C	206	LYS	3.3
9	W	192	ASP	3.2
6	F	205	GLU	3.2
3	C	51	LYS	3.2
3	Q	238	LYS	3.2
3	C	193	THR	3.2
7	G	2	GLY	3.2
3	C	239	GLN	3.2
2	P	61	SER	3.1
14	b	195	GLN	3.1
6	F	244	ASN	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	Q	236	GLN	3.1
10	J	194	ASP	3.1
6	F	2	THR	3.1
1	O	248	GLU	3.1
2	B	222	GLY	3.1
6	F	243	ILE	3.1
7	G	240	ALA	3.0
5	S	175	LEU	3.0
3	C	27	ARG	3.0
7	U	2	GLY	3.0
2	P	50	LYS	3.0
3	Q	234	ILE	3.0
1	A	248	GLU	3.0
2	B	217	LYS	3.0
1	O	50	LYS	3.0
2	B	1	GLY	3.0
12	L	172	LEU	3.0
2	P	52	THR	3.0
10	X	1	MET	3.0
8	H	219	ASN	2.9
5	E	203	GLU	2.9
7	U	222	ASP	2.9
2	P	217	LYS	2.9
3	Q	175	LYS	2.9
1	A	229	THR	2.9
5	S	233	ILE	2.9
2	P	203	SER	2.8
7	G	242	GLN	2.8
2	B	223	GLU	2.8
3	Q	237	GLU	2.8
4	R	1	ASP	2.8
4	D	169	GLU	2.8
10	J	193	ASP	2.8
3	C	240	GLU	2.8
6	F	201	GLU	2.8
3	C	237	GLU	2.8
3	Q	47	ARG	2.8
6	F	241	LYS	2.8
7	U	188	GLU	2.8
5	E	30	GLN	2.8
10	X	193	ASP	2.8
1	A	231	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	180	LYS	2.7
6	T	207	ASP	2.7
12	L	173	LYS	2.7
13	M	232	LYS	2.7
6	T	241	LYS	2.7
4	R	241	ALA	2.7
12	L	1	GLN	2.7
4	R	230	GLU	2.7
1	A	202	GLY	2.7
7	U	242	GLN	2.6
6	F	177	ASP	2.6
6	T	53	LYS	2.6
2	B	50	LYS	2.6
2	P	222	GLY	2.6
7	G	188	GLU	2.6
3	C	175	LYS	2.6
5	S	30	GLN	2.6
1	O	201	GLU	2.6
4	R	192	VAL	2.6
7	U	3	TYR	2.5
1	A	228	PRO	2.5
3	C	47	ARG	2.5
5	E	218	ASP	2.5
3	C	181	GLU	2.5
9	W	131	GLU	2.5
4	D	40	LEU	2.5
3	Q	55	THR	2.5
4	R	240	ALA	2.5
6	T	180	PRO	2.5
5	S	201	ARG	2.4
9	I	130	ASP	2.4
11	K	147	ASP	2.4
4	R	40	LEU	2.4
14	b	149	GLU	2.4
3	Q	58	THR	2.4
9	I	192	ASP	2.4
2	P	45	LEU	2.4
12	Z	165	ASN	2.4
6	T	43	VAL	2.4
4	D	123	GLU	2.4
5	S	180	LYS	2.4
10	J	24	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
11	Y	212	GLY	2.4
10	J	155	GLU	2.4
5	S	45	LEU	2.3
3	Q	171	GLU	2.3
5	E	204	SER	2.3
14	N	195	GLN	2.3
7	G	179	LYS	2.3
4	R	53	SER	2.3
5	S	36	GLY	2.3
5	E	173	ARG	2.3
1	A	36	GLY	2.3
2	B	182	ASP	2.3
5	E	227	GLU	2.3
2	P	60	THR	2.3
4	R	123	GLU	2.3
7	G	3	TYR	2.3
14	b	104	ASP	2.2
2	B	59	ASP	2.2
2	B	204	ALA	2.2
11	Y	106	ARG	2.2
6	T	203	ASN	2.2
5	S	227	GLU	2.2
12	L	165	ASN	2.2
5	S	203	GLU	2.2
4	R	217	GLN	2.2
5	E	163	ARG	2.2
13	a	233	ILE	2.2
10	J	95	ARG	2.2
2	P	44	VAL	2.2
4	R	169	GLU	2.2
3	C	33	GLY	2.2
6	T	204	LYS	2.2
3	C	34	VAL	2.2
8	V	219	ASN	2.1
11	K	106	ARG	2.1
14	N	149	GLU	2.1
7	U	124	TYR	2.1
3	C	53	GLN	2.1
5	S	72	SER	2.1
5	S	169	THR	2.1
10	J	174	MET	2.1
3	C	225	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	Q	181	GLU	2.1
2	B	203	SER	2.1
14	b	105	LYS	2.1
2	B	225	TYR	2.1
9	W	130	ASP	2.1
1	A	4	ARG	2.1
6	T	186	ARG	2.1
8	H	5	GLY	2.1
9	I	127	GLY	2.1
3	C	171	GLU	2.0
4	R	47	THR	2.0
5	S	46	VAL	2.0
4	R	242	GLU	2.0
4	R	173	ALA	2.0
2	P	4	ARG	2.0
10	X	195	PHE	2.0
5	E	201	ARG	2.0
2	P	182	ASP	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	049	K	213	18/18	0.82	0.29	2.31	35,40,41,42	0
15	049	Y	213	18/18	0.84	0.25	2.07	38,42,43,44	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.