



# Full wwPDB X-ray Structure Validation Report

Apr 23, 2024 – 10:10 pm BST


PDB ID : 8RHL  
Title : Yeast 20S proteasome in complex with a linear biarylether epoxyketone (compound 15a)  
Authors : Goetz, M.G.; Godwin, K.; Price, R.; Dorn, R.; Merrill-Steskal, G.; Hansen, H.; Klemmer, W.; Produturi, G.; Rocha, M.; Palmer, M.; Molacek, L.; Strater, Z.; Groll, M.  
Deposited on : 2023-12-15  
Resolution : 3.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

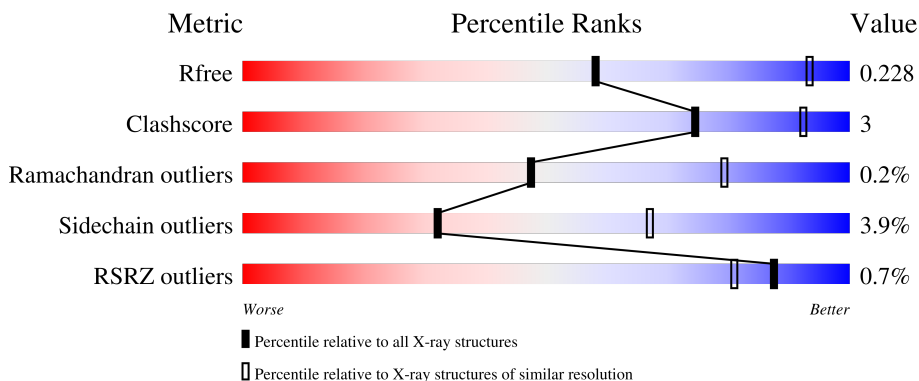
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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








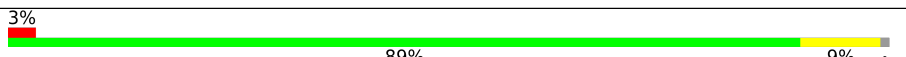

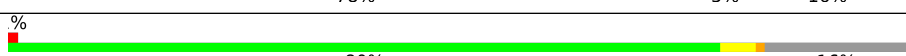

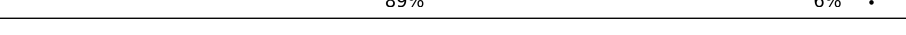

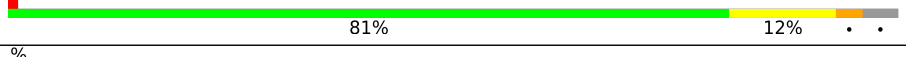


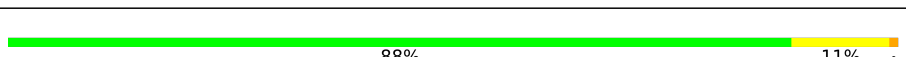
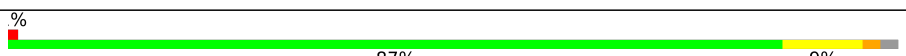









Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	 96%
1	O	250	 96%
2	B	258	 88% 6% • 5%
2	P	258	 88% 5% • 5%



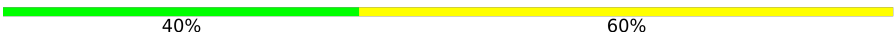
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Mol	Chain	Length	Quality of chain
3	C	254	 87% 6% • 6%
3	Q	254	 4% 87% 5% • 6%
4	D	260	 84% 6% 10%
4	R	260	 84% 6% 10%
5	E	234	 89% 9% •
5	S	234	 3% 89% 9% •
6	F	288	 78% 5% • 16%
6	T	288	 1% 80% • • 16%
7	G	252	 89% 6% •
7	U	252	 88% 7% •
8	H	232	 1% 81% 12% • •
8	V	232	 1% 81% 12% • •
9	I	205	 88% 10% •
9	W	205	 88% 11% •
10	J	198	 1% 87% 9% • •
10	X	198	 1% 88% 9% • •
11	K	212	 89% 10% •
11	Y	212	 88% 10% •
12	L	222	 91% 9%
12	Z	222	 91% 9%
13	M	246	 87% 6% 7%
13	a	246	 91% • 7%
14	N	196	 91% 8% •
14	b	196	 99% •
15	e	5	 40% 60%

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Mol	Chain	Length	Quality of chain
15	f	5	 40% 60%
15	g	5	 40% 60%
15	h	5	 40% 60%

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49514 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
			Total	C	N	O	S			
1	A	250	Total 1915	C 1219	N 315	O 377	S 4	0	0	0
1	O	250	Total 1915	C 1219	N 315	O 377	S 4	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	240	Total 1881	C 1176	N 329	O 372	S 4	0	0	0
3	Q	240	Total 1881	C 1176	N 329	O 372	S 4	0	0	0

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

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

- 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
			1684	1061	293	323	7			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	229	1790	1133	306	344	7	0	0	0
13	a	229	1790	1133	306	344	7	0	0	0

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

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

- Molecule 15 is a protein called Linear biarylether epoxyketone.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	e	5	49	35	5	9	0	0	0
15	f	5	49	35	5	9	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	g	5	Total	C	N	O	0	0	0
			49	35	5	9			
15	h	5	Total	C	N	O	0	0	0
			49	35	5	9			

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Mg	0	0
			1	1		
16	I	1	Total	Mg	0	0
			1	1		
16	K	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		
16	V	1	Total	Mg	0	0
			1	1		
16	X	1	Total	Mg	0	0
			1	1		
16	Y	1	Total	Mg	0	0
			1	1		
16	Z	1	Total	Mg	0	0
			1	1		

- Molecule 17 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	1	Total	Cl	0	0
			1	1		
17	U	1	Total	Cl	0	0
			1	1		

- Molecule 18 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
			Total	C	N	O	S		
18	K	1	12	6	1	4	1	0	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O	0	0
			1	1		
19	B	2	Total	O	0	0
			2	2		
19	C	2	Total	O	0	0
			2	2		
19	D	1	Total	O	0	0
			1	1		
19	F	1	Total	O	0	0
			1	1		
19	G	1	Total	O	0	0
			1	1		
19	H	1	Total	O	0	0
			1	1		
19	J	5	Total	O	0	0
			5	5		
19	K	2	Total	O	0	0
			2	2		
19	L	3	Total	O	0	0
			3	3		
19	M	9	Total	O	0	0
			9	9		

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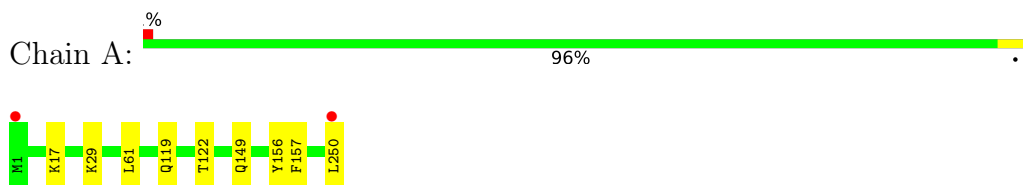
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	N	6	Total O 6 6	0	0
19	O	1	Total O 1 1	0	0
19	P	2	Total O 2 2	0	0
19	Q	5	Total O 5 5	0	0
19	R	1	Total O 1 1	0	0
19	S	2	Total O 2 2	0	0
19	U	2	Total O 2 2	0	0
19	V	2	Total O 2 2	0	0
19	W	2	Total O 2 2	0	0
19	X	5	Total O 5 5	0	0
19	Z	1	Total O 1 1	0	0
19	a	5	Total O 5 5	0	0
19	b	2	Total O 2 2	0	0
19	e	1	Total O 1 1	0	0
19	f	1	Total O 1 1	0	0
19	g	1	Total O 1 1	0	0
19	h	1	Total O 1 1	0	0

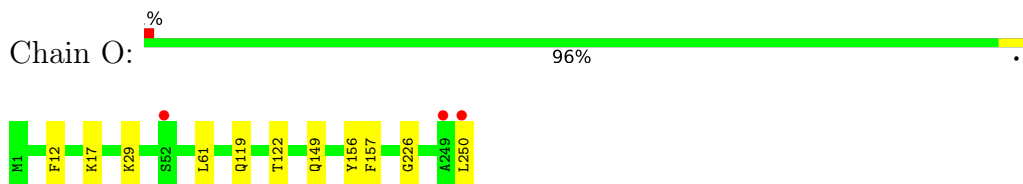
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

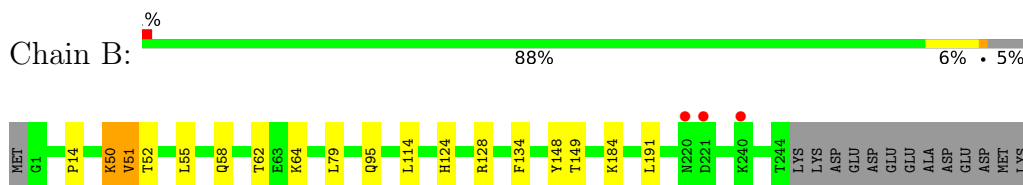
- Molecule 1: Proteasome subunit alpha type-2



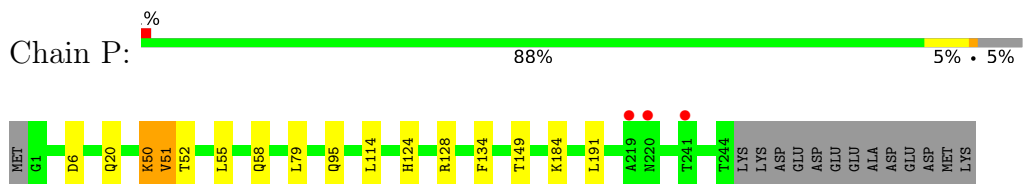
- Molecule 1: Proteasome subunit alpha type-2



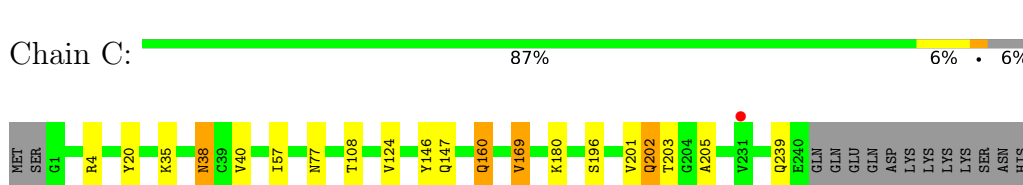
- Molecule 2: Proteasome subunit alpha type-3



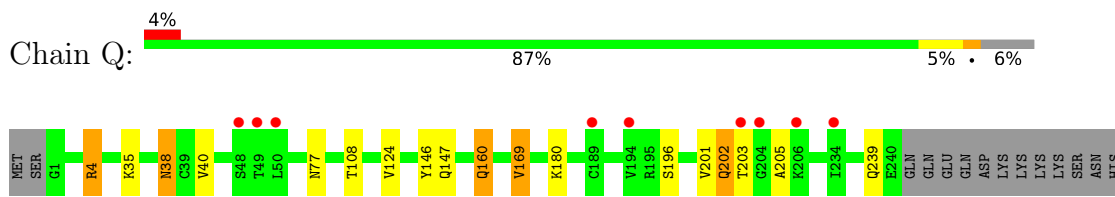
- Molecule 2: Proteasome subunit alpha type-3



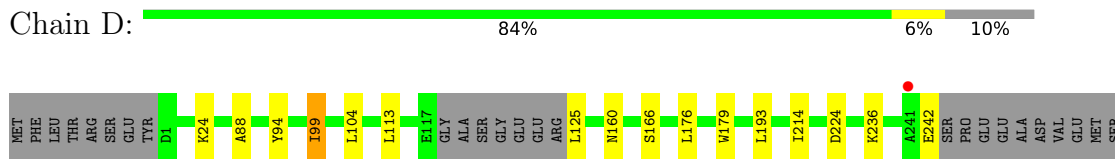
- Molecule 3: Proteasome subunit alpha type-4



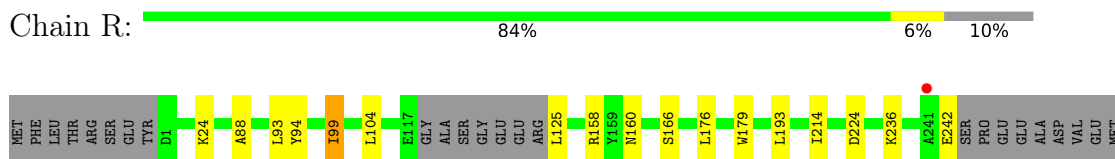
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-5

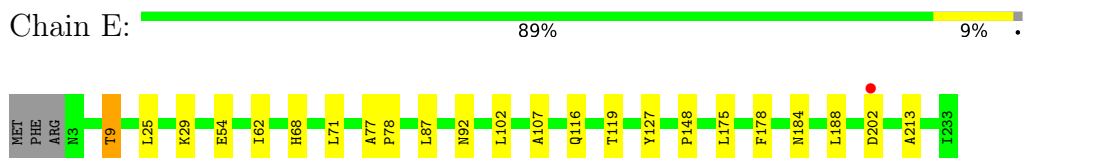


- Molecule 4: Proteasome subunit alpha type-5

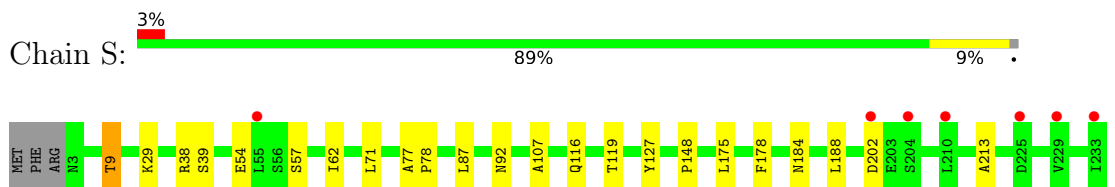


SER

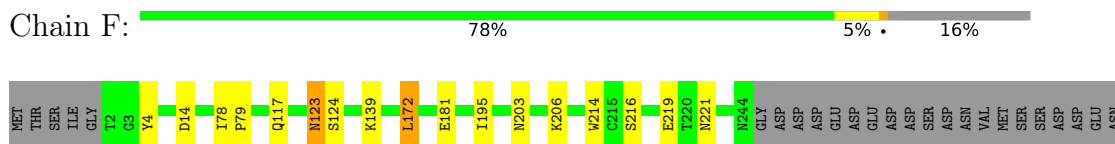
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 5: Proteasome subunit alpha type-6

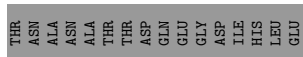
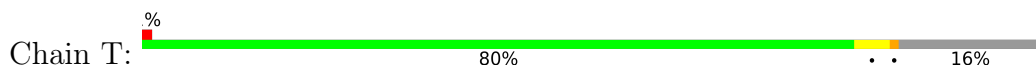


- Molecule 6: Probable proteasome subunit alpha type-7

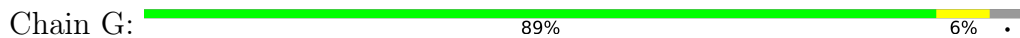


ALA  
PRO  
VAL  
ALA  
THR  
ASN  
ASN  
ALA  
ALA  
THR  
THR  
ASP  
GLN  
GLU  
GLY  
ASP  
ILE  
HIS  
LEU  
GLU

- Molecule 6: Probable proteasome subunit alpha type-7



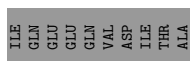
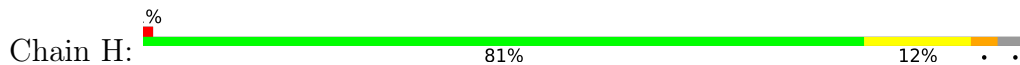
- Molecule 7: Proteasome subunit alpha type-1



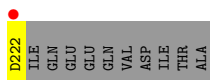
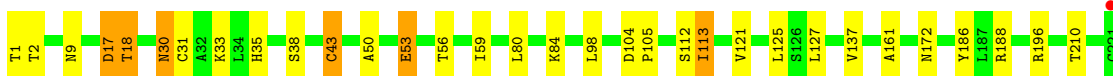
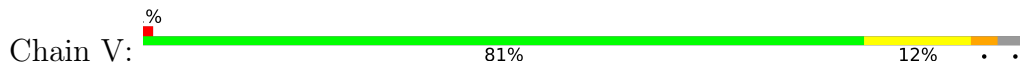
- Molecule 7: Proteasome subunit alpha type-1



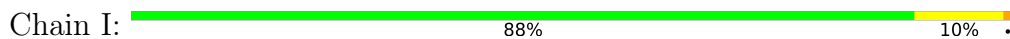
- Molecule 8: Proteasome subunit beta type-2




- Molecule 8: Proteasome subunit beta type-2



- Molecule 9: Proteasome subunit beta type-3




- Molecule 9: Proteasome subunit beta type-3

Chain W:  88% 11%




- Molecule 10: Proteasome subunit beta type-4

Chain J:  87% 9%




- Molecule 10: Proteasome subunit beta type-4

Chain X:  88% 9%




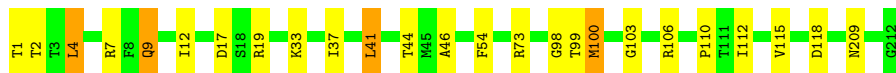
- Molecule 11: Proteasome subunit beta type-5

Chain K:  89% 10%




- Molecule 11: Proteasome subunit beta type-5

Chain Y:  88% 10%




- Molecule 12: Proteasome subunit beta type-6

Chain L:  91% 9%




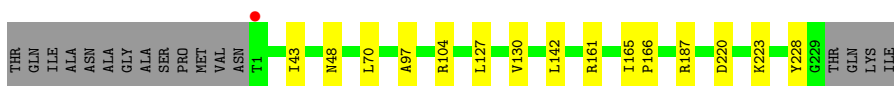
- Molecule 12: Proteasome subunit beta type-6

Chain Z:  91% 9%




- Molecule 13: Proteasome subunit beta type-7

Chain M:  87% 6% 7%




- Molecule 13: Proteasome subunit beta type-7

Chain a:  91% 7%



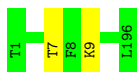
- Molecule 14: Proteasome subunit beta type-1

Chain N:  91% 8%



- Molecule 14: Proteasome subunit beta type-1

Chain b:  99%



- Molecule 15: Linear biarylether epoxyketone

Chain e:  40% 60%



- Molecule 15: Linear biarylether epoxyketone

Chain f:  40% 60%



- Molecule 15: Linear biarylether epoxyketone

Chain g:  40% 60%



- Molecule 15: Linear biarylether epoxyketone

Chain h:  40% 60%

ACE1
F2
L3
Y4
6VU5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.21Å 303.14Å 143.23Å 90.00° 113.09° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 49.72 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-3.20) 97.7 (49.72-3.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 3.19Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.184 , 0.228 0.189 , 0.228	Depositor DCC
$R_{free}$ test set	8498 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.1	Xtrriage
Anisotropy	0.646	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	49514	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, CL, PPN, MES, 6VO, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.65	0/1952	0.70	0/2642
1	O	0.65	0/1952	0.70	0/2642
2	B	0.65	0/1934	0.71	0/2618
2	P	0.66	0/1934	0.71	0/2618
3	C	0.66	0/1910	0.72	0/2586
3	Q	0.66	0/1910	0.72	0/2586
4	D	0.66	0/1837	0.71	0/2475
4	R	0.66	0/1837	0.71	0/2475
5	E	0.66	0/1800	0.71	0/2433
5	S	0.66	0/1800	0.71	0/2433
6	F	0.65	0/1932	0.70	0/2609
6	T	0.65	0/1932	0.70	0/2609
7	G	0.64	0/1945	0.70	0/2634
7	U	0.64	0/1945	0.70	0/2634
8	H	0.65	0/1715	0.75	0/2326
8	V	0.66	0/1715	0.74	0/2326
9	I	0.65	0/1611	0.72	0/2174
9	W	0.65	0/1611	0.72	0/2174
10	J	0.64	0/1589	0.70	0/2142
10	X	0.64	0/1589	0.70	0/2142
11	K	0.65	0/1681	0.73	0/2274
11	Y	0.65	0/1681	0.73	0/2274
12	L	0.64	0/1795	0.71	0/2420
12	Z	0.64	0/1795	0.71	0/2420
13	M	0.65	0/1821	0.72	0/2470
13	a	0.65	0/1821	0.72	0/2470
14	N	0.65	0/1541	0.70	0/2087
14	b	0.65	0/1541	0.70	0/2087
15	e	3.01	3/20 (15.0%)	1.40	0/26
15	f	3.16	3/20 (15.0%)	1.41	0/26
15	g	2.87	3/20 (15.0%)	1.23	0/26
15	h	3.30	3/20 (15.0%)	1.75	0/26

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.66	12/50206 (0.0%)	0.71	0/67884

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	h	4	TYR	CB-CG	-10.67	1.35	1.51
15	f	4	TYR	CB-CG	-9.94	1.36	1.51
15	e	4	TYR	CB-CG	-9.53	1.37	1.51
15	g	4	TYR	CB-CG	-8.85	1.38	1.51
15	f	3	LEU	CA-C	-7.18	1.34	1.52
15	h	3	LEU	CA-C	-6.97	1.34	1.52
15	e	3	LEU	CA-C	-6.96	1.34	1.52
15	g	3	LEU	CA-C	-6.61	1.35	1.52
15	h	4	TYR	CA-C	-5.46	1.38	1.52
15	f	4	TYR	CA-C	-5.37	1.39	1.52
15	g	4	TYR	CA-C	-5.11	1.39	1.52
15	e	4	TYR	CA-C	-5.07	1.39	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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	3	0
1	O	1915	0	1929	5	0
2	B	1904	0	1904	10	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	11	0
3	Q	1881	0	1895	9	0
4	D	1813	0	1797	8	0
4	R	1813	0	1797	10	0
5	E	1773	0	1775	12	0
5	S	1773	0	1775	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1892	0	1883	6	0
6	T	1892	0	1883	5	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	7	0
8	H	1684	0	1686	23	0
8	V	1684	0	1686	24	0
9	I	1581	0	1574	18	0
9	W	1581	0	1574	17	0
10	J	1561	0	1569	18	0
10	X	1561	0	1569	15	0
11	K	1644	0	1593	19	0
11	Y	1644	0	1592	29	0
12	L	1757	0	1711	14	0
12	Z	1757	0	1711	17	0
13	M	1790	0	1793	6	0
13	a	1790	0	1793	0	0
14	N	1512	0	1481	10	0
14	b	1512	0	1481	0	0
15	e	49	0	28	0	0
15	f	49	0	28	0	0
15	g	49	0	28	0	0
15	h	49	0	28	0	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	K	1	0	0	0	0
16	N	1	0	0	0	0
16	V	1	0	0	0	0
16	X	1	0	0	0	0
16	Y	1	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	U	1	0	0	0	0
18	K	12	0	13	0	0
19	A	1	0	0	0	0
19	B	2	0	0	2	0
19	C	2	0	0	0	0
19	D	1	0	0	0	0
19	F	1	0	0	0	0
19	G	1	0	0	0	0
19	H	1	0	0	0	0
19	J	5	0	0	0	0
19	K	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	L	3	0	0	0	0
19	M	9	0	0	0	0
19	N	6	0	0	0	0
19	O	1	0	0	0	0
19	P	2	0	0	0	0
19	Q	5	0	0	0	0
19	R	1	0	0	0	0
19	S	2	0	0	0	0
19	U	2	0	0	0	0
19	V	2	0	0	0	0
19	W	2	0	0	0	0
19	X	5	0	0	0	0
19	Z	1	0	0	0	0
19	a	5	0	0	0	0
19	b	2	0	0	0	0
19	e	1	0	0	0	0
19	f	1	0	0	0	0
19	g	1	0	0	0	0
19	h	1	0	0	0	0
All	All	49514	0	49106	266	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 (266) 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)
10:X:101:ASN:HB3	10:X:133:HIS:CD2	1.83	1.14
10:J:101:ASN:HB3	10:J:133:HIS:CD2	1.83	1.13
11:Y:1:THR:HG22	11:Y:2:THR:N	1.75	0.98
11:Y:1:THR:HG23	11:Y:33:LYS:NZ	1.90	0.87
4:R:94:TYR:HD1	12:Z:95:HIS:HD1	1.17	0.86
11:Y:1:THR:HG23	11:Y:33:LYS:HZ2	1.38	0.86
10:J:101:ASN:HB3	10:J:133:HIS:HD2	1.42	0.81
10:X:101:ASN:HB3	10:X:133:HIS:HD2	1.42	0.79
11:Y:1:THR:CG2	11:Y:2:THR:N	2.45	0.79
4:R:94:TYR:HD1	12:Z:95:HIS:ND1	1.80	0.79
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.48	0.77
11:Y:1:THR:HG23	11:Y:17:ASP:OD1	1.84	0.77
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.48	0.77
10:X:101:ASN:CB	10:X:133:HIS:CD2	2.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:152:VAL:HA	14:N:175:MET:HE1	1.70	0.73
10:J:101:ASN:CB	10:J:133:HIS:CD2	2.67	0.73
11:K:7:ARG:NH1	11:K:110:PRO:O	2.20	0.72
8:V:18:THR:HG21	8:V:172:ASN:HB2	1.71	0.72
11:Y:7:ARG:NH1	11:Y:110:PRO:O	2.22	0.72
8:H:18:THR:HG21	8:H:172:ASN:HB2	1.71	0.71
10:J:101:ASN:CB	10:J:133:HIS:HD2	2.02	0.71
8:H:50:ALA:CB	9:I:126:ILE:HG22	2.20	0.71
8:H:1:THR:HG22	8:H:2:THR:N	2.05	0.70
8:V:50:ALA:CB	9:W:126:ILE:HG22	2.21	0.70
14:N:7:THR:HG23	14:N:123:PRO:O	1.91	0.70
10:X:101:ASN:CB	10:X:133:HIS:HD2	2.03	0.68
4:D:94:TYR:HD1	12:L:95:HIS:HD1	1.42	0.68
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.78	0.66
14:N:7:THR:HG22	14:N:110:VAL:HG23	1.77	0.66
11:K:1:THR:O	11:K:130:GLY:HA3	1.96	0.65
7:G:23:PHE:O	7:G:26:THR:HB	1.97	0.64
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.78	0.64
4:D:94:TYR:HD1	12:L:95:HIS:ND1	1.95	0.64
7:U:23:PHE:O	7:U:26:THR:HB	1.97	0.64
9:W:87:THR:HG22	9:W:129:ILE:HD13	1.80	0.63
11:Y:44:THR:OG1	11:Y:100:MET:HB2	1.98	0.63
11:K:44:THR:OG1	11:K:100:MET:HB2	2.00	0.62
10:J:174:MET:HA	10:X:174:MET:HA	1.80	0.61
8:H:50:ALA:HB1	9:I:126:ILE:HG22	1.80	0.61
9:I:87:THR:HG22	9:I:129:ILE:HD13	1.80	0.61
11:Y:1:THR:HG22	11:Y:2:THR:H	1.60	0.61
11:K:99:THR:HG22	11:K:115:VAL:O	2.00	0.61
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.34	0.60
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.65	0.60
13:M:220:ASP:O	13:M:223:LYS:HG2	2.02	0.60
6:T:123:ASN:C	6:T:123:ASN:HD22	2.05	0.60
8:H:1:THR:CG2	8:H:2:THR:N	2.63	0.60
14:N:55:ILE:HD11	14:N:93:LEU:HD13	1.81	0.60
11:K:1:THR:HG22	11:K:2:THR:N	2.17	0.60
8:H:17:ASP:OD1	8:H:33:LYS:NZ	2.36	0.59
8:V:210:THR:HG21	9:W:167:SER:HB3	1.84	0.59
6:F:123:ASN:C	6:F:123:ASN:HD22	2.05	0.59
11:Y:73:ARG:HG2	11:Y:73:ARG:HH11	1.68	0.59
8:H:30:ASN:HD21	8:H:188:ARG:NH2	2.01	0.58
11:K:73:ARG:HG2	11:K:73:ARG:HH11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:17:ASP:OD1	8:V:33:LYS:NZ	2.36	0.57
11:Y:1:THR:CG2	11:Y:33:LYS:NZ	2.67	0.57
8:V:53:GLU:OE2	8:V:53:GLU:HA	2.05	0.56
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.04	0.56
9:I:98:ARG:HD2	9:I:126:ILE:HG13	1.87	0.56
8:H:30:ASN:ND2	8:H:188:ARG:NH2	2.52	0.56
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.40	0.56
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.88	0.56
9:W:98:ARG:HD2	9:W:126:ILE:HG13	1.88	0.56
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.71	0.55
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.88	0.55
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.05	0.55
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.72	0.55
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.72	0.55
6:F:4:TYR:CD1	6:F:4:TYR:N	4.06	0.55
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.89	0.55
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.42	0.55
8:H:43:CYS:SG	8:H:98:LEU:HD22	2.47	0.54
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.89	0.54
11:Y:1:THR:CG2	11:Y:2:THR:H	2.14	0.54
8:H:53:GLU:OE2	8:H:53:GLU:HA	2.07	0.54
3:C:38:ASN:C	3:C:38:ASN:HD22	2.11	0.54
12:L:8:ASN:HA	12:L:30:ILE:O	2.08	0.54
11:Y:99:THR:HG22	11:Y:115:VAL:O	2.08	0.54
6:F:123:ASN:HD22	6:F:124:SER:N	2.06	0.54
8:V:43:CYS:SG	8:V:98:LEU:HD22	2.48	0.54
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.43	0.53
6:T:123:ASN:HD22	6:T:124:SER:N	2.07	0.53
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.43	0.53
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.43	0.53
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.90	0.53
4:R:94:TYR:CD1	12:Z:95:HIS:ND1	2.64	0.53
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.90	0.53
10:J:168:LEU:O	10:J:172:MET:HB2	2.08	0.53
10:X:168:LEU:O	10:X:172:MET:HB2	2.09	0.52
11:Y:4:LEU:O	11:Y:4:LEU:HD22	2.10	0.52
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.92	0.52
2:B:64:LYS:N	19:B:301:HOH:O	2.43	0.52
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.92	0.52
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.44	0.52
3:Q:38:ASN:C	3:Q:38:ASN:HD22	2.12	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:4:LEU:HD22	11:K:4:LEU:O	2.10	0.51
11:K:4:LEU:HD22	11:K:4:LEU:C	2.31	0.51
11:Y:4:LEU:HD22	11:Y:4:LEU:C	2.30	0.51
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.10	0.51
12:Z:100:LYS:O	12:Z:104:PRO:HA	2.10	0.51
10:J:1:MET:O	10:J:2:ASP:HB2	2.11	0.51
2:P:6:ASP:OD2	3:Q:4:ARG:HG3	2.10	0.50
12:L:100:LYS:O	12:L:104:PRO:HA	2.11	0.50
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.59	0.50
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.93	0.50
8:H:32:ALA:HB2	8:H:188:ARG:NH1	2.27	0.50
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.94	0.49
8:H:35:HIS:HB2	8:H:56:THR:HG21	1.94	0.49
11:K:1:THR:CG2	11:K:2:THR:N	2.74	0.49
10:X:1:MET:O	10:X:2:ASP:HB2	2.11	0.49
13:M:228:TYR:HA	8:V:121:VAL:HG23	1.93	0.49
8:V:35:HIS:HB2	8:V:56:THR:HG21	1.94	0.49
11:Y:1:THR:CG2	11:Y:33:LYS:HZ3	2.26	0.49
14:N:36:ARG:HH21	14:N:60:GLN:HE21	1.59	0.49
14:N:14:LEU:HD11	14:N:100:ALA:HB3	1.95	0.48
8:V:50:ALA:HB1	9:W:126:ILE:HG22	1.93	0.48
10:X:101:ASN:HB3	10:X:133:HIS:NE2	2.24	0.48
7:G:78:ILE:N	7:G:79:PRO:CD	2.76	0.48
13:M:228:TYR:HA	8:V:121:VAL:CG2	2.44	0.48
8:H:35:HIS:CB	8:H:56:THR:HG21	2.43	0.48
7:U:78:ILE:N	7:U:79:PRO:CD	2.77	0.48
10:J:101:ASN:HB3	10:J:133:HIS:NE2	2.26	0.47
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.29	0.47
11:K:1:THR:HG23	11:K:33:LYS:NZ	2.29	0.47
11:K:83:LEU:HD21	11:K:99:THR:HG21	1.96	0.47
12:L:147:MET:N	12:L:148:PRO:HD2	2.29	0.47
1:O:12:PHE:H	2:P:20:GLN:HE22	1.62	0.47
8:V:35:HIS:CB	8:V:56:THR:HG21	2.44	0.47
3:C:108:THR:HG21	3:C:146:TYR:HB3	1.97	0.47
4:R:94:TYR:HD1	12:Z:95:HIS:CE1	2.32	0.47
11:Y:54:PHE:HE1	12:Z:95:HIS:CD2	2.32	0.47
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.96	0.47
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.44	0.47
8:V:30:ASN:ND2	8:V:188:ARG:NH2	2.62	0.46
11:Y:54:PHE:CE1	12:Z:95:HIS:CD2	3.04	0.46
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:19:ARG:O	14:N:33:LYS:NZ	2.46	0.46
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.97	0.46
4:D:94:TYR:CD1	12:L:95:HIS:ND1	2.80	0.46
5:E:77:ALA:N	5:E:78:PRO:CD	2.79	0.46
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	1.97	0.46
4:R:93:LEU:HG	12:Z:95:HIS:HE1	1.80	0.46
11:K:12:ILE:HG23	11:K:112:ILE:HD11	1.98	0.46
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.44	0.46
8:V:17:ASP:OD1	8:V:17:ASP:C	2.53	0.46
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.97	0.46
8:H:50:ALA:HB2	9:I:128:CYS:HB2	1.97	0.46
5:S:77:ALA:N	5:S:78:PRO:CD	2.79	0.46
7:G:43:VAL:HG11	7:G:194:VAL:HA	1.98	0.46
8:H:17:ASP:OD1	8:H:17:ASP:C	2.53	0.46
8:H:210:THR:HG21	9:I:167:SER:HB3	1.98	0.46
4:R:24:LYS:O	4:R:166:SER:HA	2.16	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.99	0.45
1:O:119:GLN:O	1:O:122:THR:HB	2.15	0.45
7:U:43:VAL:HG11	7:U:194:VAL:HA	1.97	0.45
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.99	0.45
14:N:41:ILE:HG21	14:N:78:ALA:CB	2.46	0.45
11:Y:12:ILE:HG23	11:Y:112:ILE:HD11	1.98	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.99	0.45
1:A:119:GLN:O	1:A:122:THR:HB	2.16	0.45
3:C:201:VAL:HG13	3:C:202:GLN:N	2.31	0.45
11:K:44:THR:O	11:K:99:THR:OG1	2.32	0.44
8:V:1:THR:HG22	8:V:2:THR:N	2.30	0.44
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.99	0.44
9:W:102:TYR:O	9:W:125:LEU:HD12	2.17	0.44
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.47	0.44
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.44
4:D:24:LYS:O	4:D:166:SER:HA	2.17	0.44
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.99	0.44
10:J:177:LYS:NZ	10:X:169:GLU:O	2.50	0.44
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.66	0.44
14:N:14:LEU:HD12	14:N:14:LEU:N	2.33	0.44
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.99	0.44
3:C:201:VAL:O	3:C:202:GLN:CB	2.66	0.44
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.47	0.44
11:Y:9:GLN:HE21	11:Y:9:GLN:HB3	1.66	0.44
5:E:9:THR:HG21	5:E:119:THR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.66	0.43
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.16	0.43
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.99	0.43
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.00	0.43
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.00	0.43
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.32	0.43
8:V:17:ASP:CG	8:V:33:LYS:HZ2	2.20	0.43
4:D:113:LEU:HD12	5:E:78:PRO:HB2	1.99	0.43
8:H:50:ALA:CB	9:I:126:ILE:CG2	2.94	0.43
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.52	0.43
8:H:137:VAL:HG21	8:H:161:ALA:HB2	1.99	0.43
1:O:149:GLN:O	1:O:156:TYR:HA	2.19	0.43
8:V:137:VAL:HG21	8:V:161:ALA:HB2	1.99	0.43
9:I:102:TYR:O	9:I:125:LEU:HD12	2.19	0.43
5:S:9:THR:HG21	5:S:119:THR:HA	2.00	0.43
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.01	0.43
2:B:134:PHE:O	2:B:149:THR:HA	2.18	0.43
2:P:50:LYS:O	2:P:51:VAL:C	2.57	0.43
11:Y:1:THR:HG23	11:Y:33:LYS:HZ3	1.75	0.43
11:Y:44:THR:OG1	11:Y:100:MET:N	2.49	0.43
8:V:30:ASN:HD21	8:V:188:ARG:NH2	2.16	0.43
11:Y:19:ARG:O	11:Y:33:LYS:NZ	2.51	0.43
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.99	0.43
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.00	0.43
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.00	0.43
10:J:118:GLN:HG2	10:J:133:HIS:HE1	1.84	0.43
2:P:95:GLN:HE21	9:W:68:TYR:HA	1.84	0.43
5:S:127:TYR:O	5:S:148:PRO:CB	2.67	0.43
3:C:160:GLN:HA	3:C:160:GLN:NE2	2.25	0.43
11:K:44:THR:OG1	11:K:100:MET:N	2.50	0.43
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.18	0.43
11:Y:41:LEU:HD23	11:Y:103:GLY:HA3	2.00	0.42
5:E:127:TYR:O	5:E:148:PRO:CB	2.67	0.42
11:K:46:ALA:HB3	11:K:98:GLY:O	2.20	0.42
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.17	0.42
5:S:62:ILE:HG21	5:S:213:ALA:HB2	2.01	0.42
2:B:148:TYR:OH	3:C:57:ILE:HB	2.20	0.42
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.00	0.42
11:Y:73:ARG:HH11	11:Y:73:ARG:CG	2.31	0.42
9:I:7:ASN:HA	9:I:29:GLY:O	2.19	0.42
7:U:34:LEU:C	7:U:34:LEU:HD23	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLN:O	1:A:156:TYR:HA	2.19	0.42
5:E:62:ILE:HG21	5:E:213:ALA:HB2	2.02	0.42
2:B:50:LYS:O	2:B:51:VAL:C	2.58	0.42
9:W:7:ASN:HA	9:W:29:GLY:O	2.20	0.42
8:V:222:ASP:OD1	9:W:74:LYS:NZ	2.53	0.42
5:E:127:TYR:O	5:E:148:PRO:HB2	2.20	0.42
8:H:29:LYS:NZ	9:I:150:GLU:OE2	2.52	0.42
11:K:41:LEU:HD23	11:K:103:GLY:HA3	2.01	0.42
4:R:158:ARG:O	5:S:57:SER:N	2.45	0.42
7:G:114:ASN:HD22	7:G:114:ASN:HA	1.74	0.42
10:J:75:LEU:HD12	10:J:75:LEU:HA	1.85	0.42
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.55	0.41
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.18	0.41
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.54	0.41
10:X:118:GLN:HG2	10:X:133:HIS:HE1	1.85	0.41
2:B:62:THR:HG22	19:B:301:HOH:O	2.20	0.41
4:R:99:ILE:HD11	4:R:104:LEU:HB2	2.02	0.41
3:C:35:LYS:HA	3:C:40:VAL:HA	2.03	0.41
10:J:169:GLU:O	10:X:177:LYS:NZ	2.53	0.41
7:G:34:LEU:C	7:G:34:LEU:HD23	2.41	0.41
10:J:3:ILE:HB	10:J:18:SER:HB3	2.03	0.41
5:S:38:ARG:NH1	5:S:39:SER:O	2.54	0.41
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.69	0.41
11:K:73:ARG:HH11	11:K:73:ARG:CG	2.32	0.41
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.69	0.41
3:Q:35:LYS:HA	3:Q:40:VAL:HA	2.03	0.41
8:V:210:THR:HG21	9:W:167:SER:CB	2.50	0.41
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	2.03	0.41
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.03	0.41
4:D:99:ILE:HD11	4:D:104:LEU:HB2	2.02	0.41
8:H:17:ASP:CG	8:H:33:LYS:HZ2	2.23	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.03	0.41
5:S:127:TYR:O	5:S:148:PRO:HB2	2.20	0.41
7:U:78:ILE:HG22	7:U:79:PRO:HD3	2.03	0.41
10:X:3:ILE:HB	10:X:18:SER:HB3	2.02	0.41
11:Y:99:THR:CG2	11:Y:115:VAL:O	2.69	0.41
6:F:216:SER:HB3	6:F:219:GLU:HB2	2.03	0.40
1:O:226:GLY:HA3	8:V:186:TYR:O	2.21	0.40
11:K:55:TRP:HE1	12:L:98:TYR:HH	1.69	0.40
14:N:14:LEU:HB3	14:N:34:LEU:HD22	2.03	0.40
2:P:134:PHE:O	2:P:149:THR:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:68:HIS:HE1	5:E:102:LEU:O	2.05	0.40
6:F:78:ILE:N	6:F:79:PRO:CD	2.85	0.40
10:J:118:GLN:CG	10:J:133:HIS:CE1	3.04	0.40
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.56	0.40
8:V:50:ALA:CB	9:W:126:ILE:CG2	2.94	0.40
11:Y:1:THR:CG2	11:Y:17:ASP:OD1	2.65	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%)	239 (96%)	9 (4%)	0	100	100
1	O	248/250 (99%)	239 (96%)	9 (4%)	0	100	100
2	B	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	34	69
2	P	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	34	69
3	C	238/254 (94%)	229 (96%)	6 (2%)	3 (1%)	12	47
3	Q	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	12	47
4	D	231/260 (89%)	224 (97%)	7 (3%)	0	100	100
4	R	231/260 (89%)	224 (97%)	7 (3%)	0	100	100
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	F	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
6	T	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
7	G	239/252 (95%)	232 (97%)	7 (3%)	0	100	100
7	U	239/252 (95%)	232 (97%)	7 (3%)	0	100	100
8	H	220/232 (95%)	216 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	V	220/232 (95%)	216 (98%)	4 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	29	67
10	X	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	29	67
11	K	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
12	Z	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
13	M	227/246 (92%)	218 (96%)	9 (4%)	0	100	100
13	a	227/246 (92%)	218 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
15	e	2/5 (40%)	2 (100%)	0	0	100	100
15	f	2/5 (40%)	2 (100%)	0	0	100	100
15	g	2/5 (40%)	2 (100%)	0	0	100	100
15	h	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6276/6634 (95%)	6090 (97%)	176 (3%)	10 (0%)	47	79

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
10	J	2	ASP
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
3	Q	239	GLN
3	C	205	ALA
3	C	239	GLN
3	Q	205	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	209/209 (100%)	204 (98%)	5 (2%)	49 77
1	O	209/209 (100%)	204 (98%)	5 (2%)	49 77
2	B	203/216 (94%)	195 (96%)	8 (4%)	32 67
2	P	203/216 (94%)	195 (96%)	8 (4%)	32 67
3	C	212/226 (94%)	204 (96%)	8 (4%)	33 67
3	Q	212/226 (94%)	204 (96%)	8 (4%)	33 67
4	D	194/215 (90%)	186 (96%)	8 (4%)	30 66
4	R	194/215 (90%)	186 (96%)	8 (4%)	30 66
5	E	190/193 (98%)	181 (95%)	9 (5%)	26 62
5	S	190/193 (98%)	182 (96%)	8 (4%)	30 65
6	F	201/239 (84%)	191 (95%)	10 (5%)	24 60
6	T	201/239 (84%)	191 (95%)	10 (5%)	24 60
7	G	206/210 (98%)	198 (96%)	8 (4%)	32 67
7	U	206/210 (98%)	197 (96%)	9 (4%)	28 64
8	H	181/190 (95%)	167 (92%)	14 (8%)	13 44
8	V	181/190 (95%)	168 (93%)	13 (7%)	14 47
9	I	172/173 (99%)	166 (96%)	6 (4%)	36 69
9	W	172/173 (99%)	166 (96%)	6 (4%)	36 69
10	J	173/175 (99%)	166 (96%)	7 (4%)	31 66
10	X	173/175 (99%)	166 (96%)	7 (4%)	31 66
11	K	169/169 (100%)	163 (96%)	6 (4%)	35 69
11	Y	169/169 (100%)	163 (96%)	6 (4%)	35 69
12	L	185/185 (100%)	178 (96%)	7 (4%)	33 67
12	Z	185/185 (100%)	178 (96%)	7 (4%)	33 67
13	M	195/208 (94%)	189 (97%)	6 (3%)	40 72
13	a	195/208 (94%)	189 (97%)	6 (3%)	40 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	160 (99%)	2 (1%)	71	88
14	b	162/162 (100%)	160 (99%)	2 (1%)	71	88
15	e	2/2 (100%)	2 (100%)	0	100	100
15	f	2/2 (100%)	2 (100%)	0	100	100
15	g	2/2 (100%)	2 (100%)	0	100	100
15	h	2/2 (100%)	2 (100%)	0	100	100
All	All	5312/5548 (96%)	5105 (96%)	207 (4%)	32	67

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	29	LYS
1	A	61	LEU
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	52	THR
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	114	LEU
2	B	184	LYS
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	203	THR
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	224	ASP
4	D	236	LYS
4	D	242	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	9	THR
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	9	ASN
8	H	13	VAL
8	H	17	ASP
8	H	18	THR
8	H	30	ASN
8	H	31	CYS
8	H	38	SER
8	H	43	CYS
8	H	53	GLU
8	H	59	ILE
8	H	84	LYS
8	H	113	ILE
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	I	97	ARG
9	I	125	LEU
9	I	126	ILE
9	I	171	LEU
9	I	182	TRP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	78	GLN
10	J	133	HIS
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	41	LEU
11	K	100	MET
11	K	106	ARG
11	K	118	ASP
12	L	1	GLN
12	L	23	LEU
12	L	34	SER
12	L	49	ASN
12	L	126	ASP
12	L	136	CYS
12	L	167	LYS
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	7	THR
14	N	9	LYS
1	O	17	LYS
1	O	29	LYS
1	O	61	LEU
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	52	THR
2	P	55	LEU
2	P	58	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	P	79	LEU
2	P	114	LEU
2	P	184	LYS
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	203	THR
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	224	ASP
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	14	ASP
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	125	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	U	154	TYR
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	9	ASN
8	V	17	ASP
8	V	18	THR
8	V	30	ASN
8	V	31	CYS
8	V	38	SER
8	V	43	CYS
8	V	53	GLU
8	V	59	ILE
8	V	84	LYS
8	V	113	ILE
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	97	ARG
9	W	125	LEU
9	W	126	ILE
9	W	171	LEU
9	W	182	TRP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	78	GLN
10	X	133	HIS
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	41	LEU
11	Y	100	MET
11	Y	106	ARG
11	Y	118	ASP
12	Z	1	GLN
12	Z	23	LEU
12	Z	34	SER
12	Z	49	ASN
12	Z	126	ASP

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Mol	Chain	Res	Type
12	Z	136	CYS
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	7	THR
14	b	9	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	160	ASN
4	D	198	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	147	GLN
5	E	151	ASN
5	E	184	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	175	ASN
8	H	172	ASN
10	J	55	GLN
10	J	118	GLN
10	J	133	HIS
10	J	146	HIS
10	J	191	GLN
11	K	9	GLN
11	K	85	ASN
11	K	143	ASN
11	K	176	ASN
11	K	179	HIS
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	165	ASN
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	60	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	160	ASN
4	R	198	GLN
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	147	GLN
5	S	151	ASN
5	S	184	ASN
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	175	ASN
8	V	172	ASN
9	W	71	ASN
10	X	55	GLN
10	X	118	GLN
10	X	133	HIS
10	X	146	HIS
10	X	147	HIS
10	X	191	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
11	Y	179	HIS
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN

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Mol	Chain	Res	Type
12	Z	70	ASN
12	Z	135	GLN
12	Z	159	GLN
12	Z	165	ASN
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	38	HIS
14	b	60	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](#)

4 non-standard protein/DNA/RNA residues 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	PPN	g	2	15	12,14,15	2.68	3 (25%)	13,18,20	1.16	1 (7%)
15	PPN	h	2	15	12,14,15	2.47	2 (16%)	13,18,20	1.85	4 (30%)
15	PPN	f	2	15	12,14,15	3.32	3 (25%)	13,18,20	1.63	3 (23%)
15	PPN	e	2	15	12,14,15	2.87	3 (25%)	13,18,20	1.02	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PPN	g	2	15	-	5/7/10/12	0/1/1/1
15	PPN	h	2	15	-	4/7/10/12	0/1/1/1
15	PPN	f	2	15	-	4/7/10/12	0/1/1/1
15	PPN	e	2	15	-	2/7/10/12	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	f	2	PPN	O1-N1	7.91	1.36	1.22
15	f	2	PPN	CB-CG	-6.08	1.36	1.51
15	g	2	PPN	CB-CG	-6.08	1.36	1.51
15	h	2	PPN	CB-CG	-5.90	1.37	1.51
15	e	2	PPN	CB-CG	-5.87	1.37	1.51
15	g	2	PPN	CZ-N1	-5.74	1.31	1.45
15	e	2	PPN	CZ-N1	-5.56	1.31	1.45
15	h	2	PPN	CZ-N1	-5.39	1.32	1.45
15	e	2	PPN	O1-N1	5.37	1.31	1.22
15	f	2	PPN	CZ-N1	-5.28	1.32	1.45
15	g	2	PPN	O1-N1	3.22	1.28	1.22

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	h	2	PPN	CB-CG-CD2	-3.75	113.47	120.91
15	f	2	PPN	CB-CG-CD2	-3.19	114.56	120.91
15	h	2	PPN	CB-CG-CD1	2.80	126.47	120.91
15	h	2	PPN	CG-CB-CA	2.67	119.51	114.10
15	f	2	PPN	CE1-CD1-CG	-2.49	117.60	121.03
15	h	2	PPN	CE1-CD1-CG	-2.38	117.75	121.03
15	g	2	PPN	CE1-CD1-CG	-2.13	118.10	121.03
15	f	2	PPN	CB-CA-C	2.03	115.28	111.47

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	e	2	PPN	CE1-CZ-N1-O1
15	e	2	PPN	CE2-CZ-N1-O1
15	f	2	PPN	CE1-CZ-N1-O1
15	f	2	PPN	CE2-CZ-N1-O1
15	g	2	PPN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
15	g	2	PPN	CE1-CZ-N1-O1
15	g	2	PPN	CE2-CZ-N1-O1
15	h	2	PPN	CE1-CZ-N1-O1
15	h	2	PPN	CE2-CZ-N1-O1
15	g	2	PPN	N-CA-CB-CG
15	f	2	PPN	CA-CB-CG-CD1
15	f	2	PPN	CA-CB-CG-CD2
15	h	2	PPN	CA-CB-CG-CD2
15	h	2	PPN	CA-CB-CG-CD1
15	g	2	PPN	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 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	$\# Z  > 2$
18	MES	K	301	-	12,12,12	0.84	0	14,16,16	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MES	K	301	-	-	2/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	K	301	MES	C8-C7-N4-C3
18	K	301	MES	C8-C7-N4-C5

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-0.35	2 (0%) 86 78	64, 84, 117, 167	0
1	O	250/250 (100%)	-0.20	3 (1%) 79 67	71, 92, 132, 162	0
2	B	244/258 (94%)	-0.10	3 (1%) 79 67	65, 92, 143, 194	0
2	P	244/258 (94%)	-0.13	3 (1%) 79 67	72, 91, 150, 173	0
3	C	240/254 (94%)	0.01	1 (0%) 92 89	67, 97, 146, 158	0
3	Q	240/254 (94%)	0.08	9 (3%) 40 26	76, 108, 167, 182	0
4	D	235/260 (90%)	-0.24	1 (0%) 92 89	66, 92, 120, 156	0
4	R	235/260 (90%)	-0.20	1 (0%) 92 89	71, 100, 138, 166	0
5	E	231/234 (98%)	-0.16	1 (0%) 92 89	70, 94, 121, 145	0
5	S	231/234 (98%)	0.01	7 (3%) 50 34	72, 104, 142, 175	0
6	F	243/288 (84%)	-0.33	0 100 100	64, 85, 126, 148	0
6	T	243/288 (84%)	-0.23	2 (0%) 86 78	68, 96, 135, 148	0
7	G	241/252 (95%)	-0.36	0 100 100	62, 81, 111, 142	0
7	U	241/252 (95%)	-0.28	0 100 100	64, 89, 116, 143	0
8	H	222/232 (95%)	-0.31	2 (0%) 84 75	65, 79, 105, 158	0
8	V	222/232 (95%)	-0.19	2 (0%) 84 75	72, 85, 108, 169	0
9	I	204/205 (99%)	-0.33	0 100 100	61, 78, 99, 128	0
9	W	204/205 (99%)	-0.36	0 100 100	60, 78, 101, 126	0
10	J	195/198 (98%)	-0.31	1 (0%) 91 86	62, 80, 106, 133	0
10	X	195/198 (98%)	-0.35	1 (0%) 91 86	64, 82, 105, 142	0
11	K	212/212 (100%)	-0.29	1 (0%) 91 86	61, 78, 103, 129	0
11	Y	212/212 (100%)	-0.36	0 100 100	68, 82, 110, 123	0
12	L	222/222 (100%)	-0.35	0 100 100	58, 79, 106, 117	0
12	Z	222/222 (100%)	-0.28	0 100 100	60, 80, 109, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	229/246 (93%)	-0.43	1 (0%) 92 89	59, 78, 99, 114	0
13	a	229/246 (93%)	-0.45	1 (0%) 92 89	61, 77, 100, 108	0
14	N	196/196 (100%)	-0.35	0 100 100	60, 75, 100, 124	0
14	b	196/196 (100%)	-0.19	0 100 100	65, 79, 105, 124	0
15	e	2/5 (40%)	-0.25	0 100 100	91, 91, 91, 92	0
15	f	2/5 (40%)	-0.99	0 100 100	74, 74, 74, 80	0
15	g	2/5 (40%)	-0.24	0 100 100	95, 95, 95, 96	0
15	h	2/5 (40%)	-0.95	0 100 100	80, 80, 80, 82	0
All	All	6336/6634 (95%)	-0.25	42 (0%) 87 81	58, 85, 129, 194	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	222	ASP	8.9
8	H	222	ASP	5.6
2	B	220	ASN	5.2
3	Q	50	LEU	4.3
3	Q	48	SER	4.2
5	S	233	ILE	4.2
3	Q	49	THR	3.9
8	H	221	CYS	3.7
5	S	202	ASP	3.6
1	O	250	LEU	3.5
10	J	1	MET	3.4
2	P	241	THR	3.3
8	V	221	CYS	3.2
10	X	1	MET	3.1
5	S	204	SER	3.0
3	Q	234	ILE	3.0
3	Q	204	GLY	3.0
3	Q	203	THR	2.9
13	a	1	THR	2.8
2	P	220	ASN	2.7
1	A	1	MET	2.7
3	Q	189	CYS	2.6
13	M	1	THR	2.6
5	S	229	VAL	2.6
6	T	2	THR	2.6
5	E	202	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
4	D	241	ALA	2.5
6	T	185	ALA	2.4
5	S	55	LEU	2.4
5	S	225	ASP	2.4
5	S	210	LEU	2.4
3	Q	206	LYS	2.3
1	A	250	LEU	2.3
2	B	221	ASP	2.3
2	P	219	ALA	2.2
11	K	212	GLY	2.1
1	O	249	ALA	2.1
3	Q	194	VAL	2.1
1	O	52	SER	2.0
4	R	241	ALA	2.0
2	B	240	LYS	2.0
3	C	231	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
15	PPN	g	2	14/15	0.90	0.27	97,108,115,116	0
15	PPN	e	2	14/15	0.91	0.30	101,103,114,118	0
15	PPN	h	2	14/15	0.91	0.24	85,91,112,117	0
15	PPN	f	2	14/15	0.92	0.21	80,88,106,115	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
16	MG	G	301	1/1	0.86	0.06	74,74,74,74	0
16	MG	I	301	1/1	0.87	0.56	83,83,83,83	0
17	CL	G	302	1/1	0.88	0.12	67,67,67,67	0
18	MES	K	301	12/12	0.89	0.27	101,113,120,125	0
17	CL	U	301	1/1	0.93	0.14	88,88,88,88	0
16	MG	Z	301	1/1	0.94	0.21	98,98,98,98	0
16	MG	X	201	1/1	0.94	0.24	64,64,64,64	0
16	MG	K	302	1/1	0.96	0.20	100,100,100,100	0
16	MG	N	201	1/1	0.97	0.18	68,68,68,68	0
16	MG	V	301	1/1	0.98	0.16	104,104,104,104	0
16	MG	Y	301	1/1	0.99	0.07	90,90,90,90	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.