



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 5, 2016 – 12:49 PM EST

PDB ID : 5L69
Title : Yeast 20S proteasome with mouse beta5i (1-138) and mouse beta6 (97-111; 118-133) in complex with epoxyketone inhibitor 16
Authors : Groll, M.; Huber, E.M.
Deposited on : 2016-05-28
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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

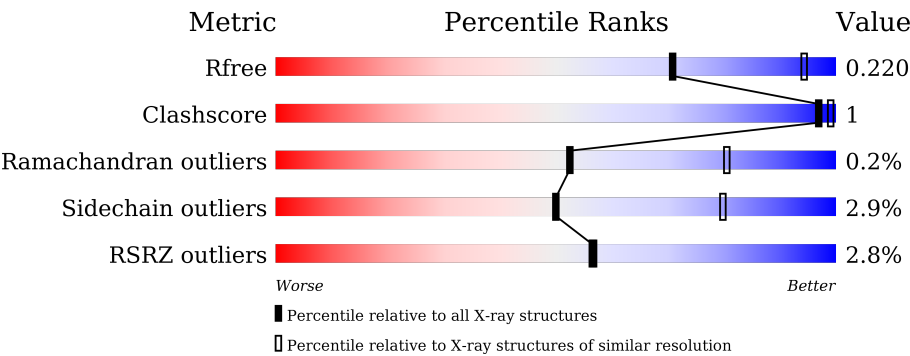
1 Overall quality at a glance i

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	<div><div>2%</div><div><div></div><div>97%</div><div></div></div><div></div></div>
1	O	250	<div><div>2%</div><div><div></div><div>98%</div><div></div></div><div></div></div>
2	B	258	<div><div>3%</div><div><div></div><div>89%</div><div></div></div><div>5% 5%</div></div>
2	P	258	<div><div>3%</div><div><div></div><div>88%</div><div></div></div><div>6% 5%</div></div>
3	C	254	<div><div>7%</div><div><div></div><div>87%</div><div></div></div><div>6% • 6%</div></div>
3	Q	254	<div><div>10%</div><div><div></div><div>87%</div><div></div></div><div>7% • 6%</div></div>

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Mol	Chain	Length	Quality of chain
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	211	
11	Y	211	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MG	Z	301	-	-	-	X
17	79P	H	301	-	-	-	X
17	79P	V	301	-	-	-	X
18	MES	K	303	-	-	-	X
18	MES	Y	302	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49884 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			

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

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

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

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

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

- Molecule 11 is a protein called Proteasome subunit beta type-8,Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1645	1039	281	313	12			
11	Y	211	Total	C	N	O	S	0	0	0
			1645	1039	281	313	12			

- Molecule 12 is a protein called Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	1	0
			1832	1159	315	351	7			

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

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

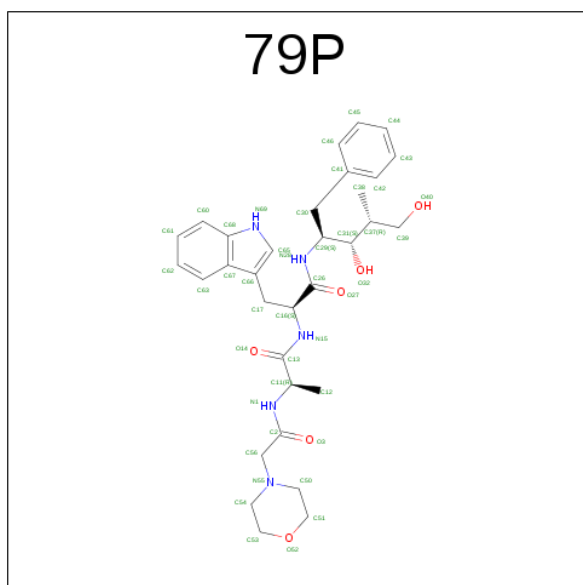
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	J	1	Total Mg 1 1	0	0
15	K	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0
15	Z	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

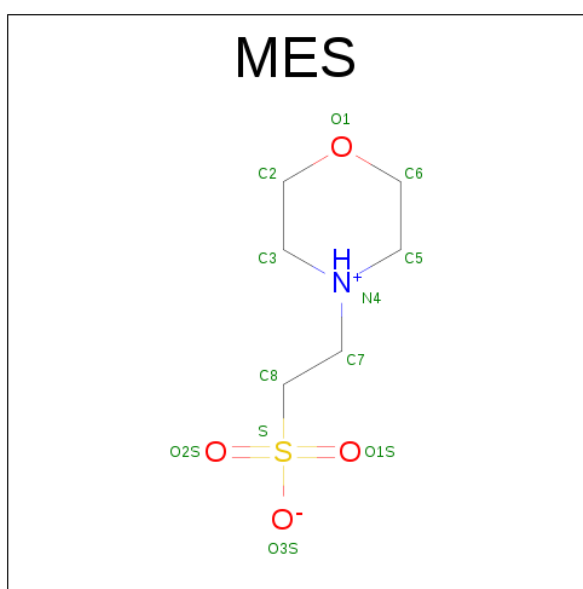
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	2	Total Cl 2 2	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is (2 {S})-3-(1 {H}-indol-3-yl)- {N}-[(2 {S},3 {S},4 {R})-4-methyl-3,5-bis(oxidanyl)-1-phenyl-pentan-2-yl]-2-[[(2 {R})-2-(2-morpholin-4-ylethanoylamino)propanoyl]amino]propanamide (three-letter code: 79P) (formula: C₃₂H₄₃N₅O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			43	32	5	6		
17	K	1	Total	C	N	O	0	0
			43	32	5	6		
17	V	1	Total	C	N	O	0	0
			43	32	5	6		
17	Y	1	Total	C	N	O	0	0
			43	32	5	6		

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	11	Total	O	0	0
			11	11		
19	B	14	Total	O	0	0
			14	14		
19	C	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	D	4	Total O 4 4	0	0
19	E	14	Total O 14 14	0	0
19	F	10	Total O 10 10	0	0
19	G	11	Total O 11 11	0	0
19	H	15	Total O 15 15	0	0
19	I	3	Total O 3 3	0	0
19	J	9	Total O 9 9	0	0
19	K	10	Total O 10 10	0	0
19	L	15	Total O 15 15	0	0
19	M	26	Total O 26 26	0	0
19	N	10	Total O 10 10	0	0
19	O	9	Total O 9 9	0	0
19	P	9	Total O 9 9	0	0
19	Q	4	Total O 4 4	0	0
19	R	5	Total O 5 5	0	0
19	S	7	Total O 7 7	0	0
19	T	6	Total O 6 6	0	0
19	U	12	Total O 12 12	0	0
19	V	13	Total O 13 13	0	0
19	W	8	Total O 8 8	0	0
19	X	9	Total O 9 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	Y	6	Total 6	O 6	0	0
19	Z	11	Total 11	O 11	0	0
19	a	17	Total 17	O 17	0	0
19	b	12	Total 12	O 12	0	0

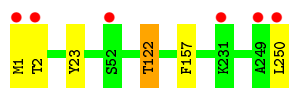
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Proteasome subunit alpha type-2



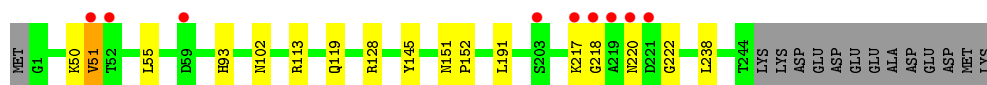
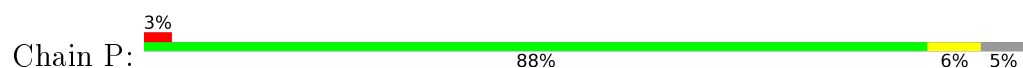
- Molecule 1: Proteasome subunit alpha type-2



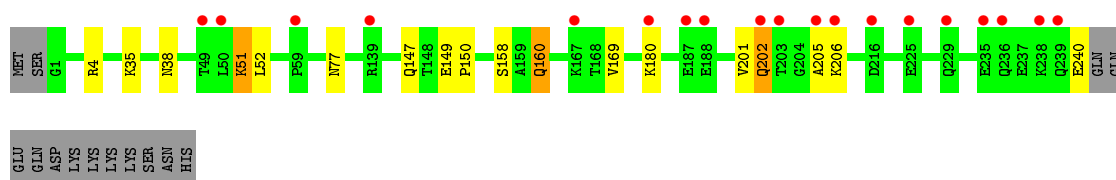
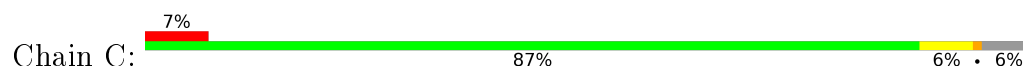
- Molecule 2: Proteasome subunit alpha type-3



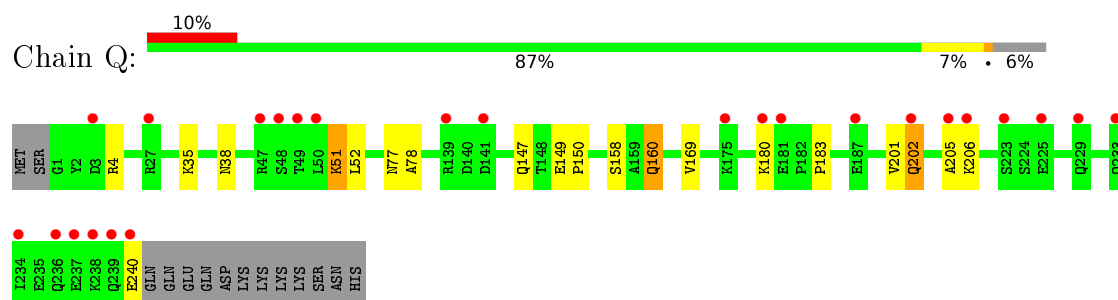
- Molecule 2: Proteasome subunit alpha type-3



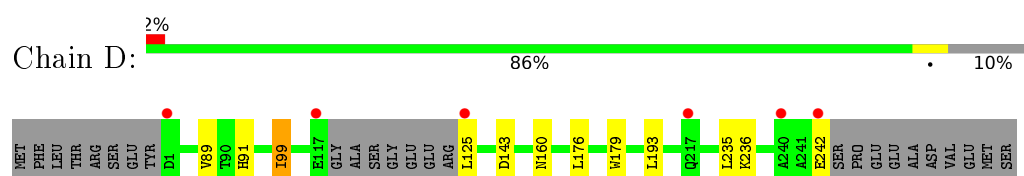
- Molecule 3: Proteasome subunit alpha type-4



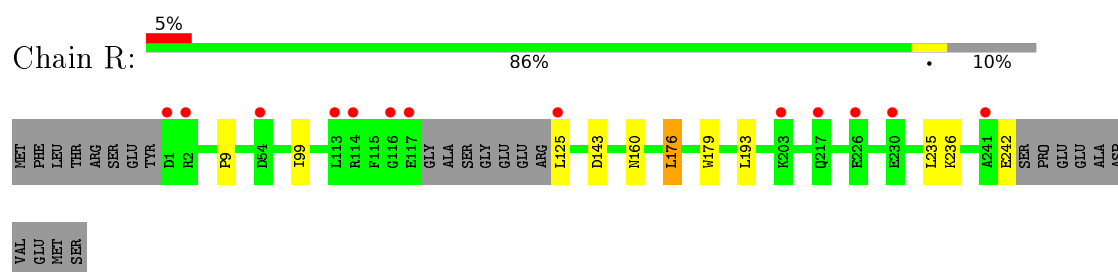
- Molecule 3: Proteasome subunit alpha type-4



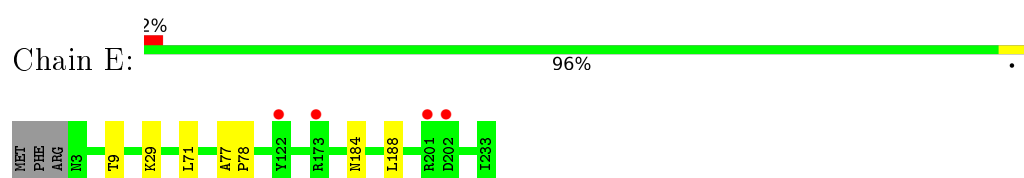
- Molecule 4: Proteasome subunit alpha type-5



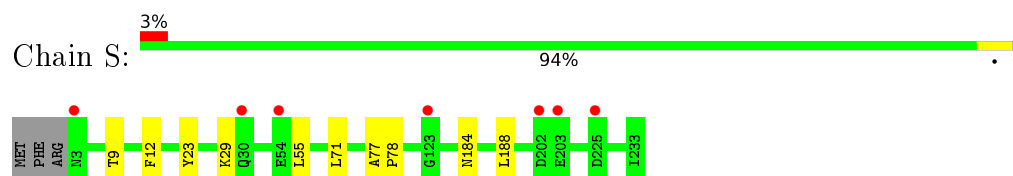
- Molecule 4: Proteasome subunit alpha type-5



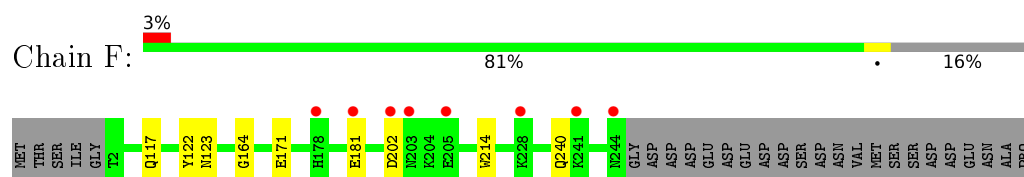
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 5: Proteasome subunit alpha type-6

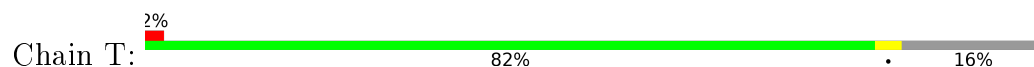


- Molecule 6: Probable proteasome subunit alpha type-7



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

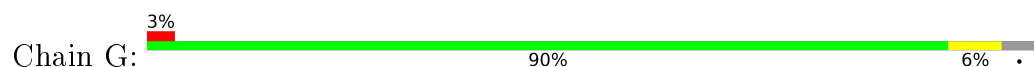
- Molecule 6: Probable proteasome subunit alpha type-7



MET THR SER ILE GLY T2 Q19 Q117 Y122 M123 E171 H178 H179 P180 E181 E205 W214 Q240 N244 GLY ASP ASP ASP ASP ASP ASP ASP SER ASP ASP ASP VAL MET SER SER ASP ASP GLU ASP ASN ALA PRO VAL ALA THR ASN ALA THR ASP

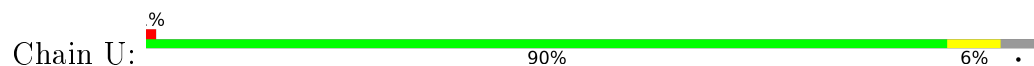
GLN
GLU
GLY
ASP
ILE
HIS
LEU
GLU

- Molecule 7: Proteasome subunit alpha type-1



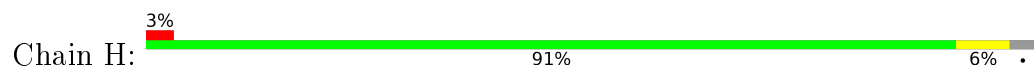
MET SER GLY ALA ALA ALA SER ALA G2 Y3 P12 F23 T26 R66 I78 P79 N83 L115 S116 Q117 R122 M125 D149 P150 E188 E208 E230 R235 A240 E241 Q242 ASP

- Molecule 7: Proteasome subunit alpha type-1



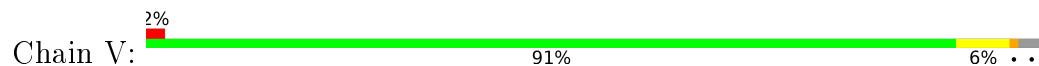
MET SER GLY ALA ALA ALA SER ALA G2 P12 F23 T26 I78 P79 N83 L115 S116 Q117 R122 M125 D149 P150 E188 D203 E208 R235 Q242 ASP

- Molecule 8: Proteasome subunit beta type-2



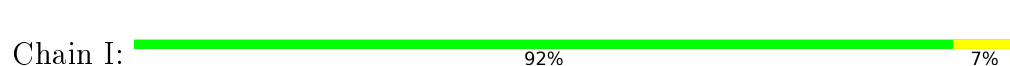
T1 T2 I3 A16 N30 H35 A50 V55 T56 L68 D104 P105 K153 R196 E215 N219 I220 C221 D222 I223 Q224 E225 E226 GLN VAL ASP ILE THR ALA

- Molecule 8: Proteasome subunit beta type-2



T1 T2 I3 N30 H35 A44 G45 A46 A50 V55 T56 L68 D104 P105 E139 K153 R196 C221 D222 I223 Q224 E225 E226 GLN VAL ASP ILE THR ALA

- Molecule 9: Proteasome subunit beta type-3



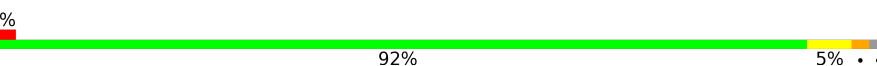
MET S1 G9 I10 V20 L26 N37 K38 K41 P118 I126 A141 E150 L171 W182 V185 I189 D204

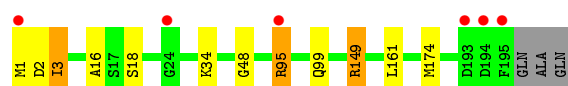
- Molecule 9: Proteasome subunit beta type-3

Chain W:  92% 7%

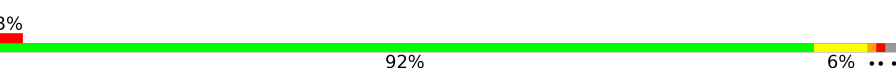


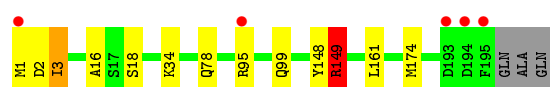
- Molecule 10: Proteasome subunit beta type-4

Chain J:  92% 5% 3%



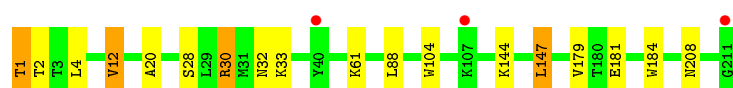
- Molecule 10: Proteasome subunit beta type-4

Chain X:  92% 6% 3%



- Molecule 11: Proteasome subunit beta type-8,Proteasome subunit beta type-5

Chain K:  91% 7% 2%



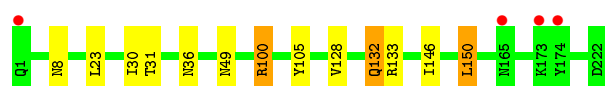
- Molecule 11: Proteasome subunit beta type-8,Proteasome subunit beta type-5

Chain Y:  92% 6% 2%

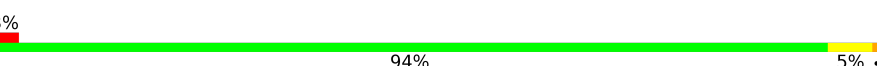


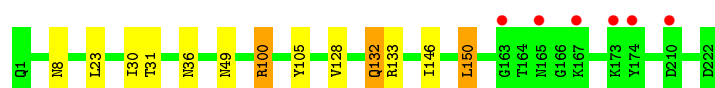
- Molecule 12: Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6

Chain L:  94% 5% 2%

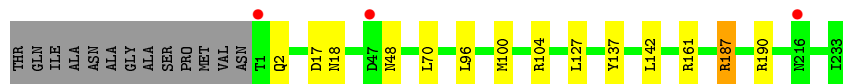
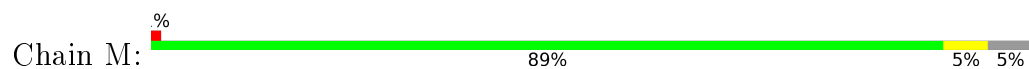


- Molecule 12: Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6

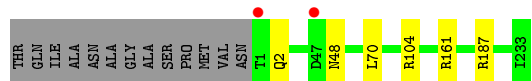
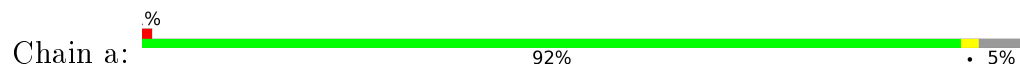
Chain Z:  94% 5% 3%



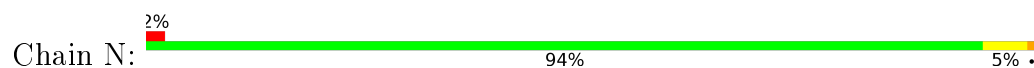
- Molecule 13: Proteasome subunit beta type-7



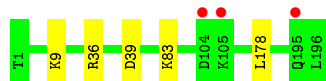
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.40 Å 298.56 Å 146.17 Å 90.00° 112.41° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.4 (15.00-2.70) 97.4 (15.00-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.69 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.192 , 0.217 0.196 , 0.220	Depositor DCC
R_{free} test set	14168 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49884	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, 79P, MES, CL

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	0.27	0/1952	0.47	0/2642
1	O	0.27	0/1952	0.47	0/2642
2	B	0.27	0/1934	0.49	0/2618
2	P	0.27	0/1934	0.48	0/2618
3	C	0.28	0/1910	0.50	0/2586
3	Q	0.28	0/1910	0.50	0/2586
4	D	0.27	0/1837	0.46	0/2475
4	R	0.26	0/1837	0.46	0/2475
5	E	0.27	0/1800	0.46	0/2433
5	S	0.27	0/1800	0.46	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.46	0/2634
7	U	0.27	0/1945	0.46	0/2634
8	H	0.27	0/1750	0.50	0/2373
8	V	0.28	0/1750	0.51	0/2373
9	I	0.27	0/1611	0.51	0/2174
9	W	0.27	0/1611	0.51	0/2174
10	J	0.27	0/1589	0.97	6/2142 (0.3%)
10	X	0.27	0/1589	0.96	6/2142 (0.3%)
11	K	0.32	1/1681 (0.1%)	0.53	1/2268 (0.0%)
11	Y	0.31	0/1681	0.53	1/2268 (0.0%)
12	L	0.28	0/1802	0.78	3/2430 (0.1%)
12	Z	0.27	0/1802	0.77	3/2430 (0.1%)
13	M	0.27	0/1855	0.51	0/2514
13	a	0.27	0/1866	0.51	0/2528
14	N	0.26	0/1541	0.48	0/2087
14	b	0.25	0/1541	0.48	0/2087
All	All	0.27	1/50289 (0.0%)	0.55	20/67984 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	2
10	X	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	32	ASN	CG-ND2	-5.68	1.18	1.32

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	100	ARG	NE-CZ-NH1	-20.68	109.96	120.30
10	J	95	ARG	NE-CZ-NH2	-20.21	110.20	120.30
10	X	149	ARG	NE-CZ-NH2	-20.17	110.21	120.30
12	Z	100	ARG	NE-CZ-NH2	-20.09	110.25	120.30
10	J	149	ARG	NE-CZ-NH1	-19.92	110.34	120.30
10	X	95	ARG	NE-CZ-NH1	-19.58	110.51	120.30
12	Z	100	ARG	NE-CZ-NH1	19.47	130.04	120.30
12	L	100	ARG	NE-CZ-NH2	19.46	130.03	120.30
10	J	149	ARG	NE-CZ-NH2	16.47	128.53	120.30
10	X	95	ARG	NE-CZ-NH2	16.39	128.50	120.30
10	J	95	ARG	NE-CZ-NH1	15.68	128.14	120.30
10	X	149	ARG	NE-CZ-NH1	15.18	127.89	120.30
10	J	149	ARG	CD-NE-CZ	9.63	137.09	123.60
10	X	149	ARG	CD-NE-CZ	9.59	137.02	123.60
12	L	100	ARG	CD-NE-CZ	9.45	136.82	123.60
10	J	95	ARG	CD-NE-CZ	9.44	136.82	123.60
12	Z	100	ARG	CD-NE-CZ	9.12	136.36	123.60
10	X	95	ARG	CD-NE-CZ	9.07	136.30	123.60
11	Y	1	THR	N-CA-C	5.21	125.06	111.00
11	K	1	THR	N-CA-C	5.13	124.84	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	149	ARG	Sidechain

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Mol	Chain	Res	Type	Group
10	J	95	ARG	Sidechain
10	X	149	ARG	Sidechain

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	3	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	4	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	5	0
6	F	1892	0	1883	2	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	4	0
8	H	1719	0	1716	7	0
8	V	1719	0	1716	10	0
9	I	1581	0	1574	9	0
9	W	1581	0	1574	8	0
10	J	1561	0	1569	4	0
10	X	1561	0	1569	5	0
11	K	1645	0	1589	12	0
11	Y	1645	0	1589	11	0
12	L	1764	0	1716	7	0
12	Z	1764	0	1716	6	0
13	M	1824	0	1832	5	0
13	a	1832	0	1845	0	0
14	N	1512	0	1481	4	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	2	0	0	0	0
16	U	1	0	0	0	0
17	H	43	0	0	1	0
17	K	43	0	0	2	0
17	V	43	0	0	0	0
17	Y	43	0	0	2	0
18	K	12	0	13	0	0
18	Y	12	0	13	0	0
19	A	11	0	0	0	0
19	B	14	0	0	1	0
19	C	7	0	0	0	0
19	D	4	0	0	0	0
19	E	14	0	0	0	0
19	F	10	0	0	0	0
19	G	11	0	0	0	0
19	H	15	0	0	0	0
19	I	3	0	0	0	0
19	J	9	0	0	0	0
19	K	10	0	0	0	0
19	L	15	0	0	0	0
19	M	26	0	0	0	0
19	N	10	0	0	0	0
19	O	9	0	0	0	0
19	P	9	0	0	1	0
19	Q	4	0	0	0	0
19	R	5	0	0	0	0
19	S	7	0	0	0	0
19	T	6	0	0	0	0
19	U	12	0	0	0	0
19	V	13	0	0	0	0
19	W	8	0	0	0	0
19	X	9	0	0	0	0
19	Y	6	0	0	0	0
19	Z	11	0	0	0	0
19	a	17	0	0	0	0
19	b	12	0	0	0	0
All	All	49884	0	49161	122	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 1.

All (122) 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:K:30:ARG:O	12:L:132:GLN:NE2	2.14	0.80
11:Y:30:ARG:O	12:Z:132:GLN:NE2	2.27	0.67
11:K:33:LYS:HE2	17:K:301:79P:C46	2.28	0.64
14:N:152:VAL:HA	14:N:175:MET:HE1	1.80	0.63
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.83	0.61
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.82	0.60
8:H:50:ALA:HB3	9:I:126:ILE:HD12	1.85	0.58
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.86	0.58
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.85	0.57
11:K:208:ASN:O	9:W:38:LYS:NZ	2.38	0.56
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.40	0.55
7:U:23:PHE:O	7:U:26:THR:HB	2.08	0.54
8:V:196:ARG:NH2	9:W:150:GLU:O	2.41	0.53
7:G:23:PHE:O	7:G:26:THR:HB	2.09	0.53
8:H:3:ILE:HG22	8:H:16:ALA:HB2	1.91	0.52
11:Y:33:LYS:HE2	17:Y:301:79P:C46	2.40	0.52
8:V:3:ILE:HG21	8:V:44:ALA:HB1	1.92	0.52
4:R:9:PRO:HA	5:S:23:TYR:CD1	2.46	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.51
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.42	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.50
8:V:3:ILE:HG21	8:V:44:ALA:CB	2.41	0.50
2:B:93:HIS:HB3	19:B:301:HOH:O	2.12	0.50
4:D:89:VAL:HG12	11:K:61:LYS:HG3	1.92	0.49
8:V:50:ALA:HB3	9:W:126:ILE:HD12	1.94	0.49
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.93	0.49
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.47	0.49
2:P:93:HIS:HB3	19:P:301:HOH:O	2.12	0.49
11:K:1:THR:HG22	11:K:2:THR:N	2.27	0.48
8:H:196:ARG:NH2	9:I:150:GLU:O	2.46	0.48
11:K:144:LYS:HB2	11:K:147:LEU:HD13	1.96	0.48
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.48	0.48
11:Y:144:LYS:HB2	11:Y:147:LEU:HD13	1.96	0.48
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.96	0.47
4:R:176:LEU:HA	5:S:55:LEU:HD21	1.97	0.47
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.97	0.46
11:K:33:LYS:HE2	17:K:301:79P:C41	2.46	0.46
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:1:THR:HG22	11:Y:2:THR:N	2.31	0.46
3:C:201:VAL:O	3:C:202:GLN:HB3	2.16	0.46
1:A:23:TYR:CD1	7:G:12:PRO:HA	2.51	0.46
12:L:8:ASN:HA	12:L:30:ILE:O	2.16	0.46
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.79	0.46
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.98	0.46
17:H:301:79P:N28	17:H:301:79P:O40	2.49	0.46
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.98	0.46
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.80	0.46
2:P:50:LYS:O	2:P:51:VAL:C	2.55	0.45
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.99	0.45
2:B:50:LYS:O	2:B:51:VAL:C	2.54	0.45
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.98	0.45
12:L:100:ARG:HD2	12:L:105:TYR:CZ	2.51	0.45
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.98	0.45
3:C:51:LYS:O	3:C:52:LEU:HB2	2.17	0.45
2:P:102:ASN:HB3	10:X:78:GLN:HE22	1.82	0.45
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.16	0.44
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.98	0.44
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.81	0.44
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.98	0.44
8:V:3:ILE:HD11	8:V:46:ALA:HB2	1.99	0.44
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.98	0.44
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.17	0.44
6:F:164:GLY:HA2	6:F:202:ASP:OD2	2.18	0.44
11:Y:104:TRP:CE2	11:Y:181:GLU:HB3	2.53	0.43
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.00	0.43
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.00	0.43
11:K:104:TRP:CE2	11:K:181:GLU:HB3	2.53	0.43
8:V:1:THR:HG22	8:V:2:THR:N	2.31	0.43
11:Y:20:ALA:HB3	11:Y:28:SER:HB3	2.00	0.43
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.00	0.43
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.19	0.43
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.00	0.43
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.43	0.43
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.00	0.43
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.01	0.43
11:Y:33:LYS:HE2	17:Y:301:79P:C41	2.49	0.43
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.84	0.43
14:N:35:THR:HG21	14:N:45:ARG:HE	1.84	0.42
11:K:20:ALA:HB3	11:K:28:SER:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:100:ARG:HD3	12:Z:105:TYR:CE2	2.54	0.42
8:H:1:THR:HG22	8:H:2:THR:N	2.35	0.42
9:I:26:LEU:HD21	9:I:185:VAL:HG23	2.01	0.42
2:P:145:TYR:OH	2:P:217:LYS:N	2.53	0.42
3:C:35:LYS:HG2	3:C:158:SER:O	2.19	0.42
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.55	0.42
2:B:145:TYR:OH	2:B:217:LYS:N	2.53	0.42
13:M:96:LEU:O	13:M:100:MET:HG2	2.20	0.42
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.84	0.42
12:L:36:ASN:HB3	13:M:137:TYR:CD1	2.55	0.42
2:P:119:GLN:CG	3:Q:78:ALA:HB1	2.49	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.41
12:L:132:GLN:HG3	12:L:133:ARG:N	2.34	0.41
8:V:35:HIS:CB	8:V:56:THR:HG21	2.50	0.41
11:Y:1:THR:CG2	11:Y:2:THR:N	2.82	0.41
12:Z:132:GLN:HG3	12:Z:133:ARG:N	2.35	0.41
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.03	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
11:Y:179:VAL:HA	11:Y:184:TRP:HA	2.03	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.02	0.41
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.34	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.41
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.55	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
11:K:1:THR:CG2	11:K:2:THR:N	2.83	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.03	0.41
13:M:17:ASP:OD1	13:M:18:ASN:N	2.53	0.41
4:R:9:PRO:HA	5:S:23:TYR:CG	2.56	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.03	0.41
11:K:179:VAL:HA	11:K:184:TRP:HA	2.03	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.40
11:K:12:VAL:HG13	11:K:179:VAL:HB	2.02	0.40
1:A:115:ALA:HB1	1:A:154:GLY:O	2.21	0.40
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.04	0.40
10:X:148:TYR:O	10:X:149:ARG:HD3	2.21	0.40
10:J:1:MET:N	10:J:48:GLY:O	2.54	0.40
5:S:12:PHE:H	6:T:19:GLN:HE22	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.52	0.40
11:Y:12:VAL:HG13	11:Y:179:VAL:HB	2.02	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%)	8 (3%)	1 (0%)	39	69
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	39	69
2	B	242/258 (94%)	232 (96%)	6 (2%)	4 (2%)	11	29
2	P	242/258 (94%)	232 (96%)	6 (2%)	4 (2%)	11	29
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	24	51
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	15	37
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	209/211 (99%)	204 (98%)	5 (2%)	0	100	100
11	Y	209/211 (99%)	204 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
13	a	232/246 (94%)	223 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6283/6612 (95%)	6125 (98%)	143 (2%)	15 (0%)	52	80

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
2	B	222	GLY
1	O	2	THR
2	P	218	GLY
2	P	222	GLY
3	C	205	ALA
3	Q	205	ALA
2	B	220	ASN
2	P	220	ASN
3	Q	183	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	74	92
1	O	209/209 (100%)	206 (99%)	3 (1%)	74	92
2	B	203/216 (94%)	199 (98%)	4 (2%)	63	87
2	P	203/216 (94%)	199 (98%)	4 (2%)	63	87
3	C	212/226 (94%)	202 (95%)	10 (5%)	32	63
3	Q	212/226 (94%)	202 (95%)	10 (5%)	32	63
4	D	194/215 (90%)	186 (96%)	8 (4%)	37	69
4	R	194/215 (90%)	186 (96%)	8 (4%)	37	69
5	E	190/193 (98%)	185 (97%)	5 (3%)	54	83
5	S	190/193 (98%)	185 (97%)	5 (3%)	54	83
6	F	201/239 (84%)	195 (97%)	6 (3%)	48	79
6	T	201/239 (84%)	195 (97%)	6 (3%)	48	79
7	G	206/210 (98%)	199 (97%)	7 (3%)	44	75
7	U	206/210 (98%)	199 (97%)	7 (3%)	44	75
8	H	185/190 (97%)	180 (97%)	5 (3%)	52	82
8	V	185/190 (97%)	179 (97%)	6 (3%)	46	77
9	I	172/173 (99%)	169 (98%)	3 (2%)	68	90
9	W	172/173 (99%)	169 (98%)	3 (2%)	68	90
10	J	173/175 (99%)	169 (98%)	4 (2%)	58	85
10	X	173/175 (99%)	169 (98%)	4 (2%)	58	85
11	K	172/172 (100%)	167 (97%)	5 (3%)	50	80
11	Y	172/172 (100%)	168 (98%)	4 (2%)	58	85
12	L	186/186 (100%)	181 (97%)	5 (3%)	52	82
12	Z	186/186 (100%)	181 (97%)	5 (3%)	52	82
13	M	199/208 (96%)	192 (96%)	7 (4%)	43	74
13	a	200/208 (96%)	194 (97%)	6 (3%)	48	79
14	N	162/162 (100%)	157 (97%)	5 (3%)	47	78
14	b	162/162 (100%)	157 (97%)	5 (3%)	47	78
All	All	5329/5548 (96%)	5176 (97%)	153 (3%)	50	80

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	55	LEU
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
6	F	117	GLN
6	F	123	ASN
6	F	171	GLU
6	F	181	GLU
6	F	214	TRP
6	F	240	GLN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG

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Mol	Chain	Res	Type
8	H	30	ASN
8	H	55	VAL
8	H	68	LEU
8	H	153	LYS
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	2	ASP
10	J	3	ILE
10	J	99	GLN
10	J	174	MET
11	K	4	LEU
11	K	12	VAL
11	K	30	ARG
11	K	88	LEU
11	K	147	LEU
12	L	23	LEU
12	L	49	ASN
12	L	128	VAL
12	L	132	GLN
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	190	ARG
14	N	9	LYS
14	N	36	ARG
14	N	39	ASP
14	N	83	LYS
14	N	178	LEU
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	55	LEU
2	P	113	ARG
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG

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Mol	Chain	Res	Type
3	Q	38	ASN
3	Q	51	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
6	T	117	GLN
6	T	123	ASN
6	T	171	GLU
6	T	181	GLU
6	T	214	TRP
6	T	240	GLN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
8	V	3	ILE
8	V	30	ASN
8	V	55	VAL
8	V	68	LEU
8	V	153	LYS
8	V	196	ARG
9	W	37	ASN

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Mol	Chain	Res	Type
9	W	171	LEU
9	W	182	TRP
10	X	2	ASP
10	X	3	ILE
10	X	99	GLN
10	X	174	MET
11	Y	4	LEU
11	Y	12	VAL
11	Y	88	LEU
11	Y	147	LEU
12	Z	23	LEU
12	Z	49	ASN
12	Z	128	VAL
12	Z	132	GLN
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	36	ARG
14	b	39	ASP
14	b	83	LYS
14	b	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
3	C	17	GLN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN

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Mol	Chain	Res	Type
4	D	91	HIS
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
11	K	175	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	109	ASN
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	194	ASN
13	M	213	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	91	HIS
4	R	225	ASN

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Mol	Chain	Res	Type
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
8	V	66	HIS
8	V	165	ASN
10	X	78	GLN
11	Y	175	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	109	ASN
13	a	48	ASN
13	a	102	GLN
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 11 are monoatomic - leaving 6 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
17	79P	H	301	8	45,46,46	1.61	7 (15%)	50,62,62	1.69	7 (14%)
17	79P	K	301	11	45,46,46	1.79	8 (17%)	50,62,62	1.59	7 (14%)
18	MES	K	303	-	12,12,12	2.19	1 (8%)	15,16,16	2.65	5 (33%)
17	79P	V	301	8	45,46,46	1.57	7 (15%)	50,62,62	1.71	8 (16%)
17	79P	Y	301	11	45,46,46	1.76	8 (17%)	50,62,62	1.66	7 (14%)
18	MES	Y	302	-	12,12,12	2.18	1 (8%)	15,16,16	1.79	3 (20%)

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
17	79P	H	301	8	-	0/41/50/50	0/4/4/4
17	79P	K	301	11	-	0/41/50/50	0/4/4/4
18	MES	K	303	-	-	0/6/14/14	0/1/1/1
17	79P	V	301	8	-	0/41/50/50	0/4/4/4
17	79P	Y	301	11	-	0/41/50/50	0/4/4/4
18	MES	Y	302	-	-	0/6/14/14	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	303	MES	C8-S	-7.43	1.66	1.77
18	Y	302	MES	C8-S	-7.24	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	301	79P	C60-C68	-5.55	1.31	1.41
17	K	301	79P	C63-C67	-5.43	1.31	1.42
17	Y	301	79P	C60-C68	-5.39	1.32	1.41
17	H	301	79P	C60-C68	-5.26	1.32	1.41
17	K	301	79P	C30-C41	-5.13	1.38	1.51
17	Y	301	79P	C63-C67	-5.09	1.31	1.42
17	V	301	79P	C60-C68	-4.93	1.32	1.41
17	Y	301	79P	C30-C41	-4.86	1.39	1.51
17	H	301	79P	C30-C41	-4.85	1.39	1.51
17	V	301	79P	C30-C41	-4.82	1.39	1.51
17	V	301	79P	C63-C67	-4.66	1.32	1.42
17	H	301	79P	C63-C67	-4.56	1.33	1.42
17	Y	301	79P	C67-C68	-4.42	1.30	1.42
17	K	301	79P	C67-C68	-4.25	1.31	1.42
17	H	301	79P	C67-C68	-3.59	1.33	1.42
17	V	301	79P	C67-C68	-3.42	1.33	1.42
17	Y	301	79P	C65-N69	-2.77	1.30	1.36
17	K	301	79P	O32-C31	-2.36	1.37	1.43
17	Y	301	79P	C68-N69	-2.31	1.31	1.38
17	K	301	79P	C65-N69	-2.22	1.32	1.36
17	K	301	79P	C68-N69	-2.20	1.31	1.38
17	K	301	79P	C65-C66	-2.20	1.31	1.37
17	H	301	79P	C68-N69	-2.17	1.31	1.38
17	Y	301	79P	C65-C66	-2.13	1.31	1.37
17	H	301	79P	C65-C66	-2.08	1.31	1.37
17	V	301	79P	C68-N69	-2.05	1.32	1.38
17	V	301	79P	C65-N69	-2.04	1.32	1.36
17	Y	301	79P	C37-C31	2.13	1.57	1.53
17	V	301	79P	C39-C37	2.16	1.55	1.52
17	H	301	79P	C37-C31	2.35	1.58	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	301	79P	C30-C29-N28	-8.38	100.90	110.17
17	V	301	79P	C30-C29-N28	-7.11	102.31	110.17
17	Y	301	79P	C30-C29-N28	-6.90	102.53	110.17
17	K	301	79P	C30-C29-N28	-6.10	103.42	110.17
17	V	301	79P	C56-N55-C50	-3.58	105.88	111.14
17	H	301	79P	C38-C37-C39	-3.08	105.68	109.73
17	V	301	79P	C56-N55-C54	-3.07	106.63	111.14
17	H	301	79P	C17-C66-C65	-2.99	124.28	127.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	301	79P	C17-C66-C65	-2.95	124.32	127.97
17	K	301	79P	C13-C11-N1	-2.94	104.25	111.63
17	Y	301	79P	C56-N55-C50	-2.85	106.95	111.14
18	K	303	MES	O2S-S-O1S	-2.63	106.53	113.96
17	K	301	79P	C56-N55-C50	-2.37	107.66	111.14
17	K	301	79P	O52-C51-C50	-2.36	106.39	111.83
17	Y	301	79P	C17-C66-C65	-2.34	125.07	127.97
17	Y	301	79P	C13-C11-N1	-2.30	105.86	111.63
17	Y	301	79P	O52-C53-C54	-2.20	106.75	111.83
18	K	303	MES	O1-C2-C3	-2.18	106.78	111.83
17	V	301	79P	O32-C31-C29	-2.10	105.47	109.59
17	Y	301	79P	C62-C61-C60	-2.10	117.43	120.45
17	H	301	79P	O32-C31-C29	-2.07	105.53	109.59
17	H	301	79P	O40-C39-C37	-2.04	106.89	111.16
17	K	301	79P	C17-C66-C65	-2.01	125.49	127.97
18	K	303	MES	O3S-S-C8	2.04	109.23	104.99
17	V	301	79P	O40-C39-C37	2.05	115.45	111.16
18	Y	302	MES	O3S-S-C8	2.08	109.31	104.99
17	H	301	79P	C41-C30-C29	2.23	116.97	113.40
17	K	301	79P	C50-N55-C54	2.38	114.20	108.87
17	V	301	79P	C53-C54-N55	2.47	113.89	110.11
17	K	301	79P	C41-C30-C29	2.57	117.51	113.40
17	V	301	79P	C31-C29-N28	2.61	115.66	110.06
17	H	301	79P	C31-C29-N28	3.49	117.54	110.06
17	Y	301	79P	C41-C30-C29	3.57	119.11	113.40
18	Y	302	MES	O2S-S-C8	3.74	109.51	106.87
18	Y	302	MES	O1S-S-C8	4.59	110.11	106.87
18	K	303	MES	O1S-S-C8	4.84	110.29	106.87
18	K	303	MES	O2S-S-C8	7.43	112.12	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	301	79P	1	0
17	K	301	79P	2	0
17	Y	301	79P	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	A	250/250 (100%)	-0.32	6 (2%) 62 62	42, 58, 96, 132	0
1	O	250/250 (100%)	-0.33	6 (2%) 62 62	45, 61, 107, 138	0
2	B	244/258 (94%)	-0.23	7 (2%) 55 55	44, 64, 107, 159	0
2	P	244/258 (94%)	-0.18	9 (3%) 45 45	47, 67, 110, 159	0
3	C	240/254 (94%)	0.04	19 (7%) 15 13	47, 72, 138, 176	0
3	Q	240/254 (94%)	0.27	25 (10%) 8 6	33, 79, 158, 203	0
4	D	235/260 (90%)	-0.21	6 (2%) 59 59	45, 68, 100, 138	0
4	R	235/260 (90%)	-0.06	13 (5%) 29 27	58, 81, 120, 154	0
5	E	231/234 (98%)	-0.21	4 (1%) 73 74	50, 68, 107, 147	0
5	S	231/234 (98%)	-0.24	7 (3%) 54 54	50, 70, 107, 142	0
6	F	243/288 (84%)	-0.33	8 (3%) 50 50	43, 63, 109, 140	0
6	T	243/288 (84%)	-0.28	6 (2%) 61 61	40, 63, 117, 148	0
7	G	241/252 (95%)	-0.33	8 (3%) 50 50	42, 59, 97, 158	0
7	U	241/252 (95%)	-0.39	3 (1%) 81 81	41, 57, 91, 132	0
8	H	226/232 (97%)	-0.33	6 (2%) 58 58	46, 58, 94, 159	0
8	V	226/232 (97%)	-0.31	4 (1%) 71 72	43, 57, 93, 170	0
9	I	204/205 (99%)	-0.57	1 (0%) 91 93	42, 56, 88, 113	0
9	W	204/205 (99%)	-0.60	1 (0%) 91 93	43, 57, 87, 111	0
10	J	195/198 (98%)	-0.31	6 (3%) 52 52	44, 62, 87, 132	0
10	X	195/198 (98%)	-0.32	5 (2%) 59 59	44, 63, 89, 144	0
11	K	211/211 (100%)	-0.37	3 (1%) 78 77	49, 64, 95, 121	0
11	Y	211/211 (100%)	-0.37	2 (0%) 85 86	48, 65, 97, 128	0
12	L	222/222 (100%)	-0.31	4 (1%) 71 72	48, 63, 109, 138	0
12	Z	222/222 (100%)	-0.30	6 (2%) 58 58	47, 64, 107, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.51	3 (1%)	79 79	40, 57, 83, 99	0
13	a	233/246 (94%)	-0.48	2 (0%)	85 86	41, 57, 81, 97	0
14	N	196/196 (100%)	-0.55	3 (1%)	76 76	36, 51, 82, 108	0
14	b	196/196 (100%)	-0.54	3 (1%)	76 76	38, 51, 82, 110	0
All	All	6342/6612 (95%)	-0.30	176 (2%)	56 57	33, 63, 107, 203	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	7.1
3	Q	238	LYS	7.0
10	J	1	MET	6.9
2	B	218	GLY	6.5
3	Q	239	GLN	6.5
12	L	174	TYR	6.4
3	Q	50	LEU	6.0
2	P	51	VAL	5.9
3	Q	206	LYS	5.7
5	E	202	ASP	5.6
2	B	221	ASP	5.5
8	H	224	GLN	5.5
6	F	202	ASP	5.4
9	W	1	SER	5.4
3	C	50	LEU	5.1
3	C	239	GLN	5.1
1	A	1	MET	5.0
2	B	51	VAL	4.8
10	X	194	ASP	4.7
6	F	203	ASN	4.6
2	B	219	ALA	4.5
3	Q	225	GLU	4.5
12	Z	174	TYR	4.5
10	J	194	ASP	4.4
8	V	224	GLN	4.4
9	I	1	SER	4.3
12	Z	173	LYS	4.2
8	V	226	GLU	4.2
1	O	1	MET	4.1
3	Q	141	ASP	4.1
3	Q	237	GLU	4.1
4	R	116	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
4	R	241	ALA	4.0
8	V	222	ASP	4.0
3	Q	236	GLN	3.9
5	S	202	ASP	3.9
6	F	181	GLU	3.9
8	H	226	GLU	3.8
2	P	221	ASP	3.8
10	X	195	PHE	3.8
3	Q	240	GLU	3.8
3	C	205	ALA	3.7
4	R	230	GLU	3.7
3	Q	48	SER	3.7
6	T	205	GLU	3.7
6	T	244	ASN	3.6
4	R	117	GLU	3.6
7	G	2	GLY	3.6
2	P	218	GLY	3.6
13	a	1	THR	3.5
3	C	206	LYS	3.5
3	C	202	GLN	3.5
1	O	231	LYS	3.5
3	C	49	THR	3.4
3	Q	49	THR	3.4
1	A	249	ALA	3.4
1	A	250	LEU	3.3
2	P	59	ASP	3.3
2	B	220	ASN	3.3
3	Q	229	GLN	3.2
4	D	117	GLU	3.2
6	F	244	ASN	3.2
10	J	195	PHE	3.2
7	G	3	TYR	3.2
3	C	238	LYS	3.1
2	P	219	ALA	3.1
11	Y	211	GLY	3.1
3	Q	180	LYS	3.0
3	Q	3	ASP	3.0
3	Q	202	GLN	3.0
12	Z	167	LYS	2.9
12	L	165	ASN	2.9
3	C	139	ARG	2.9
10	J	95	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
4	R	1	ASP	2.9
5	S	203	GLU	2.9
3	C	180	LYS	2.9
13	M	47	ASP	2.8
1	O	2	THR	2.8
3	C	225	GLU	2.8
4	R	54	ASP	2.8
8	H	215	GLU	2.8
8	H	221	CYS	2.8
3	Q	47	ARG	2.8
3	Q	205	ALA	2.7
2	P	220	ASN	2.7
1	A	201	GLU	2.7
5	S	3	ASN	2.7
13	M	1	THR	2.7
13	M	216	ASN	2.7
6	T	181	GLU	2.7
1	O	250	LEU	2.7
3	Q	27	ARG	2.7
12	Z	210	ASP	2.7
12	Z	165	ASN	2.6
1	A	248	GLU	2.6
4	R	125	LEU	2.6
4	R	226	GLU	2.6
3	C	216	ASP	2.6
14	b	104	ASP	2.5
5	E	201	ARG	2.5
2	B	242	GLY	2.5
2	P	217	LYS	2.5
11	K	107	LYS	2.5
7	U	188	GLU	2.5
7	U	242	GLN	2.5
5	S	225	ASP	2.5
12	L	173	LYS	2.5
8	H	219	ASN	2.5
14	N	181	ALA	2.4
1	O	249	ALA	2.4
7	G	241	GLU	2.4
4	R	2	ARG	2.4
8	H	222	ASP	2.4
7	G	230	GLU	2.4
11	Y	146	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
6	T	180	PRO	2.4
3	Q	234	ILE	2.4
4	R	217	GLN	2.4
10	J	193	ASP	2.3
14	b	105	LYS	2.3
7	U	203	ASP	2.3
11	K	40	TYR	2.3
3	C	167	LYS	2.3
4	R	203	LYS	2.3
5	E	122	TYR	2.3
1	A	231	LYS	2.3
4	R	114	ARG	2.3
6	T	178	HIS	2.3
4	R	113	LEU	2.3
3	C	187	GLU	2.3
3	C	235	GLU	2.3
6	F	241	LYS	2.3
6	T	2	THR	2.3
2	B	217	LYS	2.3
6	F	228	LYS	2.3
14	N	195	GLN	2.2
7	G	188	GLU	2.2
12	Z	163	GLY	2.2
5	S	30	GLN	2.2
2	P	52	THR	2.2
13	a	47	ASP	2.2
12	L	1	GLN	2.2
4	D	217	GLN	2.2
3	C	188	GLU	2.2
3	Q	139	ARG	2.2
7	G	68	ARG	2.2
3	Q	233	GLN	2.2
3	C	236	GLN	2.2
2	P	203	SER	2.2
3	Q	175	LYS	2.2
4	D	1	ASP	2.2
7	G	242	GLN	2.2
8	V	221	CYS	2.2
5	S	54	GLU	2.1
6	F	205	GLU	2.1
10	J	24	GLY	2.1
11	K	211	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	203	THR	2.1
3	Q	187	GLU	2.1
4	D	242	GLU	2.1
6	F	178	HIS	2.1
3	Q	181	GLU	2.1
7	G	240	ALA	2.1
3	Q	223	SER	2.1
3	C	59	PRO	2.1
4	D	240	ALA	2.1
4	D	125	LEU	2.1
14	N	105	LYS	2.1
5	E	173	ARG	2.1
5	S	123	GLY	2.1
10	X	193	ASP	2.1
10	X	95	ARG	2.0
3	C	229	GLN	2.0
14	b	195	GLN	2.0
1	O	52	SER	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, 95th 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 ²)	Q<0.9
17	79P	V	301	43/43	0.75	0.37	7.52	56,61,89,91	43
18	MES	Y	302	12/12	0.89	0.32	6.29	65,68,78,78	0
18	MES	K	303	12/12	0.89	0.25	5.37	60,66,69,75	12

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
17	79P	H	301	43/43	0.82	0.34	4.90	59,64,93,94	43
15	MG	Z	301	1/1	0.91	0.27	3.69	75,75,75,75	0
17	79P	Y	301	43/43	0.92	0.19	1.78	52,62,83,87	0
17	79P	K	301	43/43	0.93	0.20	1.57	55,62,88,94	0
15	MG	N	201	1/1	0.98	0.13	0.71	59,59,59,59	0
15	MG	G	301	1/1	0.89	0.14	0.09	65,65,65,65	0
15	MG	K	302	1/1	0.97	0.08	-0.86	59,59,59,59	0
15	MG	I	301	1/1	0.97	0.10	-0.87	60,60,60,60	0
15	MG	L	301	1/1	0.97	0.09	-1.83	68,68,68,68	0
15	MG	I	302	1/1	0.99	0.05	-2.43	59,59,59,59	0
16	CL	U	301	1/1	0.98	0.10	-	48,48,48,48	0
16	CL	G	302	1/1	0.99	0.10	-	50,50,50,50	0
16	CL	G	303	1/1	0.99	0.12	-	55,55,55,55	0
15	MG	J	201	1/1	0.99	0.18	-	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.