



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:44 am GMT

PDB ID : 5L5F
Title : Yeast 20S proteasome with human beta5i (1-138) and human beta6 (97-111; 118-133) in complex with bortezomib
Authors : Groll, M.; Huber, E.M.
Deposited on : 2016-05-28
Resolution : 2.50 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

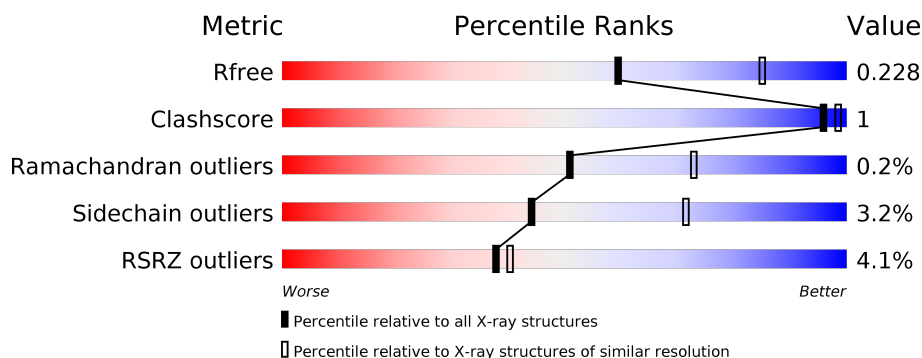
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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>4%</div> <div>98%</div> <div>•</div> </div>
1	O	250	<div> <div>4%</div> <div>98%</div> <div>•</div> </div>
2	B	258	<div> <div>6%</div> <div>88%</div> <div>6% • 5%</div> </div>
2	P	258	<div> <div>5%</div> <div>88%</div> <div>7% • 5%</div> </div>
3	C	254	<div> <div>12%</div> <div>87%</div> <div>6% • 6%</div> </div>
3	Q	254	<div> <div>12%</div> <div>87%</div> <div>6% • 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	J	201	-	-	-	X
17	BO2	N	201	-	-	-	X
17	BO2	Y	301	-	-	-	X
17	BO2	b	201	-	-	-	X

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 50436 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
			1640	1035	282	311	12			
11	Y	211	Total	C	N	O	S	0	0	0
			1640	1035	282	311	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	0	0
			1824	1154	312	351	7			

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

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

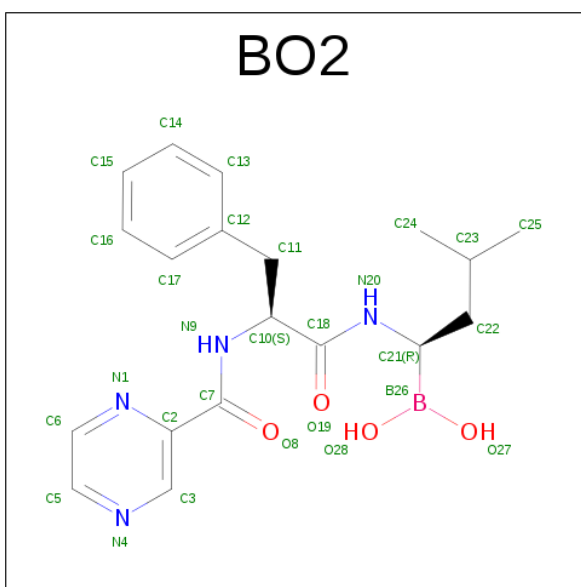
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	J	1	Total Mg 1 1	0	0
15	K	1	Total Mg 1 1	0	0
15	b	1	Total Mg 1 1	0	0
15	I	1	Total Mg 1 1	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	1	Total Cl 1 1	0	0
16	b	1	Total Cl 1 1	0	0
16	N	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (three-letter code: BO2) (formula: C₁₉H₂₅BN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
17	K	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
17	N	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
17	V	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
17	Y	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
17	b	1	Total	B	C	N	O	0	0
			28	1	19	4	4		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	39	Total	O	0	0
			39	39		
18	B	26	Total	O	0	0
			26	26		
18	C	19	Total	O	0	0
			19	19		
18	D	13	Total	O	0	0
			13	13		
18	E	14	Total	O	0	0
			14	14		
18	F	34	Total	O	0	0
			34	34		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	G	42	Total O 42 42	0	0
18	H	63	Total O 63 63	0	0
18	I	38	Total O 38 38	0	0
18	J	30	Total O 30 30	0	0
18	K	26	Total O 26 26	0	0
18	L	42	Total O 42 42	0	0
18	M	55	Total O 55 55	0	0
18	N	30	Total O 30 30	0	0
18	O	33	Total O 33 33	0	0
18	P	20	Total O 20 20	0	0
18	Q	13	Total O 13 13	0	0
18	R	14	Total O 14 14	0	0
18	S	17	Total O 17 17	0	0
18	T	27	Total O 27 27	0	0
18	U	43	Total O 43 43	0	0
18	V	46	Total O 46 46	0	0
18	W	36	Total O 36 36	0	0
18	X	29	Total O 29 29	0	0
18	Y	24	Total O 24 24	0	0
18	Z	30	Total O 30 30	0	0
18	a	41	Total O 41 41	0	0

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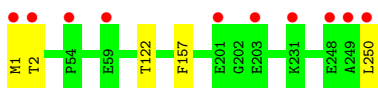
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	b	40	Total	O	0	0
			40	40		

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 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.

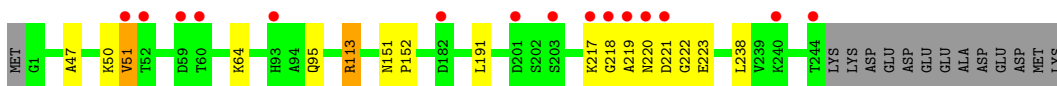
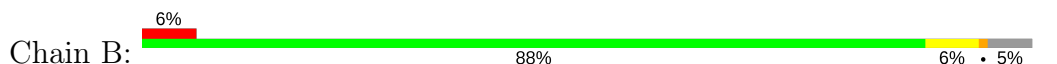
- Molecule 1: Proteasome subunit alpha type-2



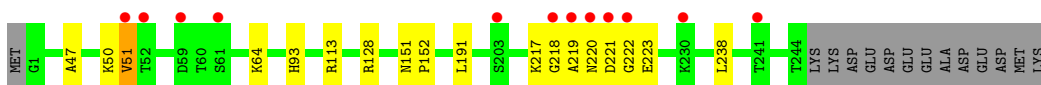
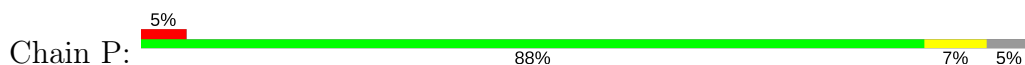
- Molecule 1: Proteasome subunit alpha type-2



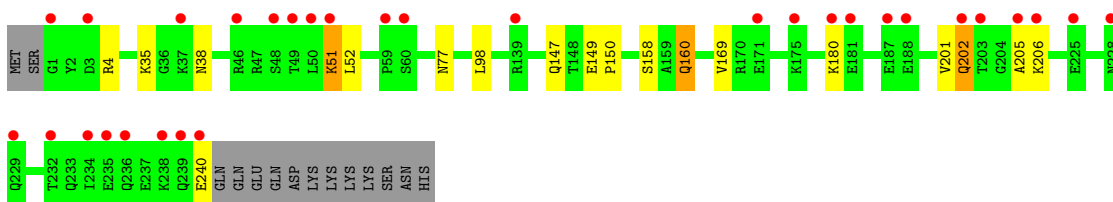
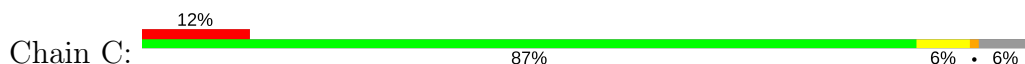
- Molecule 2: Proteasome subunit alpha type-3



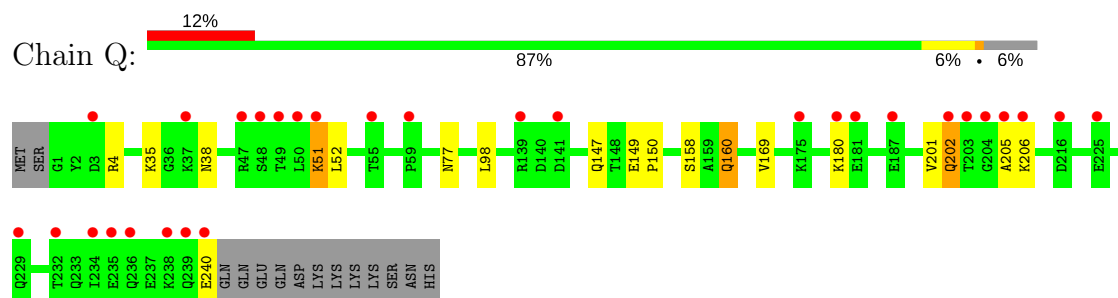
- Molecule 2: Proteasome subunit alpha type-3



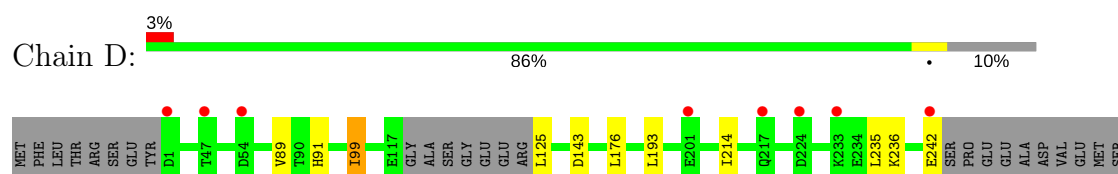
- Molecule 3: Proteasome subunit alpha type-4



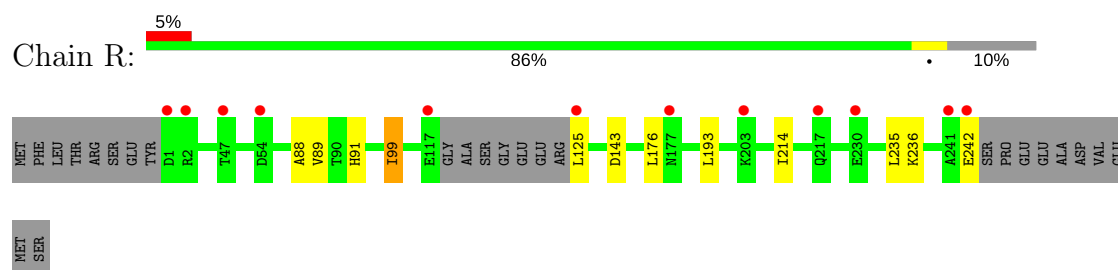
- Molecule 3: Proteasome subunit alpha type-4



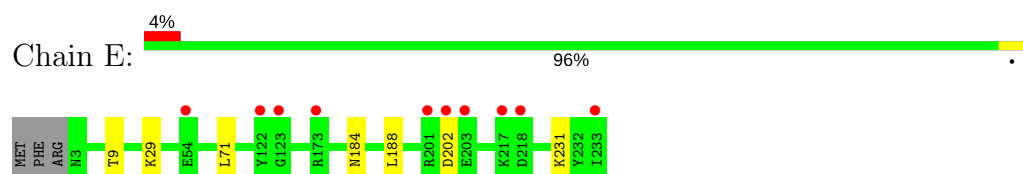
- Molecule 4: Proteasome subunit alpha type-5



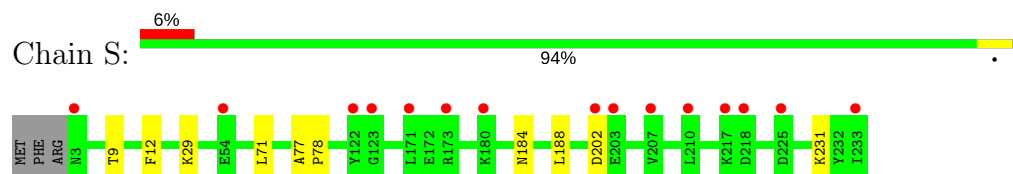
- Molecule 4: Proteasome subunit alpha type-5



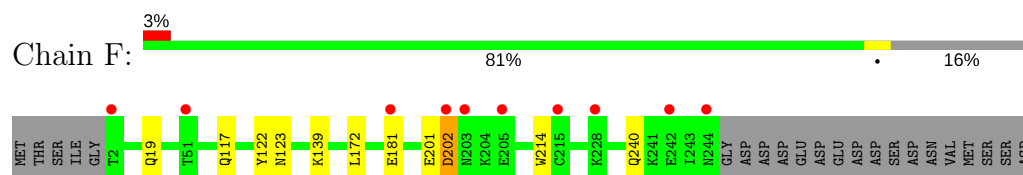
- Molecule 5: Proteasome subunit alpha type-6

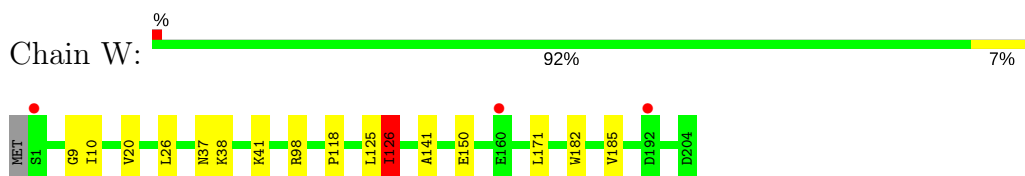


- Molecule 5: Proteasome subunit alpha type-6

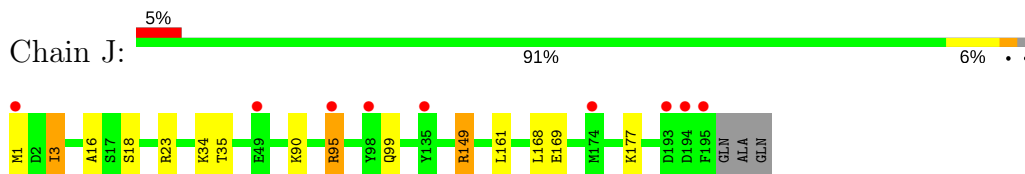


- Molecule 6: Probable proteasome subunit alpha type-7

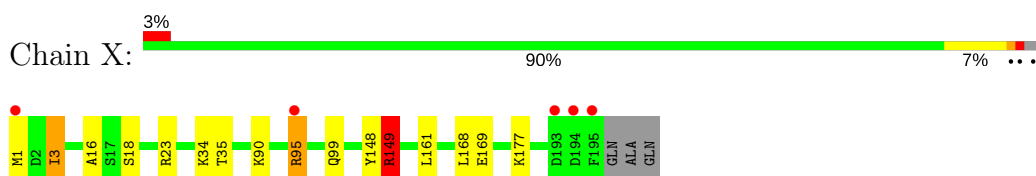




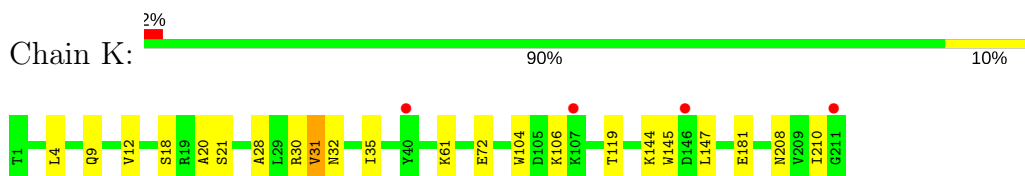
- Molecule 10: Proteasome subunit beta type-4



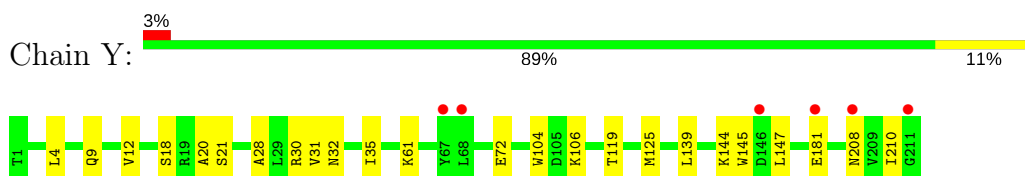
- Molecule 10: Proteasome subunit beta type-4



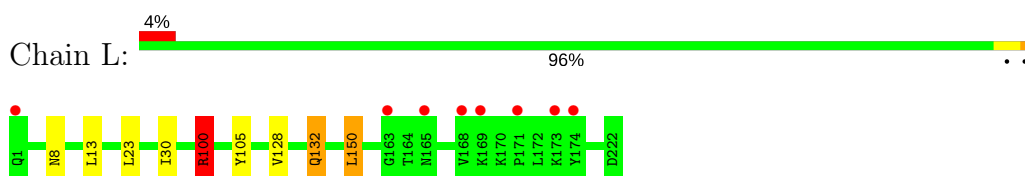
- Molecule 11: Proteasome subunit beta type-8, Proteasome subunit beta type-5



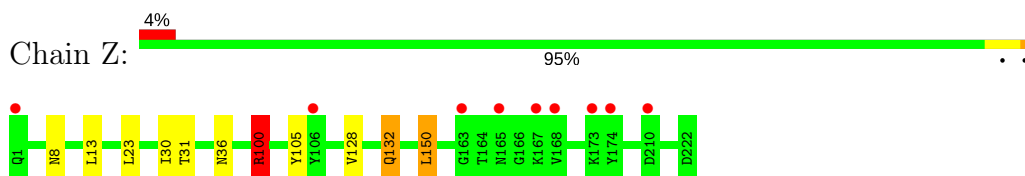
- Molecule 11: Proteasome subunit beta type-8, Proteasome subunit beta type-5



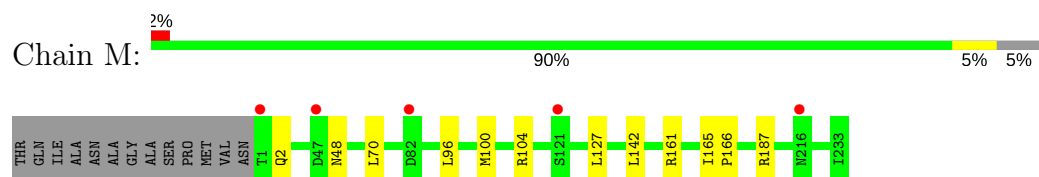
- Molecule 12: Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6



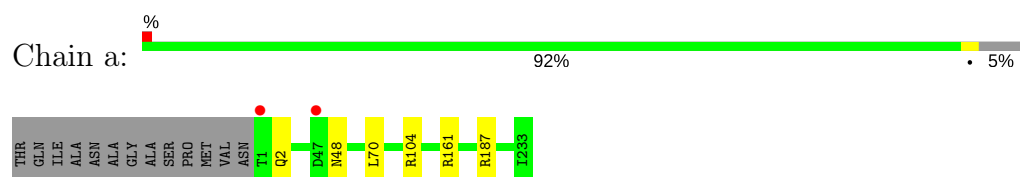
- Molecule 12: Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6



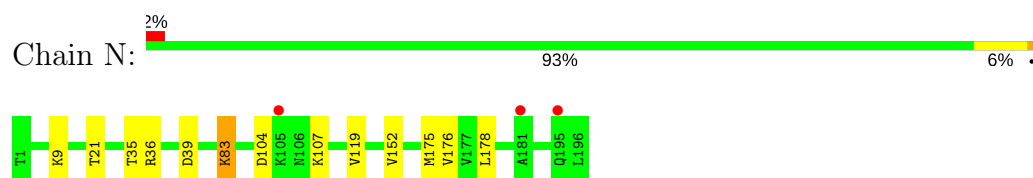
- Molecule 13: Proteasome subunit beta type-7



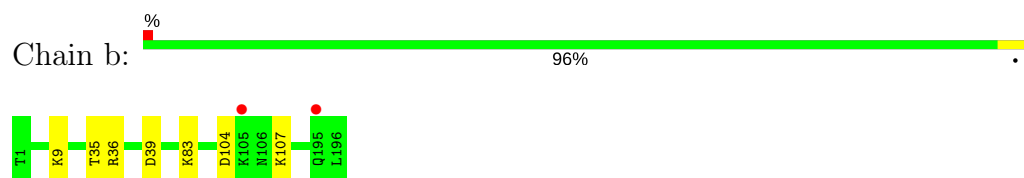
- Molecule 13: Proteasome subunit beta type-7



- 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	135.51Å 300.91Å 144.92Å 90.00° 112.59° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (15.00-2.50) 98.3 (15.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.205 , 0.228 0.207 , 0.228	Depositor DCC
R_{free} test set	17997 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.7	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	50436	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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: BO2, MG, 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	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.49	0/2618
2	P	0.27	0/1934	0.49	0/2618
3	C	0.27	0/1910	0.50	0/2586
3	Q	0.28	0/1910	0.50	0/2586
4	D	0.27	0/1837	0.47	0/2475
4	R	0.27	0/1837	0.47	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	0.74	4/2634 (0.2%)
7	U	0.28	0/1945	0.78	4/2634 (0.2%)
8	H	0.25	0/1750	0.47	0/2373
8	V	0.25	0/1750	0.47	0/2373
9	I	0.26	0/1611	0.56	2/2174 (0.1%)
9	W	0.27	0/1611	0.55	2/2174 (0.1%)
10	J	0.27	0/1589	0.97	6/2142 (0.3%)
10	X	0.27	0/1589	0.94	6/2142 (0.3%)
11	K	0.26	0/1677	0.50	0/2263
11	Y	0.27	0/1677	0.50	0/2263
12	L	0.28	0/1802	0.73	3/2430 (0.1%)
12	Z	0.27	0/1802	0.73	3/2430 (0.1%)
13	M	0.27	0/1855	0.51	0/2514
13	a	0.27	0/1855	0.51	0/2514
14	N	0.25	0/1541	0.47	0/2087
14	b	0.26	0/1541	0.47	0/2087
All	All	0.27	0/50270	0.57	30/67960 (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
7	G	0	1
10	J	0	2
10	X	0	2
12	L	0	1
12	Z	0	1
All	All	0	7

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	68	ARG	NE-CZ-NH2	-22.78	108.91	120.30
10	J	95	ARG	NE-CZ-NH2	-20.69	109.95	120.30
7	G	68	ARG	NE-CZ-NH1	-20.68	109.96	120.30
10	J	149	ARG	NE-CZ-NH1	-20.55	110.03	120.30
12	Z	100	ARG	NE-CZ-NH2	-20.30	110.15	120.30
10	X	149	ARG	NE-CZ-NH2	-19.98	110.31	120.30
12	L	100	ARG	NE-CZ-NH1	-19.75	110.42	120.30
10	X	95	ARG	NE-CZ-NH1	-18.80	110.90	120.30
7	U	68	ARG	NE-CZ-NH1	17.92	129.26	120.30
7	G	68	ARG	NE-CZ-NH2	17.61	129.11	120.30
12	Z	100	ARG	NE-CZ-NH1	16.48	128.54	120.30
12	L	100	ARG	NE-CZ-NH2	16.34	128.47	120.30
10	J	149	ARG	NE-CZ-NH2	16.17	128.39	120.30
10	X	95	ARG	NE-CZ-NH2	15.86	128.23	120.30
10	X	149	ARG	NE-CZ-NH1	15.00	127.80	120.30
10	J	95	ARG	NE-CZ-NH1	13.80	127.20	120.30
7	U	68	ARG	CD-NE-CZ	10.81	138.74	123.60
9	I	126	ILE	CG1-CB-CG2	-10.73	87.78	111.40
10	J	95	ARG	CD-NE-CZ	10.55	138.37	123.60
10	J	149	ARG	CD-NE-CZ	10.28	137.99	123.60
9	W	126	ILE	CG1-CB-CG2	-10.24	88.88	111.40
7	G	68	ARG	CD-NE-CZ	10.11	137.75	123.60
10	X	149	ARG	CD-NE-CZ	9.55	136.97	123.60
12	Z	100	ARG	CD-NE-CZ	9.09	136.32	123.60
10	X	95	ARG	CD-NE-CZ	8.96	136.15	123.60
12	L	100	ARG	CD-NE-CZ	8.83	135.96	123.60
7	U	68	ARG	CG-CD-NE	-7.41	96.23	111.80
7	G	68	ARG	CG-CD-NE	5.35	123.03	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	126	ILE	CA-CB-CG1	5.20	120.87	111.00
9	I	126	ILE	CA-CB-CG1	5.08	120.64	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	68	ARG	Sidechain
10	J	149	ARG	Sidechain
10	J	95	ARG	Sidechain
12	L	100	ARG	Sidechain
10	X	149	ARG	Sidechain
10	X	95	ARG	Sidechain
12	Z	100	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	1	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	7	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	0	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	3	0
8	H	1719	0	1718	6	0
8	V	1719	0	1718	5	0
9	I	1581	0	1574	11	0
9	W	1581	0	1574	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	1561	0	1569	9	0
10	X	1561	0	1569	10	0
11	K	1640	0	1580	9	0
11	Y	1640	0	1580	11	0
12	L	1764	0	1716	4	0
12	Z	1764	0	1716	5	0
13	M	1824	0	1832	3	0
13	a	1824	0	1832	0	0
14	N	1512	0	1480	4	0
14	b	1512	0	1480	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	J	1	0	0	0	0
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
15	b	1	0	0	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	H	28	0	25	0	0
17	K	28	0	25	0	0
17	N	28	0	25	1	0
17	V	28	0	25	0	0
17	Y	28	0	25	0	0
17	b	28	0	25	0	0
18	A	39	0	0	0	0
18	B	26	0	0	2	0
18	C	19	0	0	0	0
18	D	13	0	0	0	0
18	E	14	0	0	0	0
18	F	34	0	0	1	0
18	G	42	0	0	0	0
18	H	63	0	0	0	0
18	I	38	0	0	0	0
18	J	30	0	0	0	0
18	K	26	0	0	0	0
18	L	42	0	0	0	0
18	M	55	0	0	0	0
18	N	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	O	33	0	0	0	0
18	P	20	0	0	1	0
18	Q	13	0	0	0	0
18	R	14	0	0	0	0
18	S	17	0	0	0	0
18	T	27	0	0	0	0
18	U	43	0	0	0	0
18	V	46	0	0	0	0
18	W	36	0	0	0	0
18	X	29	0	0	0	0
18	Y	24	0	0	0	0
18	Z	30	0	0	0	0
18	a	41	0	0	0	0
18	b	40	0	0	0	0
All	All	50436	0	49256	123	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 (123) 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)
9:W:98:ARG:HD2	9:W:126:ILE:HD12	1.68	0.75
9:I:98:ARG:HD2	9:I:126:ILE:HD12	1.69	0.74
10:X:3:ILE:HD11	10:X:168:LEU:HD13	1.71	0.72
10:J:3:ILE:HD11	10:J:168:LEU:HD13	1.71	0.71
9:W:125:LEU:HD23	9:W:126:ILE:HG22	1.72	0.70
11:K:72:GLU:OE1	11:K:106:LYS:NZ	2.21	0.68
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.75	0.68
11:Y:72:GLU:OE1	11:Y:106:LYS:NZ	2.21	0.67
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.75	0.67
10:X:23:ARG:NH2	11:Y:119:THR:OG1	2.28	0.66
10:J:23:ARG:NH2	11:K:119:THR:OG1	2.25	0.65
11:Y:31:VAL:HA	12:Z:132:GLN:HE22	1.62	0.64
9:W:125:LEU:CD2	9:W:126:ILE:HG22	2.30	0.62
11:K:31:VAL:HA	12:L:132:GLN:HE22	1.65	0.61
10:J:3:ILE:CD1	10:J:168:LEU:HD13	2.31	0.61
10:X:3:ILE:CD1	10:X:168:LEU:HD13	2.31	0.60
9:I:125:LEU:HD23	9:I:126:ILE:HG22	1.84	0.59
14:N:152:VAL:HA	14:N:175:MET:HE1	1.85	0.58
9:I:125:LEU:CD2	9:I:126:ILE:HG22	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:ARG:NE	18:B:301:HOH:O	2.35	0.56
11:K:104:TRP:CE2	11:K:181:GLU:HB3	2.41	0.56
9:W:98:ARG:HD2	9:W:126:ILE:CD1	2.35	0.56
11:Y:104:TRP:CE2	11:Y:181:GLU:HB3	2.41	0.55
4:R:89:VAL:HG12	11:Y:61:LYS:HG3	1.88	0.54
2:P:93:HIS:HB3	18:P:301:HOH:O	2.10	0.53
7:G:23:PHE:O	7:G:26:THR:HB	2.09	0.52
4:D:89:VAL:HG12	11:K:61:LYS:HG3	1.91	0.52
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.52
8:H:196:ARG:NH2	9:I:150:GLU:O	2.42	0.52
11:Y:9:GLN:HB2	11:Y:145:TRP:O	2.11	0.51
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.94	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.50
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.50
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.94	0.50
8:V:84:LYS:HA	8:V:113:ILE:HD11	1.94	0.49
11:K:9:GLN:HB2	11:K:145:TRP:O	2.11	0.49
10:X:3:ILE:HG22	10:X:18:SER:HB3	1.93	0.49
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.93	0.49
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.93	0.49
10:X:3:ILE:HG22	10:X:18:SER:CB	2.43	0.49
10:J:3:ILE:HG22	10:J:18:SER:CB	2.43	0.49
8:H:84:LYS:HA	8:H:113:ILE:HD11	1.95	0.49
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.78	0.48
10:J:3:ILE:HG22	10:J:18:SER:HB3	1.93	0.48
11:Y:20:ALA:HB3	11:Y:28:ALA:HB3	1.95	0.48
3:C:51:LYS:O	3:C:52:LEU:HB2	2.12	0.48
11:K:20:ALA:HB3	11:K:28:ALA:HB3	1.94	0.48
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.46	0.48
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.43	0.48
12:Z:100:ARG:HD3	12:Z:105:TYR:CE2	2.49	0.48
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.13	0.48
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.96	0.48
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.78	0.47
8:V:196:ARG:NH2	9:W:150:GLU:O	2.47	0.47
6:F:19:GLN:NE2	18:F:301:HOH:O	2.47	0.47
12:L:100:ARG:HD2	12:L:105:TYR:CZ	2.50	0.46
5:S:12:PHE:H	6:T:19:GLN:HE22	1.64	0.46
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.97	0.46
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.99	0.45
8:H:53:GLU:O	8:H:57:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:208:ASN:O	9:W:38:LYS:NZ	2.49	0.45
9:I:98:ARG:HD2	9:I:126:ILE:CD1	2.44	0.45
9:W:98:ARG:CD	9:W:126:ILE:CD1	2.94	0.45
2:B:217:LYS:C	2:B:219:ALA:H	2.20	0.45
10:J:177:LYS:NZ	10:X:169:GLU:O	2.50	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.97	0.45
2:P:50:LYS:O	2:P:51:VAL:C	2.55	0.45
10:X:148:TYR:O	10:X:149:ARG:HD3	2.16	0.44
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.98	0.44
2:B:50:LYS:O	2:B:51:VAL:C	2.56	0.44
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.53	0.44
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.00	0.44
2:P:217:LYS:C	2:P:219:ALA:H	2.20	0.44
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.00	0.44
8:V:53:GLU:O	8:V:57:GLN:HG2	2.18	0.44
9:W:126:ILE:HD13	9:W:126:ILE:HG21	1.42	0.44
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.99	0.43
11:K:144:LYS:HB2	11:K:147:LEU:HD13	2.01	0.43
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.00	0.43
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.01	0.43
3:C:35:LYS:HG2	3:C:158:SER:O	2.19	0.43
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.49	0.43
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.00	0.43
2:B:221:ASP:O	2:B:223:GLU:N	2.52	0.43
2:P:221:ASP:O	2:P:223:GLU:N	2.52	0.43
2:B:95:GLN:NE2	18:B:302:HOH:O	2.52	0.43
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.01	0.43
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.19	0.42
11:Y:144:LYS:HB2	11:Y:147:LEU:HD13	2.01	0.42
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.02	0.42
14:N:21:THR:O	17:N:201:BO2:H3	2.19	0.42
6:F:202:ASP:OD1	6:F:202:ASP:N	2.53	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.19	0.42
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.00	0.42
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.02	0.42
10:J:169:GLU:O	10:X:177:LYS:NZ	2.52	0.42
9:I:26:LEU:HD21	9:I:185:VAL:HG23	2.02	0.42
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.02	0.42
3:C:201:VAL:O	3:C:202:GLN:HB3	2.19	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.02	0.41
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.50	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.02	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.41
6:T:202:ASP:N	6:T:202:ASP:OD1	2.53	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.03	0.41
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.56	0.41
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.85	0.41
13:M:96:LEU:O	13:M:100:MET:HG2	2.21	0.41
11:Y:125:MET:SD	11:Y:139:LEU:HB3	2.61	0.41
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.36	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.21	0.41
9:W:98:ARG:NE	9:W:126:ILE:HD11	2.36	0.40
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.86	0.40
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.56	0.40
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.52	0.40
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.04	0.40
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	38 59
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	38 59
2	B	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	11 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	11	18
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	22	39
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	22	39
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (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%)	219 (98%)	5 (2%)	0	100	100
8	V	224/232 (97%)	219 (98%)	5 (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%)	3 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	209/211 (99%)	203 (97%)	6 (3%)	0	100	100
11	Y	209/211 (99%)	202 (97%)	7 (3%)	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%)	224 (97%)	7 (3%)	0	100	100
13	a	231/246 (94%)	224 (97%)	7 (3%)	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	6282/6612 (95%)	6134 (98%)	134 (2%)	14 (0%)	51	73

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	222	GLY
3	C	202	GLN

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

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%)	71	90
1	O	209/209 (100%)	206 (99%)	3 (1%)	71	90
2	B	203/216 (94%)	200 (98%)	3 (2%)	70	89
2	P	203/216 (94%)	200 (98%)	3 (2%)	70	89
3	C	212/226 (94%)	201 (95%)	11 (5%)	27	49
3	Q	212/226 (94%)	201 (95%)	11 (5%)	27	49
4	D	194/215 (90%)	185 (95%)	9 (5%)	31	55
4	R	194/215 (90%)	185 (95%)	9 (5%)	31	55
5	E	190/193 (98%)	183 (96%)	7 (4%)	39	66
5	S	190/193 (98%)	183 (96%)	7 (4%)	39	66
6	F	201/239 (84%)	192 (96%)	9 (4%)	32	56
6	T	201/239 (84%)	192 (96%)	9 (4%)	32	56
7	G	206/210 (98%)	199 (97%)	7 (3%)	42	69
7	U	206/210 (98%)	200 (97%)	6 (3%)	48	75
8	H	185/190 (97%)	181 (98%)	4 (2%)	57	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	185/190 (97%)	181 (98%)	4 (2%)	57	82
9	I	172/173 (99%)	168 (98%)	4 (2%)	56	81
9	W	172/173 (99%)	168 (98%)	4 (2%)	56	81
10	J	173/175 (99%)	169 (98%)	4 (2%)	56	81
10	X	173/175 (99%)	169 (98%)	4 (2%)	56	81
11	K	170/170 (100%)	161 (95%)	9 (5%)	26	48
11	Y	170/170 (100%)	162 (95%)	8 (5%)	30	54
12	L	186/186 (100%)	182 (98%)	4 (2%)	57	82
12	Z	186/186 (100%)	182 (98%)	4 (2%)	57	82
13	M	199/208 (96%)	193 (97%)	6 (3%)	46	74
13	a	199/208 (96%)	193 (97%)	6 (3%)	46	74
14	N	162/162 (100%)	155 (96%)	7 (4%)	33	58
14	b	162/162 (100%)	155 (96%)	7 (4%)	33	58
All	All	5324/5544 (96%)	5152 (97%)	172 (3%)	44	71

All (172) 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	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	98	LEU
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

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Mol	Chain	Res	Type
4	D	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
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
5	E	202	ASP
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	214	TRP
6	F	240	GLN
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	31	CYS
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
9	I	182	TRP
10	J	3	ILE
10	J	35	THR
10	J	90	LYS
10	J	99	GLN

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Mol	Chain	Res	Type
11	K	4	LEU
11	K	12	VAL
11	K	18	SER
11	K	21	SER
11	K	30	ARG
11	K	31	VAL
11	K	32	ASN
11	K	35	ILE
11	K	210	ILE
12	L	23	LEU
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
14	N	9	LYS
14	N	35	THR
14	N	36	ARG
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	113	ARG
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	77	ASN
3	Q	98	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS

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Mol	Chain	Res	Type
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	214	ILE
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
5	S	202	ASP
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	214	TRP
6	T	240	GLN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	31	CYS
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
9	W	182	TRP
10	X	3	ILE
10	X	35	THR

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Mol	Chain	Res	Type
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	12	VAL
11	Y	18	SER
11	Y	21	SER
11	Y	30	ARG
11	Y	32	ASN
11	Y	35	ILE
11	Y	210	ILE
12	Z	23	LEU
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	35	THR
14	b	36	ARG
14	b	39	ASP
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
3	C	17	GLN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN

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Mol	Chain	Res	Type
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	146	GLN
4	D	210	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	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	66	HIS
8	H	86	HIS
9	I	37	ASN
11	K	9	GLN
11	K	32	ASN
11	K	175	ASN
12	L	3	ASN
12	L	70	ASN
12	L	79	HIS
12	L	95	HIS
12	L	132	GLN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS

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Mol	Chain	Res	Type
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	15	GLN
4	R	91	HIS
4	R	146	GLN
4	R	225	ASN
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	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
8	V	86	HIS
9	W	37	ASN
11	Y	9	GLN
11	Y	32	ASN
11	Y	175	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	132	GLN
13	a	48	ASN
13	a	102	GLN

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Mol	Chain	Res	Type
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 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	BO2	H	301	8	27,29,29	1.57	5 (18%)	30,38,38	1.22	3 (10%)
17	BO2	K	301	11	27,29,29	1.56	5 (18%)	30,38,38	1.16	2 (6%)
17	BO2	N	201	14	27,29,29	1.53	5 (18%)	30,38,38	1.14	3 (10%)
17	BO2	V	301	8	27,29,29	1.57	5 (18%)	30,38,38	1.22	3 (10%)
17	BO2	Y	301	11	27,29,29	1.57	5 (18%)	30,38,38	1.17	2 (6%)
17	BO2	b	201	14	27,29,29	1.54	5 (18%)	30,38,38	1.17	3 (10%)

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	BO2	H	301	8	-	0/22/28/28	0/2/2/2
17	BO2	K	301	11	-	0/22/28/28	0/2/2/2
17	BO2	N	201	14	-	0/22/28/28	0/2/2/2
17	BO2	V	301	8	-	0/22/28/28	0/2/2/2
17	BO2	Y	301	11	-	0/22/28/28	0/2/2/2
17	BO2	b	201	14	-	0/22/28/28	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	301	BO2	C2-C7	-4.47	1.39	1.50
17	K	301	BO2	C2-C7	-4.45	1.40	1.50
17	N	201	BO2	C2-C7	-4.38	1.40	1.50
17	b	201	BO2	C2-C7	-4.37	1.40	1.50
17	H	301	BO2	C2-C7	-4.36	1.40	1.50
17	V	301	BO2	C2-C7	-4.34	1.40	1.50
17	b	201	BO2	C11-C12	-4.19	1.41	1.51
17	H	301	BO2	C11-C12	-4.14	1.41	1.51
17	V	301	BO2	C11-C12	-4.12	1.41	1.51
17	N	201	BO2	C11-C12	-4.06	1.41	1.51
17	K	301	BO2	C11-C12	-3.88	1.42	1.51
17	Y	301	BO2	C11-C12	-3.87	1.42	1.51
17	N	201	BO2	C5-N4	2.00	1.39	1.33
17	b	201	BO2	C5-N4	2.04	1.39	1.33
17	H	301	BO2	C5-N4	2.33	1.40	1.33
17	K	301	BO2	C5-N4	2.37	1.40	1.33
17	V	301	BO2	C5-N4	2.38	1.40	1.33
17	Y	301	BO2	C5-N4	2.40	1.40	1.33
17	b	201	BO2	C3-N4	2.80	1.40	1.34
17	N	201	BO2	C3-N4	2.80	1.40	1.34
17	N	201	BO2	C6-N1	2.84	1.40	1.34
17	K	301	BO2	C6-N1	2.87	1.40	1.34
17	b	201	BO2	C6-N1	2.89	1.40	1.34
17	Y	301	BO2	C6-N1	2.89	1.40	1.34
17	V	301	BO2	C6-N1	2.97	1.41	1.34
17	H	301	BO2	C6-N1	2.98	1.41	1.34
17	H	301	BO2	C3-N4	3.09	1.40	1.34
17	V	301	BO2	C3-N4	3.09	1.40	1.34
17	K	301	BO2	C3-N4	3.17	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	301	BO2	C3-N4	3.27	1.41	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	201	BO2	C11-C10-N9	-2.28	105.96	110.80
17	K	301	BO2	C6-C5-N4	-2.23	119.17	121.97
17	Y	301	BO2	C6-C5-N4	-2.23	119.18	121.97
17	H	301	BO2	C6-C5-N4	-2.21	119.20	121.97
17	N	201	BO2	C11-C10-N9	-2.17	106.19	110.80
17	V	301	BO2	C6-C5-N4	-2.17	119.25	121.97
17	b	201	BO2	C6-C5-N4	-2.12	119.31	121.97
17	V	301	BO2	C12-C11-C10	-2.11	107.50	113.41
17	N	201	BO2	C6-C5-N4	-2.06	119.39	121.97
17	H	301	BO2	C12-C11-C10	-2.04	107.69	113.41
17	N	201	BO2	C6-N1-C2	2.99	120.89	116.94
17	b	201	BO2	C6-N1-C2	3.03	120.96	116.94
17	K	301	BO2	C6-N1-C2	3.37	121.41	116.94
17	Y	301	BO2	C6-N1-C2	3.44	121.50	116.94
17	H	301	BO2	C6-N1-C2	3.53	121.61	116.94
17	V	301	BO2	C6-N1-C2	3.54	121.62	116.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	N	201	BO2	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.11	10 (4%)	39 41	33, 48, 85, 125	0
1	O	250/250 (100%)	-0.07	10 (4%)	39 41	36, 53, 100, 134	0
2	B	244/258 (94%)	0.05	15 (6%)	22 22	34, 55, 103, 153	0
2	P	244/258 (94%)	0.07	12 (4%)	30 32	37, 57, 101, 153	0
3	C	240/254 (94%)	0.37	31 (12%)	4 3	33, 61, 130, 171	0
3	Q	240/254 (94%)	0.48	30 (12%)	4 4	26, 70, 149, 191	0
4	D	235/260 (90%)	-0.04	8 (3%)	46 48	39, 58, 89, 130	0
4	R	235/260 (90%)	0.12	12 (5%)	29 30	47, 66, 108, 146	0
5	E	231/234 (98%)	0.06	10 (4%)	36 38	39, 61, 100, 147	0
5	S	231/234 (98%)	0.10	15 (6%)	20 20	42, 64, 105, 139	0
6	F	243/288 (84%)	-0.12	10 (4%)	38 40	33, 53, 103, 128	0
6	T	243/288 (84%)	-0.05	12 (4%)	30 32	34, 59, 114, 144	0
7	G	241/252 (95%)	-0.20	7 (2%)	52 55	31, 49, 87, 144	0
7	U	241/252 (95%)	-0.13	9 (3%)	42 44	34, 50, 84, 128	0
8	H	226/232 (97%)	-0.24	6 (2%)	55 58	27, 44, 82, 150	0
8	V	226/232 (97%)	-0.19	7 (3%)	49 52	30, 46, 80, 157	0
9	I	204/205 (99%)	-0.41	2 (0%)	82 83	30, 44, 74, 98	0
9	W	204/205 (99%)	-0.38	3 (1%)	74 75	31, 46, 76, 98	0
10	J	195/198 (98%)	-0.17	9 (4%)	33 35	32, 49, 73, 121	0
10	X	195/198 (98%)	-0.22	5 (2%)	56 59	33, 50, 75, 130	0
11	K	211/211 (100%)	0.00	4 (1%)	67 69	36, 54, 89, 105	0
11	Y	211/211 (100%)	0.01	6 (2%)	53 56	38, 57, 91, 113	0
12	L	222/222 (100%)	0.07	8 (3%)	43 45	38, 52, 98, 131	0
12	Z	222/222 (100%)	0.02	9 (4%)	38 40	32, 54, 99, 133	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.36	5 (2%)	64 66	30, 48, 71, 88	0
13	a	233/246 (94%)	-0.32	2 (0%)	84 85	30, 48, 71, 87	0
14	N	196/196 (100%)	-0.38	3 (1%)	74 75	28, 41, 70, 99	0
14	b	196/196 (100%)	-0.37	2 (1%)	82 83	30, 42, 72, 103	0
All	All	6342/6612 (95%)	-0.08	262 (4%)	38 40	26, 52, 99, 191	0

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	218	GLY	10.0
10	J	1	MET	9.4
12	L	174	TYR	8.9
12	Z	174	TYR	7.5
10	X	1	MET	7.4
2	P	221	ASP	7.4
12	L	165	ASN	7.3
2	B	218	GLY	7.1
3	C	202	GLN	6.9
2	P	51	VAL	6.9
2	B	221	ASP	6.8
9	W	1	SER	6.6
3	Q	206	LYS	6.4
9	I	1	SER	6.3
1	O	249	ALA	6.2
3	C	238	LYS	6.1
3	Q	239	GLN	5.9
1	O	2	THR	5.8
3	Q	240	GLU	5.7
1	A	1	MET	5.7
2	P	219	ALA	5.4
3	C	235	GLU	5.3
3	Q	50	LEU	5.1
1	O	1	MET	5.1
2	B	219	ALA	5.1
3	C	239	GLN	5.1
2	B	51	VAL	5.0
5	S	202	ASP	5.0
6	F	215	CYS	4.9
1	A	249	ALA	4.9
3	Q	202	GLN	4.8
12	Z	168	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
12	Z	173	LYS	4.8
14	N	195	GLN	4.7
3	C	206	LYS	4.7
3	C	49	THR	4.6
3	Q	225	GLU	4.6
1	A	2	THR	4.5
3	Q	238	LYS	4.5
3	C	50	LEU	4.5
12	L	173	LYS	4.4
10	J	194	ASP	4.4
7	U	2	GLY	4.4
3	Q	236	GLN	4.4
12	Z	165	ASN	4.4
8	V	226	GLU	4.3
3	Q	141	ASP	4.3
10	X	195	PHE	4.2
3	Q	49	THR	4.2
4	R	217	GLN	4.2
10	X	194	ASP	4.2
3	C	225	GLU	4.2
5	S	173	ARG	4.1
1	O	250	LEU	4.1
2	P	59	ASP	4.1
7	G	2	GLY	4.0
6	F	244	ASN	3.9
7	U	242	GLN	3.9
1	O	52	SER	3.9
2	P	52	THR	3.9
4	R	241	ALA	3.8
8	V	224	GLN	3.8
8	H	226	GLU	3.8
6	T	244	ASN	3.7
12	L	163	GLY	3.7
6	F	181	GLU	3.7
3	C	236	GLN	3.7
1	A	250	LEU	3.6
4	R	1	ASP	3.6
3	C	234	ILE	3.6
5	E	202	ASP	3.6
3	C	59	PRO	3.6
3	Q	232	THR	3.5
3	Q	204	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
12	Z	167	LYS	3.5
6	F	202	ASP	3.5
10	X	193	ASP	3.5
4	D	242	GLU	3.5
14	b	195	GLN	3.5
5	E	217	LYS	3.4
3	C	180	LYS	3.4
3	Q	234	ILE	3.4
2	B	60	THR	3.4
8	H	224	GLN	3.3
2	B	220	ASN	3.3
5	E	122	TYR	3.3
2	B	217	LYS	3.3
6	T	181	GLU	3.3
2	P	220	ASN	3.3
13	a	1	THR	3.2
3	C	171	GLU	3.2
1	O	231	LYS	3.2
4	R	117	GLU	3.2
7	U	222	ASP	3.2
8	V	222	ASP	3.2
5	S	3	ASN	3.2
6	F	203	ASN	3.1
10	J	95	ARG	3.1
3	C	205	ALA	3.1
3	Q	205	ALA	3.1
11	K	146	ASP	3.1
5	E	233	ILE	3.1
4	R	54	ASP	3.1
8	H	221	CYS	3.1
12	L	1	GLN	3.0
8	V	221	CYS	3.0
6	F	205	GLU	3.0
3	Q	51	LYS	3.0
5	S	233	ILE	3.0
5	E	201	ARG	3.0
3	Q	235	GLU	2.9
6	F	2	THR	2.9
3	Q	181	GLU	2.9
5	S	203	GLU	2.9
10	J	193	ASP	2.9
4	R	125	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	60	SER	2.9
2	B	59	ASP	2.9
12	Z	163	GLY	2.8
2	B	52	THR	2.8
3	Q	203	THR	2.8
3	Q	48	SER	2.8
2	B	182	ASP	2.8
11	Y	68	LEU	2.8
7	G	3	TYR	2.8
6	T	2	THR	2.8
3	Q	175	LYS	2.8
5	E	173	ARG	2.8
3	C	203	THR	2.8
7	G	242	GLN	2.7
3	Q	47	ARG	2.7
7	U	181	LYS	2.7
14	b	105	LYS	2.7
5	E	203	GLU	2.7
6	T	243	ILE	2.7
7	G	179	LYS	2.7
11	Y	146	ASP	2.7
1	O	53	SER	2.7
10	J	174	MET	2.7
8	H	222	ASP	2.7
3	Q	180	LYS	2.6
10	J	195	PHE	2.6
6	T	180	PRO	2.6
5	E	54	GLU	2.6
1	O	4	ARG	2.6
3	Q	139	ARG	2.6
2	P	222	GLY	2.6
5	E	123	GLY	2.6
12	L	169	LYS	2.6
3	C	139	ARG	2.6
5	S	207	VAL	2.6
1	O	248	GLU	2.6
3	Q	187	GLU	2.6
6	T	205	GLU	2.6
2	P	203	SER	2.6
11	Y	211	GLY	2.6
2	B	240	LYS	2.6
11	Y	67	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
6	F	51	THR	2.5
11	K	211	GLY	2.5
2	P	230	LYS	2.5
12	L	171	PRO	2.5
7	U	241	GLU	2.5
5	S	180	LYS	2.5
6	T	241	LYS	2.5
8	V	223	ILE	2.5
2	B	203	SER	2.5
7	U	230	GLU	2.5
7	G	181	LYS	2.5
4	R	230	GLU	2.5
7	U	188	GLU	2.5
12	Z	1	GLN	2.4
1	A	248	GLU	2.4
10	X	95	ARG	2.4
14	N	105	LYS	2.4
9	I	192	ASP	2.4
3	C	1	GLY	2.4
7	U	51	PRO	2.4
3	C	51	LYS	2.4
6	T	215	CYS	2.4
6	T	230	ASP	2.4
1	A	201	GLU	2.4
7	U	3	TYR	2.4
10	J	135	TYR	2.4
3	C	175	LYS	2.4
5	S	217	LYS	2.4
13	M	82	ASP	2.4
5	S	54	GLU	2.4
3	Q	59	PRO	2.4
3	C	48	SER	2.4
3	C	181	GLU	2.4
5	S	171	LEU	2.4
12	Z	210	ASP	2.3
5	S	225	ASP	2.3
2	B	244	THR	2.3
2	B	93	HIS	2.3
6	F	242	GLU	2.3
3	C	46	ARG	2.3
6	F	228	LYS	2.3
2	P	241	THR	2.3

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Mol	Chain	Res	Type	RSRZ
13	M	1	THR	2.3
9	W	192	ASP	2.3
11	K	107	LYS	2.3
1	O	201	GLU	2.3
3	C	240	GLU	2.3
8	H	145	ASP	2.3
6	T	178	HIS	2.3
2	B	201	ASP	2.2
3	Q	37	LYS	2.2
3	C	228	ASN	2.2
4	R	242	GLU	2.2
5	E	218	ASP	2.2
3	Q	229	GLN	2.2
11	K	40	TYR	2.2
3	C	232	THR	2.2
3	C	3	ASP	2.2
12	L	168	VAL	2.2
3	C	187	GLU	2.2
11	Y	181	GLU	2.2
8	H	219	ASN	2.2
13	M	47	ASP	2.2
3	Q	55	THR	2.2
4	R	177	ASN	2.2
5	S	210	LEU	2.2
4	D	217	GLN	2.1
5	S	122	TYR	2.1
4	D	54	ASP	2.1
1	A	54	PRO	2.1
4	R	47	THR	2.1
4	R	203	LYS	2.1
13	M	121	SER	2.1
3	Q	3	ASP	2.1
7	G	222	ASP	2.1
6	T	201	GLU	2.1
9	W	160	GLU	2.1
14	N	181	ALA	2.1
3	C	188	GLU	2.1
8	V	91	GLN	2.1
4	D	47	THR	2.1
4	R	2	ARG	2.1
13	M	216	ASN	2.1
4	D	1	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	229	GLN	2.1
4	D	224	ASP	2.1
5	S	218	ASP	2.1
2	P	61	SER	2.1
6	T	166	GLN	2.1
1	A	59	GLU	2.1
10	J	49	GLU	2.1
12	Z	106	TYR	2.0
7	G	188	GLU	2.0
3	C	37	LYS	2.0
8	V	145	ASP	2.0
13	a	47	ASP	2.0
1	A	231	LYS	2.0
11	Y	208	ASN	2.0
3	Q	216	ASP	2.0
1	A	203	GLU	2.0
4	D	201	GLU	2.0
5	S	123	GLY	2.0
10	J	98	TYR	2.0
4	D	233	LYS	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
15	MG	J	201	1/1	0.89	0.36	10.01	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
17	BO2	b	201	28/28	0.88	0.19	3.27	29,39,48,49	0
17	BO2	N	201	28/28	0.86	0.20	2.76	24,37,47,47	0
17	BO2	Y	301	28/28	0.91	0.23	2.14	30,40,49,52	0
17	BO2	V	301	28/28	0.92	0.19	1.72	37,39,57,59	0
17	BO2	H	301	28/28	0.91	0.18	1.59	33,38,56,58	0
17	BO2	K	301	28/28	0.91	0.20	1.21	26,36,46,47	0
15	MG	G	301	1/1	0.92	0.14	0.50	46,46,46,46	0
15	MG	b	203	1/1	0.99	0.12	0.09	30,30,30,30	0
16	CL	N	203	1/1	1.00	0.09	-0.85	39,39,39,39	0
15	MG	N	202	1/1	0.99	0.10	-1.10	31,31,31,31	0
15	MG	Z	301	1/1	0.96	0.10	-1.83	51,51,51,51	0
15	MG	K	302	1/1	0.98	0.05	-2.16	46,46,46,46	0
15	MG	L	301	1/1	0.99	0.05	-2.47	49,49,49,49	0
16	CL	b	202	1/1	0.99	0.05	-2.59	41,41,41,41	0
15	MG	I	301	1/1	0.99	0.04	-2.85	46,46,46,46	0
16	CL	G	302	1/1	1.00	0.07	-	38,38,38,38	0
16	CL	U	301	1/1	0.99	0.15	-	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.