



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:43 PM UTC

PDB ID : 6HTB / pdb_00006htb
Title : Yeast 20S proteasome with human beta2c (S171G)
Authors : Huber, E.M.; Groll, M.
Deposited on : 2018-10-03
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

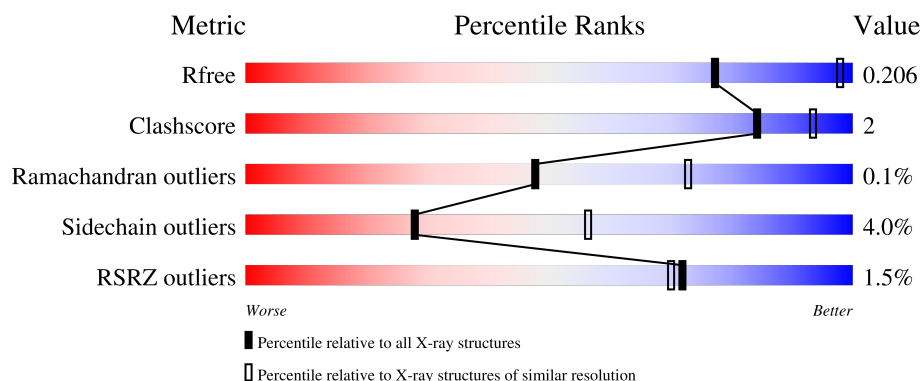
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	2% 92% ...
1	O	250	4% 89% 5% . .
2	B	258	3% 86% 8% . 5%
2	P	258	4% 84% 8% . 5%
3	C	254	2% 83% 10% . 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	 3% 84% 8% • 6%
4	D	260	 2% 84% 5% • 10%
4	R	260	 84% 6% 10%
5	E	234	 94% 5% •
5	S	234	 92% 7% •
6	F	288	 % 80% • 16%
6	T	288	 2% 80% • 16%
7	G	252	 % 89% 6% •
7	U	252	 % 89% 6% •
8	H	234	 % 78% 13% • 6%
8	V	234	 3% 80% 11% • 6%
9	I	205	 89% 10% •
9	W	205	 91% 8%
10	J	198	 2% 93% 5% • •
10	X	198	 % 94% • • •
11	K	212	 96% •
11	Y	212	 96% •
12	L	222	 93% 7%
12	Z	222	 91% 8%
13	M	246	 2% 87% • 9%
13	a	246	 2% 88% • 9%
14	N	196	 % 93% 6% •
14	b	196	 % 92% 7% •

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49877 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	240	Total	C	N	O	S	0	0	0
			1842	1171	305	362	4			
1	O	240	Total	C	N	O	S	0	0	0
			1842	1171	305	362	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-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	219	Total	C	N	O	S	0	0	0
			1648	1038	282	316	12			
8	V	219	Total	C	N	O	S	0	0	0
			1648	1038	282	316	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	171	GLY	SER	engineered mutation	UNP Q99436
V	171	GLY	SER	engineered mutation	UNP Q99436

- 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			
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	224	Total	C	N	O	S	0	0	0
			1753	1108	300	338	7			
13	a	224	Total	C	N	O	S	0	0	0
			1753	1108	300	338	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 (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	35	Total O 35 35	0	0
17	B	34	Total O 34 34	0	0
17	C	34	Total O 34 34	0	0
17	D	31	Total O 31 31	0	0
17	E	20	Total O 20 20	0	0
17	F	25	Total O 25 25	0	0
17	G	40	Total O 40 40	0	0
17	H	27	Total O 27 27	0	0
17	I	36	Total O 36 36	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	41	Total 41	O 41	0	0
17	K	54	Total 54	O 54	0	0
17	L	33	Total 33	O 33	0	0
17	M	36	Total 36	O 36	0	0
17	N	34	Total 34	O 34	0	0
17	O	17	Total 17	O 17	0	0
17	P	24	Total 24	O 24	0	0
17	Q	26	Total 26	O 26	0	0
17	R	25	Total 25	O 25	0	0
17	S	23	Total 23	O 23	0	0
17	T	29	Total 29	O 29	0	0
17	U	35	Total 35	O 35	0	0
17	V	26	Total 26	O 26	0	0
17	W	44	Total 44	O 44	0	0
17	X	45	Total 45	O 45	0	0
17	Y	41	Total 41	O 41	0	0
17	Z	41	Total 41	O 41	0	0
17	a	44	Total 44	O 44	0	0
17	b	31	Total 31	O 31	0	0

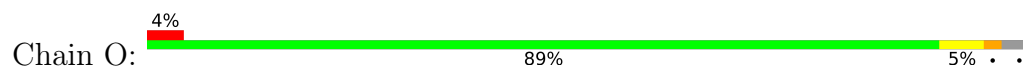
3 Residue-property plots [i](#)

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

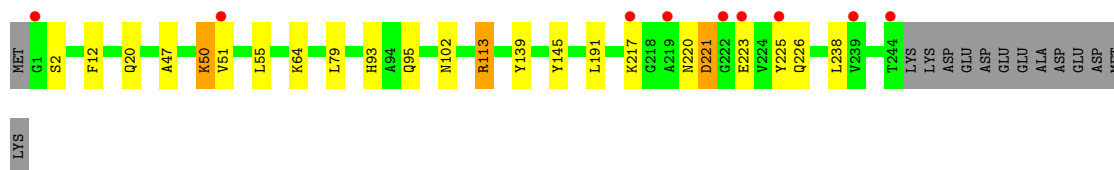
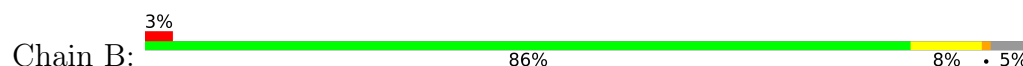
- Molecule 1: Proteasome subunit alpha type-2



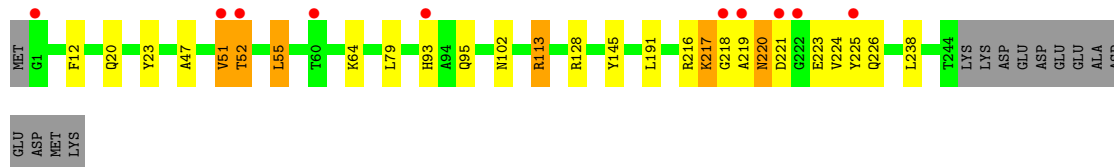
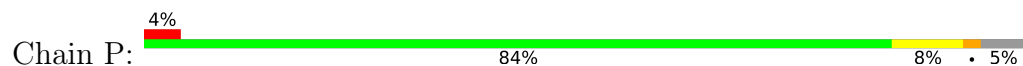
- Molecule 1: Proteasome subunit alpha type-2



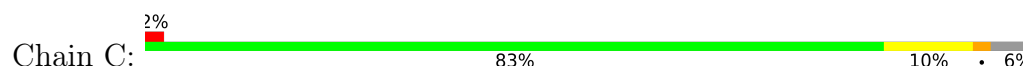
- Molecule 2: Proteasome subunit alpha type-3

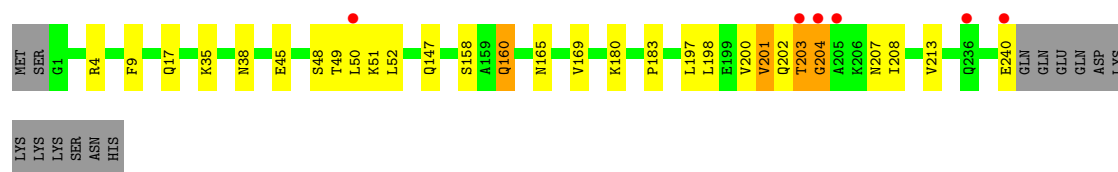


- Molecule 2: Proteasome subunit alpha type-3

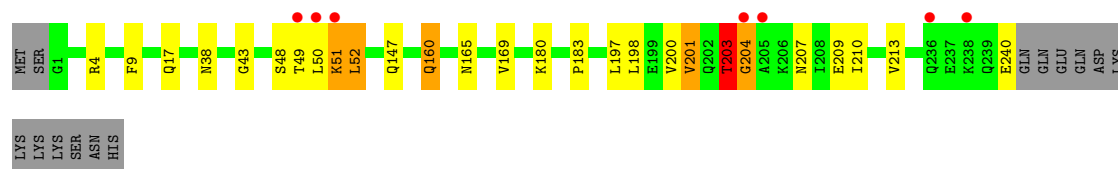
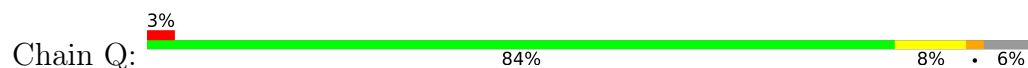


- Molecule 3: Proteasome subunit alpha type-4

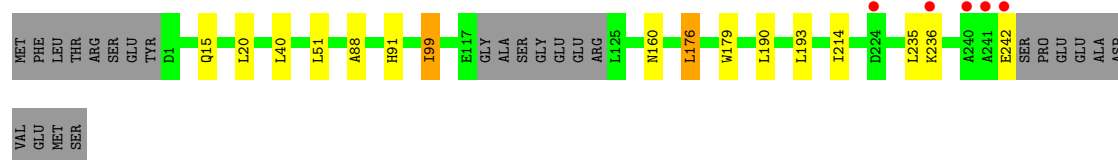
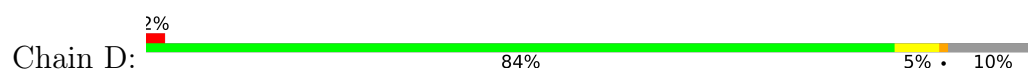




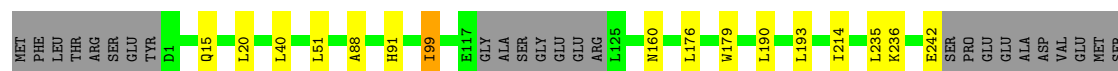
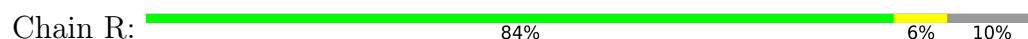
• Molecule 3: Proteasome subunit alpha type-4



• Molecule 4: Proteasome subunit alpha type-5



• Molecule 4: Proteasome subunit alpha type-5



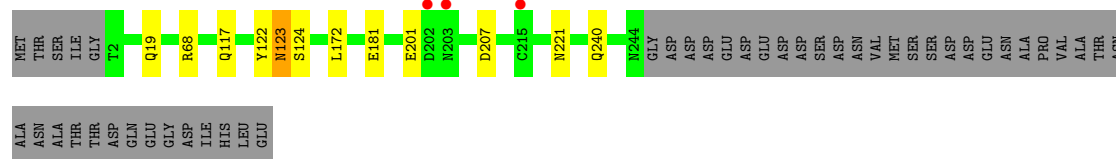
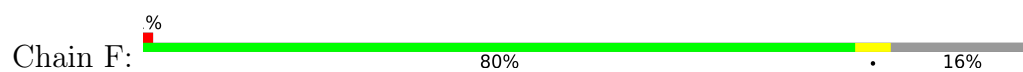
• Molecule 5: Proteasome subunit alpha type-6



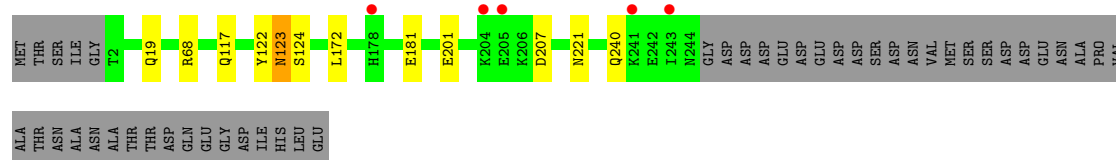
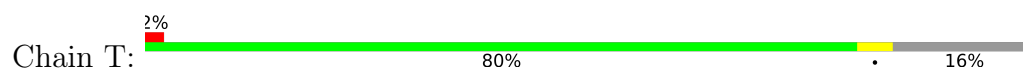
• Molecule 5: Proteasome subunit alpha type-6



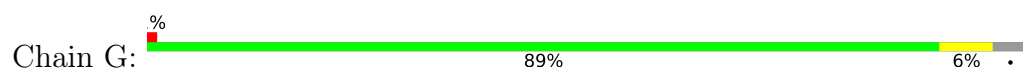
• Molecule 6: Probable proteasome subunit alpha type-7



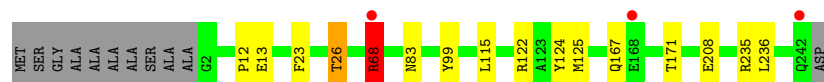
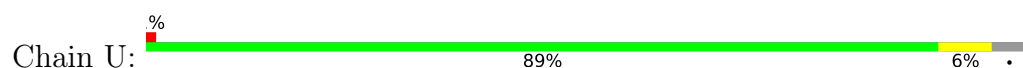
- Molecule 6: Probable proteasome subunit alpha type-7



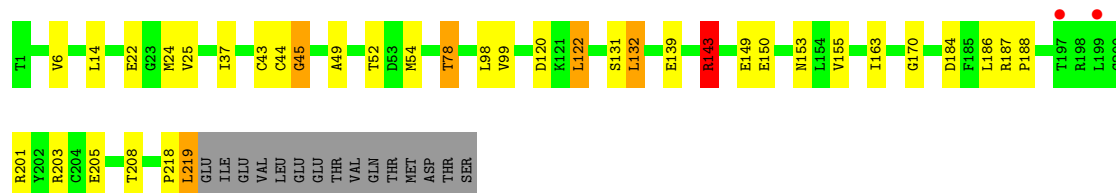
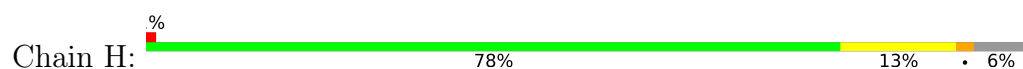
- Molecule 7: Proteasome subunit alpha type-1



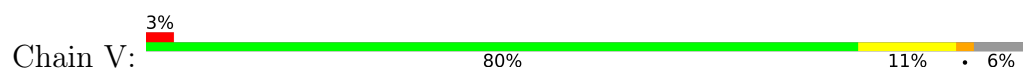
- Molecule 7: Proteasome subunit alpha type-1

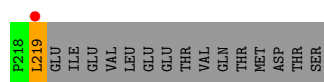


- Molecule 8: Proteasome subunit beta type-7



- Molecule 8: Proteasome subunit beta type-7





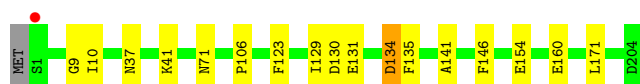
- Molecule 9: Proteasome subunit beta type-3

Chain I: 89% 10% .



- Molecule 9: Proteasome subunit beta type-3

Chain W: 91% 8%



- Molecule 10: Proteasome subunit beta type-4

Chain J: 2% 93% 5% ..



- Molecule 10: Proteasome subunit beta type-4

Chain X: % 94% . . .



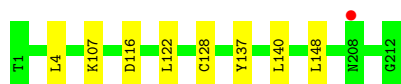
- Molecule 11: Proteasome subunit beta type-5

Chain K: 96% .

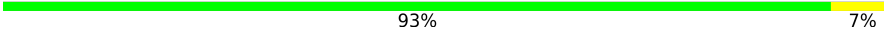


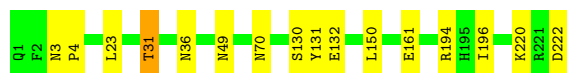
- Molecule 11: Proteasome subunit beta type-5

Chain Y: 96% .



- Molecule 12: Proteasome subunit beta type-6

Chain L:  93% 7%



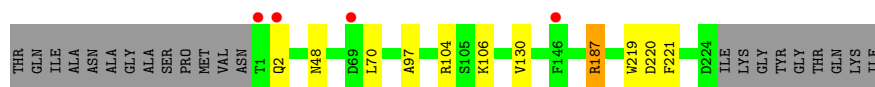
- Molecule 12: Proteasome subunit beta type-6

Chain Z:  91% 8%



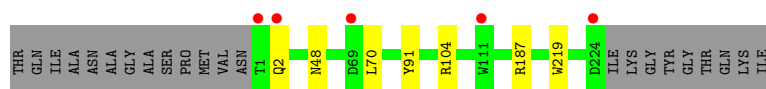
- Molecule 13: Proteasome subunit beta type-7

Chain M:  87% 2% 9%

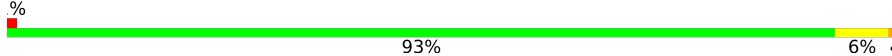


- Molecule 13: Proteasome subunit beta type-7

Chain a:  88% 2% 9%

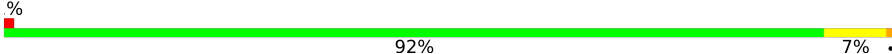


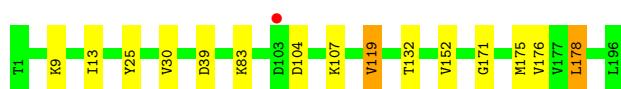
- Molecule 14: Proteasome subunit beta type-1

Chain N:  93% 6%



- Molecule 14: Proteasome subunit beta type-1

Chain b:  92% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.68Å 300.58Å 145.05Å 90.00° 113.06° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (15.00-2.70) 98.2 (15.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.193 , 0.220 (Not available) , 0.206	Depositor DCC
R_{free} test set	14322 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.689	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.9	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	49877	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.60	0/1876	0.84	2/2535 (0.1%)
1	O	0.61	0/1876	0.87	6/2535 (0.2%)
2	B	0.60	0/1934	0.83	1/2618 (0.0%)
2	P	0.59	0/1934	0.88	4/2618 (0.2%)
3	C	0.58	0/1910	0.85	3/2586 (0.1%)
3	Q	0.58	0/1910	0.88	3/2586 (0.1%)
4	D	0.51	0/1837	0.79	0/2475
4	R	0.50	0/1837	0.78	0/2475
5	E	0.52	0/1800	0.75	0/2433
5	S	0.52	0/1800	0.76	0/2433
6	F	0.52	0/1932	0.79	0/2609
6	T	0.53	0/1932	0.79	0/2609
7	G	0.52	0/1945	0.81	1/2634 (0.0%)
7	U	0.54	1/1945 (0.1%)	0.85	6/2634 (0.2%)
8	H	0.69	0/1675	1.03	8/2267 (0.4%)
8	V	0.52	1/1675 (0.1%)	0.94	4/2267 (0.2%)
9	I	0.71	0/1611	0.87	3/2174 (0.1%)
9	W	0.64	0/1611	0.87	3/2174 (0.1%)
10	J	0.52	0/1589	0.77	0/2142
10	X	0.52	0/1589	0.77	0/2142
11	K	0.49	0/1681	0.78	0/2274
11	Y	0.49	0/1681	0.78	0/2274
12	L	0.49	0/1795	0.76	0/2420
12	Z	0.50	0/1795	0.76	0/2420
13	M	0.56	0/1783	0.81	1/2420 (0.0%)
13	a	0.53	0/1783	0.79	0/2420
14	N	0.49	0/1541	0.77	0/2087
14	b	0.49	0/1541	0.77	0/2087
All	All	0.55	2/49818 (0.0%)	0.82	45/67348 (0.1%)

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
7	U	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	68	ARG	CZ-NH2	-6.15	1.25	1.33
8	V	35	HIS	CE1-NE2	5.26	1.37	1.32

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	204	GLY	N-CA-C	13.11	127.01	111.93
8	H	143	ARG	NE-CZ-NH2	12.48	130.43	119.20
8	H	143	ARG	NE-CZ-NH1	-11.73	109.77	121.50
8	V	219	LEU	CD1-CG-CD2	-11.29	85.96	110.80
8	H	219	LEU	CD1-CG-CD2	-10.55	87.58	110.80
9	W	134	ASP	N-CA-C	9.35	121.24	111.14
1	A	2	THR	N-CA-C	-8.93	93.67	108.76
7	G	68	ARG	NE-CZ-NH2	8.70	127.03	119.20
7	U	68	ARG	CG-CD-NE	-8.22	93.91	112.00
2	P	55	LEU	N-CA-C	8.13	122.47	112.54
8	H	143	ARG	CD-NE-CZ	7.67	135.13	124.40
8	V	143	ARG	NE-CZ-NH2	-7.67	112.30	119.20
9	I	127	GLY	N-CA-C	7.53	125.89	115.27
1	O	2	THR	N-CA-C	-7.39	96.86	108.90
7	U	68	ARG	NE-CZ-NH2	-7.35	112.58	119.20
7	U	68	ARG	NE-CZ-NH1	7.31	128.81	121.50
8	V	143	ARG	CD-NE-CZ	6.79	133.90	124.40
1	O	3	ASP	N-CA-C	-6.75	96.62	108.23
8	H	37	ILE	N-CA-C	-6.57	105.30	111.48
7	U	68	ARG	CD-NE-CZ	6.46	133.44	124.40
2	P	224	VAL	N-CA-C	6.42	117.94	109.21
3	C	203	THR	N-CA-C	6.17	117.53	108.14
2	P	217	LYS	N-CA-C	-6.13	105.67	113.02
8	H	49	ALA	N-CA-C	6.08	117.90	111.28
2	P	221	ASP	N-CA-C	5.99	119.83	111.74
3	C	201	VAL	N-CA-C	5.92	116.70	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	204	GLY	N-CA-C	5.90	120.15	112.25
1	A	3	ASP	N-CA-C	-5.87	99.57	108.67
7	U	68	ARG	CA-CB-CG	-5.77	102.56	114.10
2	B	220	ASN	N-CA-C	-5.72	101.38	109.96
9	W	130	ASP	N-CA-C	-5.51	99.53	108.52
1	O	218	ASN	CB-CA-C	-5.47	103.86	110.15
7	U	68	ARG	CB-CG-CD	5.43	123.78	111.30
9	W	129	ILE	N-CA-C	5.41	116.03	108.89
8	V	143	ARG	NE-CZ-NH1	5.41	126.91	121.50
13	M	220	ASP	N-CA-C	5.32	117.83	111.71
9	I	130	ASP	N-CA-C	-5.30	99.14	108.20
1	O	232	GLY	CA-C-N	-5.28	114.29	119.99
1	O	232	GLY	C-N-CA	-5.28	114.29	119.99
9	I	133	LYS	N-CA-C	5.27	117.94	111.82
1	O	105	PRO	O-C-N	5.13	123.56	121.15
3	Q	203	THR	CA-C-N	5.10	124.94	120.10
3	Q	203	THR	C-N-CA	5.10	124.94	120.10
8	H	22	GLU	N-CA-C	-5.02	99.23	108.02
8	H	45	GLY	N-CA-C	5.01	119.91	111.04

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	68	ARG	Sidechain
7	U	68	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	1842	0	1855	8	0
1	O	1842	0	1855	18	0
2	B	1904	0	1904	24	0
2	P	1904	0	1904	23	0
3	C	1881	0	1895	17	0
3	Q	1881	0	1894	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1813	0	1797	7	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	8	0
5	S	1773	0	1775	8	0
6	F	1892	0	1883	4	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	8	0
8	H	1648	0	1673	23	0
8	V	1648	0	1673	20	0
9	I	1581	0	1574	14	0
9	W	1581	0	1574	8	0
10	J	1561	0	1569	4	0
10	X	1561	0	1569	3	0
11	K	1644	0	1595	3	0
11	Y	1644	0	1595	3	0
12	L	1757	0	1711	10	0
12	Z	1757	0	1711	9	0
13	M	1753	0	1754	6	0
13	a	1753	0	1754	2	0
14	N	1512	0	1481	8	0
14	b	1512	0	1481	11	0
15	G	1	0	0	0	0
15	I	2	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	W	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	A	35	0	0	0	0
17	B	34	0	0	3	0
17	C	34	0	0	0	0
17	D	31	0	0	0	0
17	E	20	0	0	0	0
17	F	25	0	0	0	0
17	G	40	0	0	0	0
17	H	27	0	0	0	0
17	I	36	0	0	0	0
17	J	41	0	0	0	0
17	K	54	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	L	33	0	0	0	0
17	M	36	0	0	1	0
17	N	34	0	0	0	0
17	O	17	0	0	0	0
17	P	24	0	0	2	0
17	Q	26	0	0	0	0
17	R	25	0	0	0	0
17	S	23	0	0	1	0
17	T	29	0	0	0	0
17	U	35	0	0	0	0
17	V	26	0	0	0	0
17	W	44	0	0	0	0
17	X	45	0	0	0	0
17	Y	41	0	0	0	0
17	Z	41	0	0	0	0
17	a	44	0	0	0	0
17	b	31	0	0	0	0
All	All	49877	0	48733	227	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 2.

All (227) 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)
3:Q:197:LEU:O	3:Q:201:VAL:CG2	1.85	1.23
3:Q:197:LEU:O	3:Q:201:VAL:HG23	0.94	1.12
3:Q:203:THR:HG22	3:Q:204:GLY:H	1.22	1.02
3:Q:197:LEU:C	3:Q:201:VAL:HG23	1.84	1.00
3:Q:165:ASN:HB2	3:Q:200:VAL:HG11	1.50	0.94
2:B:145:TYR:OH	2:B:217:LYS:N	2.01	0.93
2:B:145:TYR:OH	2:B:217:LYS:HB2	1.69	0.91
3:C:203:THR:HG22	3:C:204:GLY:N	1.89	0.88
3:C:202:GLN:O	3:C:203:THR:OG1	1.93	0.87
3:C:203:THR:CG2	3:C:204:GLY:H	1.87	0.87
3:C:203:THR:HG22	3:C:204:GLY:H	1.39	0.85
1:A:4:ARG:HB2	2:B:2:SER:OG	1.77	0.85
3:Q:209:GLU:O	3:Q:210:ILE:HD13	1.77	0.84
3:Q:165:ASN:CB	3:Q:200:VAL:HG11	2.07	0.84
2:B:145:TYR:OH	2:B:217:LYS:CB	2.26	0.83
8:V:143:ARG:NH1	8:V:150:GLU:OE1	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:220:LYS:HE3	12:L:222:ASP:OD1	1.80	0.81
2:P:51:VAL:HG12	2:P:52:THR:H	1.45	0.81
12:Z:220:LYS:HE3	12:Z:222:ASP:OD1	1.83	0.79
2:P:219:ALA:HB3	2:P:223:GLU:O	1.82	0.78
3:Q:203:THR:HG22	3:Q:204:GLY:N	2.02	0.74
8:H:143:ARG:NH1	8:H:150:GLU:OE1	2.23	0.72
2:P:51:VAL:HG12	2:P:52:THR:N	2.03	0.71
8:H:149:GLU:O	8:H:153:ASN:ND2	2.20	0.71
1:A:4:ARG:CB	2:B:2:SER:OG	2.38	0.70
8:V:184:ASP:HB3	8:V:186:LEU:HD11	1.73	0.70
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.56	0.70
8:H:184:ASP:HB3	8:H:186:LEU:HD11	1.76	0.68
2:B:221:ASP:C	17:B:301:HOH:O	2.22	0.68
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.58	0.67
2:B:12:PHE:H	3:C:17:GLN:HE22	1.43	0.67
7:G:68:ARG:NH1	14:N:39:ASP:OD2	2.29	0.66
3:C:48:SER:HB2	3:C:207:ASN:HD21	1.62	0.64
1:A:4:ARG:HD3	5:E:122:TYR:HD2	1.63	0.64
2:P:225:TYR:CE1	2:P:226:GLN:O	2.51	0.64
3:C:165:ASN:HB2	3:C:200:VAL:HG11	1.80	0.63
1:O:12:PHE:H	2:P:20:GLN:HE22	1.45	0.63
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.45	0.63
5:E:12:PHE:H	6:F:19:GLN:HE22	1.45	0.63
2:B:145:TYR:OH	2:B:217:LYS:CA	2.47	0.62
5:S:12:PHE:H	6:T:19:GLN:HE22	1.45	0.62
2:B:145:TYR:HH	2:B:217:LYS:H	1.43	0.62
1:A:4:ARG:HB2	2:B:2:SER:CB	2.28	0.61
3:Q:197:LEU:HB3	3:Q:201:VAL:HG21	1.82	0.61
1:O:1:MET:HE3	7:U:124:TYR:HE2	1.64	0.61
8:H:219:LEU:HD11	9:I:194:VAL:HG23	1.82	0.61
3:C:202:GLN:O	3:C:202:GLN:HG3	1.99	0.61
7:G:23:PHE:O	7:G:26:THR:HB	2.01	0.60
14:b:152:VAL:HA	14:b:175:MET:HE1	1.83	0.60
8:H:132:LEU:HD22	14:N:25:TYR:CE1	2.37	0.59
3:Q:197:LEU:C	3:Q:201:VAL:CG2	2.56	0.59
1:O:230:ASP:N	1:O:230:ASP:OD1	2.36	0.59
1:A:12:PHE:H	2:B:20:GLN:HE22	1.50	0.59
8:H:218:PRO:C	8:H:219:LEU:HG	2.28	0.59
3:Q:48:SER:HB2	3:Q:207:ASN:ND2	2.18	0.59
8:V:132:LEU:HD22	14:b:25:TYR:CE1	2.37	0.59
1:O:2:THR:OG1	1:O:4:ARG:HD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.49	0.58
3:Q:200:VAL:HG12	3:Q:200:VAL:O	2.02	0.58
2:B:51:VAL:O	2:B:51:VAL:HG22	2.02	0.58
14:N:152:VAL:HA	14:N:175:MET:HE1	1.85	0.58
2:B:139:TYR:OH	2:B:217:LYS:HE2	2.04	0.57
8:H:184:ASP:HB3	8:H:186:LEU:CD1	2.34	0.57
9:I:15:THR:HG23	9:I:120:ILE:HG12	1.86	0.57
7:G:99:TYR:O	8:H:78:THR:HB	2.04	0.57
13:M:221:PHE:CE2	14:b:30:VAL:HG21	2.39	0.57
8:V:184:ASP:HB3	8:V:186:LEU:CD1	2.34	0.57
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.17	0.57
2:P:51:VAL:O	2:P:52:THR:HG23	2.04	0.57
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.87	0.57
2:P:93:HIS:HB3	17:P:301:HOH:O	2.04	0.56
7:U:23:PHE:O	7:U:26:THR:HB	2.04	0.56
2:B:50:LYS:O	2:B:51:VAL:HG12	2.06	0.56
7:U:68:ARG:NH1	14:b:39:ASP:OD2	2.39	0.56
8:H:45:GLY:HA3	8:H:52:THR:HG21	1.88	0.55
6:T:123:ASN:C	6:T:123:ASN:HD22	2.15	0.55
3:Q:203:THR:CG2	3:Q:204:GLY:H	2.03	0.55
2:P:51:VAL:C	2:P:52:THR:HG23	2.31	0.55
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.88	0.55
2:B:145:TYR:HH	2:B:217:LYS:CB	2.19	0.55
9:I:120:ILE:HD12	9:I:136:ILE:HG12	1.88	0.55
1:O:1:MET:CE	7:U:124:TYR:HE2	2.18	0.55
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.42	0.55
6:F:123:ASN:C	6:F:123:ASN:HD22	2.15	0.55
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.19	0.55
8:H:143:ARG:NH1	8:H:150:GLU:CD	2.65	0.54
12:Z:31:THR:HG22	12:Z:36:ASN:HD21	1.73	0.54
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.55	0.53
2:P:216:ARG:HB3	2:P:218:GLY:H	1.73	0.53
3:Q:204:GLY:O	3:Q:207:ASN:N	2.41	0.53
12:L:31:THR:HG22	12:L:36:ASN:HD21	1.73	0.53
2:P:220:ASN:OD1	2:P:220:ASN:N	2.42	0.53
8:V:45:GLY:HA3	8:V:52:THR:HG21	1.90	0.53
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.92	0.52
8:V:186:LEU:N	8:V:186:LEU:HD12	2.24	0.52
8:V:143:ARG:NH1	8:V:150:GLU:CD	2.68	0.52
6:T:123:ASN:HD22	6:T:124:SER:N	2.08	0.52
3:C:197:LEU:HD13	3:C:208:ILE:HG23	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1:MET:HG3	6:T:122:TYR:CE1	2.45	0.51
8:H:186:LEU:HD12	8:H:186:LEU:N	2.26	0.51
3:Q:48:SER:HB2	3:Q:207:ASN:HD21	1.76	0.51
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.58	0.51
1:O:2:THR:OG1	1:O:4:ARG:HG2	2.11	0.51
1:A:4:ARG:HD3	5:E:122:TYR:CD2	2.45	0.51
2:P:145:TYR:OH	2:P:217:LYS:HB2	2.11	0.51
1:O:218:ASN:O	1:O:233:PRO:HD2	2.11	0.50
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.93	0.50
2:P:217:LYS:C	2:P:219:ALA:H	2.20	0.50
3:C:45:GLU:HG3	3:C:201:VAL:HG22	1.92	0.50
9:I:123:PHE:CD1	9:I:123:PHE:N	2.80	0.50
6:F:123:ASN:HD22	6:F:124:SER:N	2.10	0.50
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.47	0.49
13:M:221:PHE:HE2	14:b:30:VAL:HG21	1.75	0.49
8:H:25:VAL:HG11	9:I:146:PHE:CD2	2.47	0.49
3:Q:197:LEU:HB3	3:Q:201:VAL:CG2	2.42	0.49
8:H:143:ARG:NH1	8:H:150:GLU:OE2	2.46	0.49
3:C:9:PHE:H	4:D:15:GLN:HE22	1.60	0.49
13:M:106:LYS:HE3	17:M:330:HOH:O	2.13	0.49
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.48	0.48
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.96	0.48
8:H:44:CYS:HB2	8:H:99:VAL:HB	1.95	0.48
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.49	0.48
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.11	0.47
8:H:120:ASP:HB3	8:H:122:LEU:HD22	1.96	0.47
8:V:44:CYS:HB2	8:V:99:VAL:HB	1.95	0.47
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.96	0.47
9:W:134:ASP:OD1	9:W:135:PHE:N	2.47	0.47
8:V:205:GLU:O	8:V:208:THR:OG1	2.30	0.47
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.45	0.47
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.97	0.47
3:Q:198:LEU:HD23	3:Q:198:LEU:HA	1.74	0.47
1:O:5:TYR:HB3	1:O:126:GLY:CA	2.44	0.47
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.50	0.47
2:B:113:ARG:NE	17:B:302:HOH:O	2.47	0.47
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.45	0.47
1:O:2:THR:OG1	1:O:4:ARG:CG	2.63	0.47
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.97	0.46
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.97	0.46
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:217:LYS:C	2:P:219:ALA:N	2.73	0.46
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.97	0.46
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.97	0.46
8:V:25:VAL:HG11	9:W:146:PHE:CD2	2.50	0.46
8:H:205:GLU:O	8:H:208:THR:OG1	2.33	0.46
2:B:145:TYR:CZ	2:B:217:LYS:HB2	2.49	0.46
8:V:187:ARG:HA	8:V:188:PRO:HA	1.78	0.46
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.64	0.46
1:O:5:TYR:HB3	1:O:126:GLY:HA2	1.98	0.45
9:W:106:PRO:HD2	9:W:123:PHE:HB2	1.97	0.45
12:L:196:ILE:HD11	8:V:24:MET:HE2	1.98	0.45
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.81	0.45
2:B:225:TYR:CE1	2:B:226:GLN:O	2.69	0.45
8:H:6:VAL:HG22	8:H:155:VAL:CG2	2.47	0.45
3:C:203:THR:HG23	3:C:204:GLY:H	1.75	0.45
8:V:6:VAL:HG22	8:V:155:VAL:CG2	2.47	0.45
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.51	0.45
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.15	0.44
2:P:51:VAL:O	2:P:52:THR:OG1	2.22	0.44
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.14	0.44
5:S:147:GLN:NE2	17:S:302:HOH:O	2.50	0.44
1:A:1:MET:HG3	6:F:122:TYR:CE1	2.52	0.44
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.99	0.44
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.47	0.44
1:O:1:MET:HE3	7:U:124:TYR:CE2	2.50	0.44
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.83	0.43
9:I:37:ASN:C	9:I:37:ASN:HD22	2.26	0.43
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.49	0.43
2:P:220:ASN:O	2:P:223:GLU:HG2	2.18	0.43
7:U:99:TYR:O	8:V:78:THR:HB	2.19	0.43
14:b:13:ILE:HG21	14:b:175:MET:HE2	2.00	0.43
2:B:50:LYS:C	2:B:51:VAL:HG12	2.43	0.43
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.16	0.43
3:C:202:GLN:C	3:C:203:THR:HG1	2.01	0.43
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.99	0.43
8:H:54:MET:HG3	9:I:95:TYR:CG	2.54	0.43
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.53	0.43
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.00	0.43
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.00	0.42
1:O:4:ARG:HD3	5:S:122:TYR:CD2	2.52	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.84	0.42
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.42
5:S:98:PHE:O	13:a:91:TYR:HA	2.19	0.42
8:V:203:ARG:HH11	9:W:154:GLU:CD	2.28	0.42
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.55	0.42
8:V:153:ASN:N	8:V:153:ASN:HD22	2.17	0.42
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.48	0.42
8:V:149:GLU:O	8:V:153:ASN:ND2	2.53	0.42
3:C:198:LEU:HA	3:C:198:LEU:HD23	1.81	0.42
12:Z:131:TYR:O	12:Z:132:GLU:HG3	2.20	0.42
8:H:139:GLU:OE2	8:H:139:GLU:HA	2.20	0.41
12:L:194:ARG:O	8:V:25:VAL:HA	2.19	0.41
3:C:35:LYS:HG2	3:C:158:SER:O	2.20	0.41
3:C:48:SER:HB2	3:C:207:ASN:ND2	2.33	0.41
3:Q:43:GLY:HA2	3:Q:210:ILE:HD13	2.01	0.41
1:A:4:ARG:HB3	2:B:2:SER:OG	2.19	0.41
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.02	0.41
4:D:91:HIS:HB3	4:D:99:ILE:HG22	2.03	0.41
3:Q:209:GLU:C	3:Q:210:ILE:HD13	2.44	0.41
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.03	0.41
2:B:93:HIS:HB3	17:B:302:HOH:O	2.20	0.41
8:H:25:VAL:HA	12:Z:194:ARG:O	2.20	0.41
8:H:203:ARG:HH11	9:I:154:GLU:CD	2.28	0.41
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.03	0.41
1:O:4:ARG:HD3	5:S:122:TYR:HD2	1.86	0.41
8:H:187:ARG:HA	8:H:188:PRO:HA	1.80	0.41
12:L:131:TYR:O	12:L:132:GLU:HG3	2.21	0.41
14:N:133:PHE:HA	14:b:132:THR:O	2.21	0.41
14:b:176:VAL:HG12	14:b:178:LEU:HD13	2.02	0.41
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.03	0.41
13:M:187:ARG:HG3	14:b:25:TYR:CE1	2.56	0.41
2:P:113:ARG:NE	17:P:301:HOH:O	2.43	0.41
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.03	0.41
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.56	0.41
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.19	0.41
8:V:139:GLU:OE2	8:V:139:GLU:HA	2.20	0.41
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.86	0.41
5:S:68:HIS:HE1	5:S:102:LEU:O	2.04	0.41
1:O:2:THR:OG1	1:O:4:ARG:CD	2.69	0.40
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.86	0.40
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.57	0.40
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.04	0.40
2:P:51:VAL:O	2:P:52:THR:CB	2.68	0.40
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.69	0.40
7:G:165:LYS:HD2	7:G:205:LEU:HD22	2.04	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	236/250 (94%)	230 (98%)	6 (2%)	0	100	100
1	O	236/250 (94%)	229 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	237 (98%)	5 (2%)	0	100	100
2	P	242/258 (94%)	237 (98%)	3 (1%)	2 (1%)	16	37
3	C	238/254 (94%)	236 (99%)	1 (0%)	1 (0%)	30	54
3	Q	238/254 (94%)	234 (98%)	2 (1%)	2 (1%)	16	37
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	217/234 (93%)	215 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	V	217/234 (93%)	216 (100%)	1 (0%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	198 (98%)	4 (2%)	0	100	100
10	J	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	205 (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	222/246 (90%)	215 (97%)	7 (3%)	0	100	100
13	a	222/246 (90%)	216 (97%)	6 (3%)	0	100	100
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6228/6618 (94%)	6106 (98%)	117 (2%)	5 (0%)	48	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	52	THR
3	Q	203	THR
2	P	51	VAL
3	Q	183	PRO
3	C	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	201/209 (96%)	193 (96%)	8 (4%)	28	56
1	O	201/209 (96%)	195 (97%)	6 (3%)	36	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	203/216 (94%)	194 (96%)	9 (4%)	25	53
2	P	203/216 (94%)	196 (97%)	7 (3%)	32	62
3	C	212/226 (94%)	200 (94%)	12 (6%)	18	43
3	Q	212/226 (94%)	199 (94%)	13 (6%)	17	40
4	D	194/215 (90%)	183 (94%)	11 (6%)	18	43
4	R	194/215 (90%)	183 (94%)	11 (6%)	18	43
5	E	190/193 (98%)	183 (96%)	7 (4%)	30	59
5	S	190/193 (98%)	183 (96%)	7 (4%)	30	59
6	F	201/239 (84%)	192 (96%)	9 (4%)	24	52
6	T	201/239 (84%)	192 (96%)	9 (4%)	24	52
7	G	206/210 (98%)	197 (96%)	9 (4%)	25	53
7	U	206/210 (98%)	197 (96%)	9 (4%)	25	53
8	H	179/194 (92%)	169 (94%)	10 (6%)	19	44
8	V	179/194 (92%)	168 (94%)	11 (6%)	17	40
9	I	172/173 (99%)	167 (97%)	5 (3%)	37	67
9	W	172/173 (99%)	168 (98%)	4 (2%)	44	73
10	J	173/175 (99%)	168 (97%)	5 (3%)	37	67
10	X	173/175 (99%)	168 (97%)	5 (3%)	37	67
11	K	169/169 (100%)	164 (97%)	5 (3%)	36	66
11	Y	169/169 (100%)	164 (97%)	5 (3%)	36	66
12	L	185/185 (100%)	179 (97%)	6 (3%)	34	64
12	Z	185/185 (100%)	179 (97%)	6 (3%)	34	64
13	M	192/208 (92%)	187 (97%)	5 (3%)	40	70
13	a	192/208 (92%)	187 (97%)	5 (3%)	40	70
14	N	162/162 (100%)	157 (97%)	5 (3%)	35	65
14	b	162/162 (100%)	157 (97%)	5 (3%)	35	65
All	All	5278/5548 (95%)	5069 (96%)	209 (4%)	28	56

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	THR

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Mol	Chain	Res	Type
1	A	4	ARG
1	A	6	SER
1	A	59	GLU
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	79	LEU
2	B	102	ASN
2	B	113	ARG
2	B	191	LEU
2	B	221	ASP
2	B	223	GLU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	49	THR
3	C	50	LEU
3	C	51	LYS
3	C	52	LEU
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	213	VAL
3	C	240	GLU
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	99	ILE
4	D	176	LEU
4	D	190	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	55	LEU
5	E	71	LEU

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Mol	Chain	Res	Type
5	E	188	LEU
5	E	207	VAL
5	E	231	LYS
6	F	68	ARG
6	F	117	GLN
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	207	ASP
6	F	221	ASN
6	F	240	GLN
7	G	13	GLU
7	G	26	THR
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	14	LEU
8	H	24	MET
8	H	43	CYS
8	H	78	THR
8	H	98	LEU
8	H	122	LEU
8	H	131	SER
8	H	132	LEU
8	H	143	ARG
8	H	201	ARG
9	I	37	ASN
9	I	120	ILE
9	I	131	GLU
9	I	160	GLU
9	I	171	LEU
10	J	2	ASP
10	J	3	ILE
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU

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Mol	Chain	Res	Type
11	K	107	LYS
11	K	116	ASP
11	K	140	LEU
11	K	148	LEU
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	130	SER
12	L	150	LEU
12	L	161	GLU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	187	ARG
14	N	9	LYS
14	N	104	ASP
14	N	107	LYS
14	N	119	VAL
14	N	178	LEU
1	O	4	ARG
1	O	59	GLU
1	O	122	THR
1	O	157	PHE
1	O	230	ASP
1	O	250	LEU
2	P	55	LEU
2	P	79	LEU
2	P	102	ASN
2	P	113	ARG
2	P	191	LEU
2	P	220	ASN
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	49	THR
3	Q	50	LEU
3	Q	51	LYS
3	Q	52	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL

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Mol	Chain	Res	Type
3	Q	180	LYS
3	Q	201	VAL
3	Q	213	VAL
3	Q	240	GLU
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	99	ILE
4	R	176	LEU
4	R	190	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	55	LEU
5	S	71	LEU
5	S	188	LEU
5	S	207	VAL
5	S	231	LYS
6	T	68	ARG
6	T	117	GLN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	207	ASP
6	T	221	ASN
6	T	240	GLN
7	U	13	GLU
7	U	26	THR
7	U	83	ASN
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	14	LEU
8	V	24	MET

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Mol	Chain	Res	Type
8	V	43	CYS
8	V	78	THR
8	V	98	LEU
8	V	131	SER
8	V	132	LEU
8	V	143	ARG
8	V	153	ASN
8	V	201	ARG
8	V	219	LEU
9	W	37	ASN
9	W	131	GLU
9	W	160	GLU
9	W	171	LEU
10	X	2	ASP
10	X	3	ILE
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	107	LYS
11	Y	116	ASP
11	Y	140	LEU
11	Y	148	LEU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	130	SER
12	Z	150	LEU
12	Z	161	GLU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	187	ARG
14	b	9	LYS
14	b	104	ASP
14	b	107	LYS
14	b	119	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (153) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	176	GLN
2	B	232	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	165	ASN
3	C	207	ASN
4	D	15	GLN
4	D	91	HIS
4	D	106	GLN
4	D	146	GLN
4	D	160	ASN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN

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Mol	Chain	Res	Type
8	H	35	HIS
8	H	80	ASN
9	I	37	ASN
9	I	63	ASN
9	I	203	GLN
10	J	10	GLN
10	J	55	GLN
10	J	61	GLN
10	J	63	ASN
10	J	112	ASN
11	K	9	GLN
11	K	85	ASN
11	K	143	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	79	HIS
12	L	80	ASN
12	L	155	ASN
12	L	158	ASN
12	L	159	GLN
13	M	48	ASN
13	M	102	GLN
13	M	194	ASN
13	M	213	GLN
14	N	69	GLN
14	N	141	ASN
14	N	161	GLN
1	O	218	ASN
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	176	GLN
2	P	232	GLN
3	Q	17	GLN

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Mol	Chain	Res	Type
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	202	GLN
4	R	15	GLN
4	R	91	HIS
4	R	106	GLN
4	R	146	GLN
4	R	160	ASN
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
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
8	V	80	ASN
8	V	153	ASN
9	W	37	ASN
9	W	63	ASN
9	W	88	GLN
9	W	203	GLN
10	X	10	GLN

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Mol	Chain	Res	Type
10	X	55	GLN
10	X	63	ASN
10	X	86	GLN
10	X	112	ASN
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	153	GLN
12	Z	155	ASN
12	Z	158	ASN
12	Z	159	GLN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	149	HIS
14	b	69	GLN
14	b	141	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	240/250 (96%)	-0.16	5 (2%) 63 61	40, 58, 95, 134	0
1	O	240/250 (96%)	-0.04	9 (3%) 44 40	44, 65, 111, 144	0
2	B	244/258 (94%)	-0.04	9 (3%) 45 41	38, 58, 105, 154	0
2	P	244/258 (94%)	-0.13	10 (4%) 41 37	42, 59, 103, 153	0
3	C	240/254 (94%)	-0.13	6 (2%) 58 55	37, 60, 120, 152	0
3	Q	240/254 (94%)	-0.03	7 (2%) 53 50	42, 69, 147, 174	0
4	D	235/260 (90%)	-0.30	5 (2%) 63 61	42, 59, 91, 134	0
4	R	235/260 (90%)	-0.25	0 100 100	46, 65, 103, 134	0
5	E	231/234 (98%)	-0.21	1 (0%) 88 87	44, 61, 98, 138	0
5	S	231/234 (98%)	-0.08	1 (0%) 88 87	44, 66, 102, 142	0
6	F	243/288 (84%)	-0.23	3 (1%) 76 75	38, 55, 105, 133	0
6	T	243/288 (84%)	-0.17	5 (2%) 63 61	38, 62, 114, 144	0
7	G	241/252 (95%)	-0.34	2 (0%) 82 81	36, 51, 86, 135	0
7	U	241/252 (95%)	-0.24	3 (1%) 76 75	40, 55, 86, 128	0
8	H	219/234 (93%)	-0.27	2 (0%) 81 80	32, 51, 101, 114	0
8	V	219/234 (93%)	-0.16	7 (3%) 50 46	37, 55, 110, 127	0
9	I	204/205 (99%)	-0.53	1 (0%) 87 86	33, 47, 72, 93	0
9	W	204/205 (99%)	-0.53	1 (0%) 87 86	36, 48, 79, 102	0
10	J	195/198 (98%)	-0.39	3 (1%) 72 70	36, 50, 75, 128	0
10	X	195/198 (98%)	-0.39	2 (1%) 79 78	36, 52, 77, 138	0
11	K	212/212 (100%)	-0.53	0 100 100	31, 48, 70, 91	0
11	Y	212/212 (100%)	-0.50	1 (0%) 87 86	37, 49, 72, 93	0
12	L	222/222 (100%)	-0.38	0 100 100	36, 51, 84, 115	0
12	Z	222/222 (100%)	-0.42	0 100 100	37, 51, 84, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	224/246 (91%)	-0.32	4 (1%) 67 65	35, 54, 80, 112	0
13	a	224/246 (91%)	-0.32	5 (2%) 62 59	35, 51, 75, 107	0
14	N	196/196 (100%)	-0.48	1 (0%) 87 86	33, 46, 75, 104	0
14	b	196/196 (100%)	-0.47	1 (0%) 87 86	34, 47, 74, 110	0
All	All	6292/6618 (95%)	-0.28	94 (1%) 72 70	31, 55, 98, 174	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	5.2
13	a	1	THR	5.0
10	J	1	MET	4.6
3	Q	50	LEU	4.5
13	M	1	THR	4.1
1	O	2	THR	3.8
2	B	51	VAL	3.8
2	B	219	ALA	3.5
6	T	205	GLU	3.5
2	P	219	ALA	3.5
6	T	243	ILE	3.4
3	C	203	THR	3.4
2	B	1	GLY	3.3
8	V	219	LEU	3.3
13	a	2	GLN	3.3
2	B	217	LYS	3.2
1	A	1	MET	3.2
2	P	225	TYR	3.2
4	D	240	ALA	3.2
2	P	1	GLY	3.2
8	V	196	GLY	3.2
3	Q	205	ALA	3.1
2	B	223	GLU	3.0
4	D	241	ALA	3.0
1	O	219	PRO	3.0
2	P	51	VAL	2.9
8	H	199	LEU	2.9
2	P	221	ASP	2.9
6	T	204	LYS	2.9
10	J	98	TYR	2.9
14	b	103	ASP	2.9
6	T	241	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	O	1	MET	2.8
2	B	222	GLY	2.7
1	O	249	ALA	2.7
3	Q	204	GLY	2.6
2	P	60	THR	2.6
10	X	98	TYR	2.6
3	C	50	LEU	2.6
4	D	242	GLU	2.5
1	A	231	LYS	2.4
1	O	209	ILE	2.4
8	V	204	CYS	2.4
1	A	201	GLU	2.4
13	a	111	TRP	2.4
1	O	95	THR	2.4
3	C	240	GLU	2.4
2	P	218	GLY	2.4
3	C	205	ALA	2.4
3	Q	49	THR	2.3
2	P	222	GLY	2.3
7	U	242	GLN	2.3
2	B	239	VAL	2.3
8	V	199	LEU	2.3
1	O	96	SER	2.3
5	E	122	TYR	2.3
8	V	217	THR	2.3
7	U	168	GLU	2.3
6	F	202	ASP	2.3
9	I	1	SER	2.3
13	a	69	ASP	2.3
13	M	2	GLN	2.3
6	F	203	ASN	2.3
4	D	224	ASP	2.3
8	V	198	ARG	2.3
3	C	236	GLN	2.2
3	C	204	GLY	2.2
14	N	103	ASP	2.2
2	P	93	HIS	2.2
2	P	52	THR	2.2
8	V	197	THR	2.2
7	G	68	ARG	2.2
2	B	225	TYR	2.2
5	S	122	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	231	LYS	2.2
3	Q	238	LYS	2.1
13	a	224	ASP	2.1
9	W	1	SER	2.1
8	H	197	THR	2.1
6	F	215	CYS	2.1
1	A	53	SER	2.1
6	T	178	HIS	2.1
7	U	68	ARG	2.1
3	Q	236	GLN	2.1
11	Y	208	ASN	2.1
13	M	69	ASP	2.0
1	A	249	ALA	2.0
1	O	53	SER	2.0
3	Q	51	LYS	2.0
7	G	2	GLY	2.0
13	M	146	PHE	2.0
10	J	2	ASP	2.0
4	D	236	LYS	2.0
2	B	244	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å ²)	Q<0.9
15	MG	Z	301	1/1	0.83	0.16	70,70,70,70	0
15	MG	I	301	1/1	0.88	0.16	69,69,69,69	0
16	CL	U	301	1/1	0.96	0.14	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	L	301	1/1	0.97	0.12	72,72,72,72	0
16	CL	G	302	1/1	0.97	0.07	66,66,66,66	0
15	MG	W	301	1/1	0.97	0.12	64,64,64,64	0
15	MG	G	301	1/1	0.98	0.06	58,58,58,58	0
15	MG	N	201	1/1	0.98	0.04	64,64,64,64	0
15	MG	K	301	1/1	0.98	0.06	57,57,57,57	0
15	MG	I	302	1/1	0.99	0.03	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.