



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:05 PM UTC

PDB ID : 5M2B / pdb_00005m2b
Title : Yeast 20S proteasome with human beta5i (1-138) and human beta6 (97-111; 118-133) in complex with thiazole based inhibitor Ro19
Authors : Groll, M.
Deposited on : 2016-10-12
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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

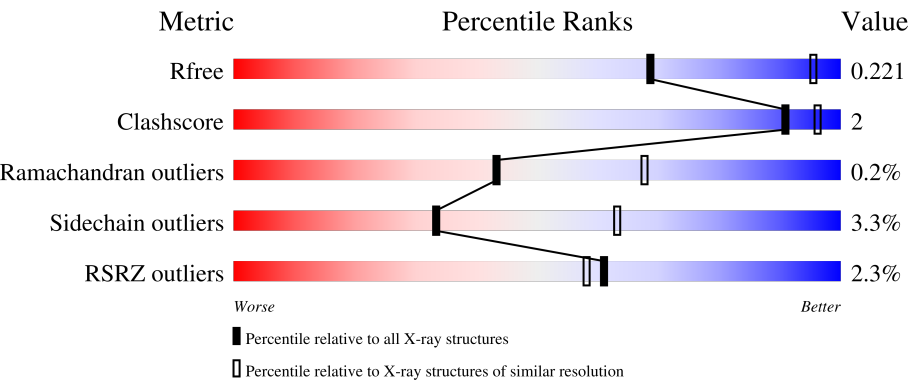
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	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	0% 98% ..
1	O	250	0% 97% ..
2	B	258	3% 87% 7% • 5%
2	P	258	2% 86% 8% • 5%
3	C	254	6% 87% 6% • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	 6% 87% 6% • 6%
4	D	260	 2% 84% 6% 10%
4	R	260	 6% 85% 5% 10%
5	E	234	 2% 95% • •
5	S	234	 3% 94% 5% •
6	F	288	 % 81% • 16%
6	T	288	 3% 81% • 16%
7	G	252	 % 91% • •
7	U	252	 % 90% 5% • •
8	H	232	 2% 91% 6% • •
8	V	232	 2% 91% 6% • •
9	I	205	 91% 8%
9	W	205	 91% 8%
10	J	198	 % 91% 5% • •
10	X	198	 3% 91% 6% • • •
11	K	211	 % 89% 9% •
11	Y	211	 2% 90% 9% •
12	L	222	 2% 92% 7% •
12	Z	222	 3% 93% 7%
13	M	246	 2% 89% 5% 5%
13	a	246	 % 89% 5% • 5%
14	N	196	 % 94% 5% •
14	b	196	 94% 5% •

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49899 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,Proteasome subunit beta type-6,Proteasome subunit beta type,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			

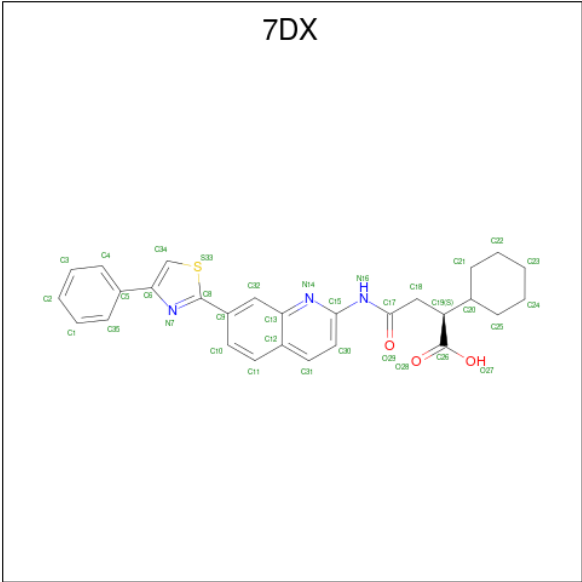
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is (2 {S})-2-cyclohexyl-4-oxidanilidene-4-[[7-(4-phenyl-1,3-thiazol-2-yl)quinolin-2-yl]amino]butanoic acid (CCD ID: 7DX) (formula: C₂₈H₂₇N₃O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	K	1	Total	C	N	O	S	0	0
			35	28	3	3	1		
17	Y	1	Total	C	N	O	S	0	0
			35	28	3	3	1		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	20	Total	O	0	0
			20	20		
18	B	13	Total	O	0	0
			13	13		
18	C	12	Total	O	0	0
			12	12		
18	D	12	Total	O	0	0
			12	12		
18	E	8	Total	O	0	0
			8	8		
18	F	14	Total	O	0	0
			14	14		
18	G	18	Total	O	0	0
			18	18		
18	H	22	Total	O	0	0
			22	22		
18	I	17	Total	O	0	0
			17	17		
18	J	18	Total	O	0	0
			18	18		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	K	15	Total 15	O 15	0	0
18	L	15	Total 15	O 15	0	0
18	M	25	Total 25	O 25	0	0
18	N	19	Total 19	O 19	0	0
18	O	18	Total 18	O 18	0	0
18	P	16	Total 16	O 16	0	0
18	Q	4	Total 4	O 4	0	0
18	R	15	Total 15	O 15	0	0
18	S	7	Total 7	O 7	0	0
18	T	11	Total 11	O 11	0	0
18	U	25	Total 25	O 25	0	0
18	V	17	Total 17	O 17	0	0
18	W	20	Total 20	O 20	0	0
18	X	20	Total 20	O 20	0	0
18	Y	11	Total 11	O 11	0	0
18	Z	13	Total 13	O 13	0	0
18	a	22	Total 22	O 22	0	0
18	b	19	Total 19	O 19	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.

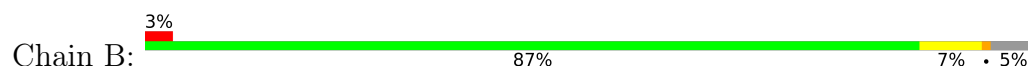
- Molecule 1: Proteasome subunit alpha type-2



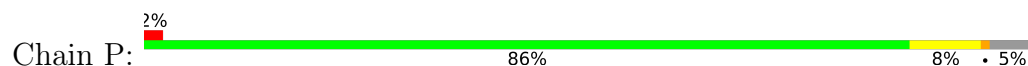
- Molecule 1: Proteasome subunit alpha type-2



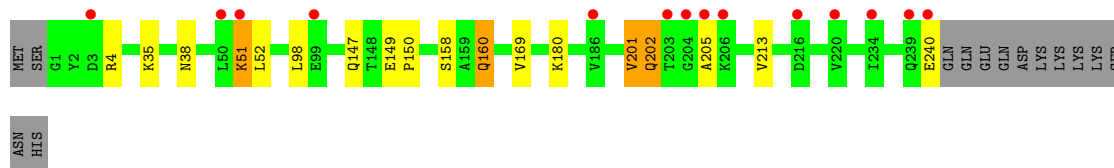
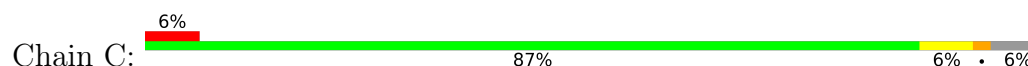
- Molecule 2: Proteasome subunit alpha type-3



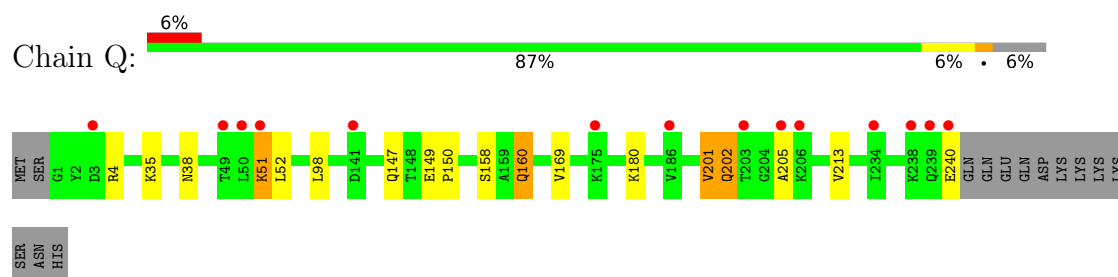
- Molecule 2: Proteasome subunit alpha type-3



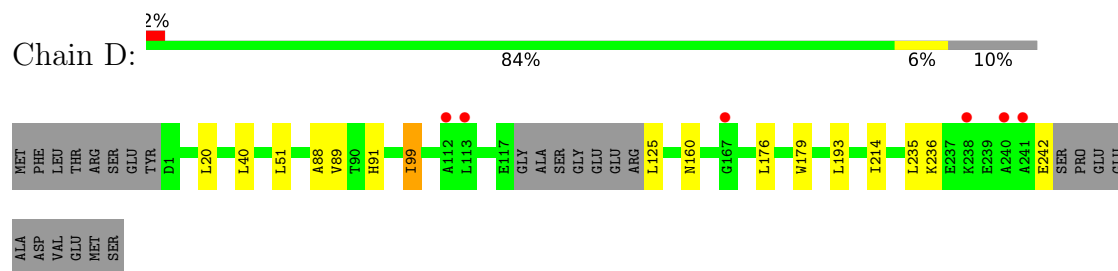
- Molecule 3: Proteasome subunit alpha type-4



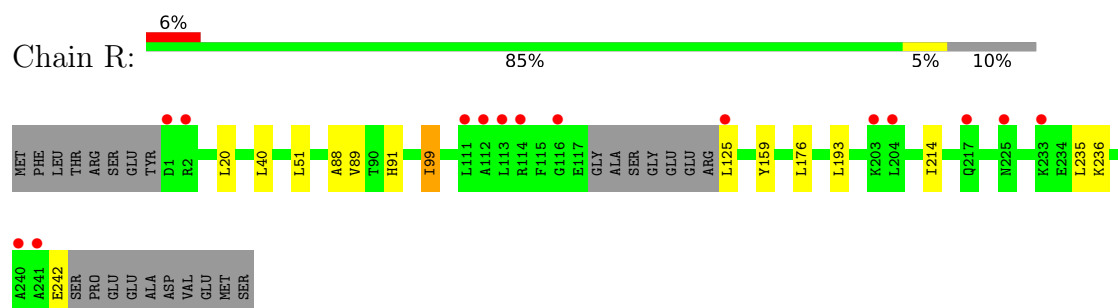
- Molecule 3: Proteasome subunit alpha type-4



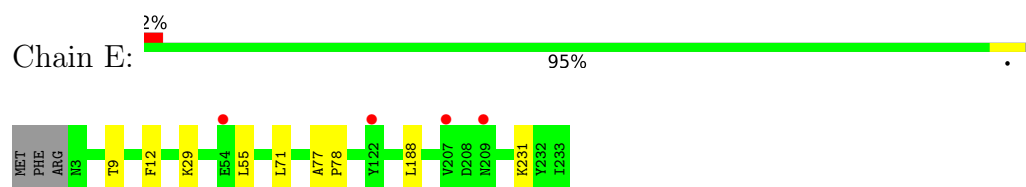
- Molecule 4: Proteasome subunit alpha type-5



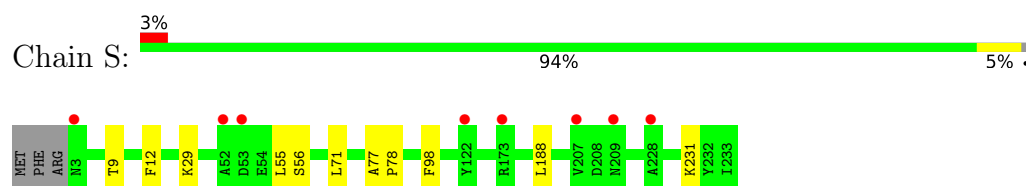
- Molecule 4: Proteasome subunit alpha type-5



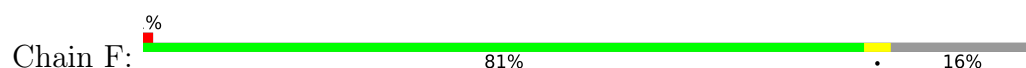
- Molecule 5: Proteasome subunit alpha type-6

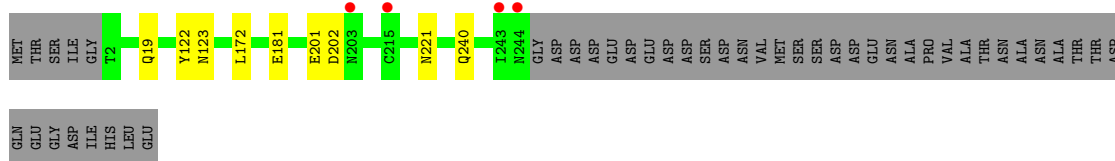


- Molecule 5: Proteasome subunit alpha type-6

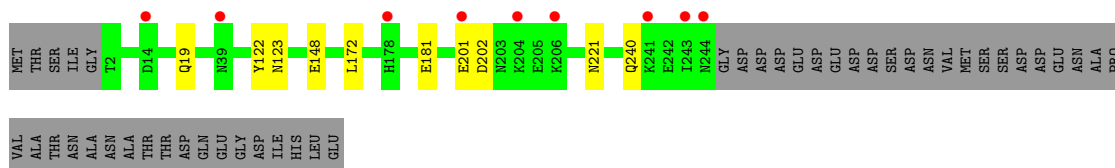
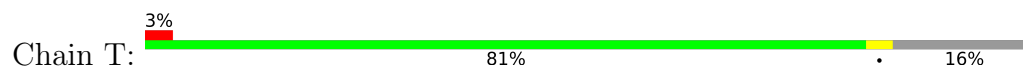


- Molecule 6: Probable proteasome subunit alpha type-7





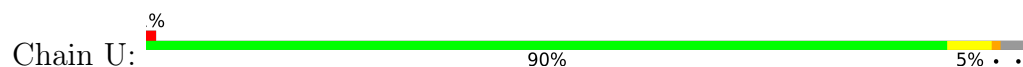
- Molecule 6: Probable proteasome subunit alpha type-7



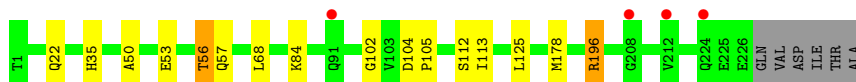
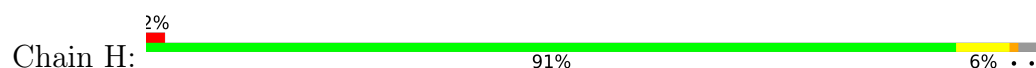
- Molecule 7: Proteasome subunit alpha type-1



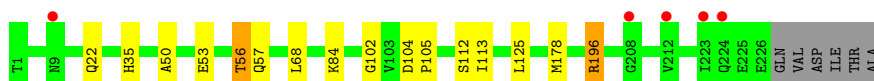
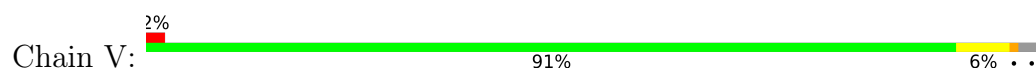
- Molecule 7: Proteasome subunit alpha type-1



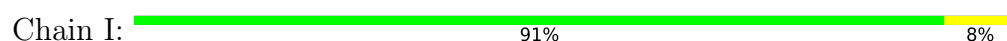
- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2



- Molecule 9: Proteasome subunit beta type-3





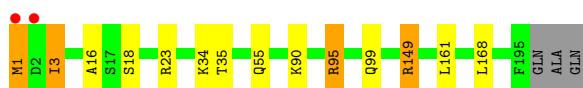
- Molecule 9: Proteasome subunit beta type-3

Chain W: 91% 8%



- Molecule 10: Proteasome subunit beta type-4

Chain J: 91% 5% . .



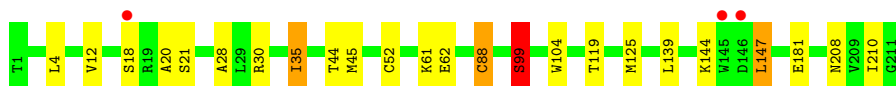
- Molecule 10: Proteasome subunit beta type-4

Chain X: 91% 3% 6% . . .



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

Chain K: 89% 9% .



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

Chain Y: 90% 2% 9% .

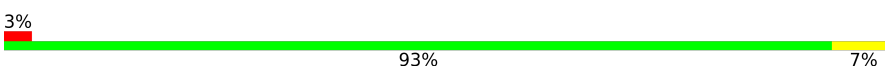


- Molecule 12: Proteasome subunit beta type-6, Proteasome subunit beta type, Proteasome subunit beta type-6, Proteasome subunit beta type, Proteasome subunit beta type-6

Chain L: 92% 2% 7% .



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

Chain Z: 



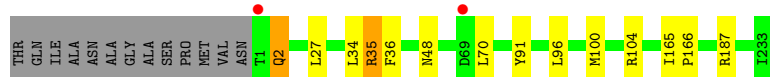
- Molecule 13: Proteasome subunit beta type-7

Chain M: 

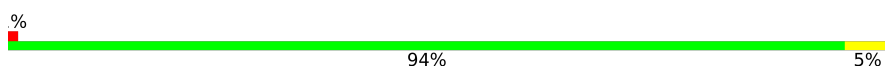


- Molecule 13: Proteasome subunit beta type-7

Chain a: 

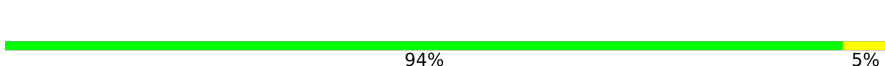


- Molecule 14: Proteasome subunit beta type-1

Chain N: 



- Molecule 14: Proteasome subunit beta type-1

Chain b: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.16Å 301.15Å 145.98Å 90.00° 112.81° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.7 (15.00-2.70) 96.1 (15.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.200 , 0.218 0.204 , 0.221	Depositor DCC
R_{free} test set	14094 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	49899	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 2.29% 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: CL, MG, 7DX

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	0.36	0/1952	0.68	0/2642
1	O	0.36	0/1952	0.68	0/2642
2	B	0.45	0/1934	0.68	0/2618
2	P	0.41	0/1934	0.68	0/2618
3	C	0.41	0/1910	0.69	1/2586 (0.0%)
3	Q	0.41	0/1910	0.69	1/2586 (0.0%)
4	D	0.40	0/1837	0.65	0/2475
4	R	0.40	0/1837	0.65	0/2475
5	E	0.41	0/1800	0.65	0/2433
5	S	0.41	0/1800	0.65	0/2433
6	F	0.41	0/1932	0.68	0/2609
6	T	0.40	0/1932	0.69	0/2609
7	G	0.41	0/1945	0.67	0/2634
7	U	0.39	0/1945	0.76	4/2634 (0.2%)
8	H	0.34	0/1750	0.69	0/2373
8	V	0.34	0/1750	0.68	0/2373
9	I	0.34	0/1611	0.72	0/2174
9	W	0.34	0/1611	0.71	0/2174
10	J	0.41	0/1589	0.84	6/2142 (0.3%)
10	X	0.42	0/1589	0.82	6/2142 (0.3%)
11	K	0.43	0/1677	0.74	1/2263 (0.0%)
11	Y	0.39	0/1677	0.73	0/2263
12	L	0.37	0/1802	0.79	5/2430 (0.2%)
12	Z	0.37	0/1802	0.75	5/2430 (0.2%)
13	M	0.35	0/1855	0.69	0/2514
13	a	0.38	0/1855	0.72	1/2514 (0.0%)
14	N	0.34	0/1541	0.68	0/2087
14	b	0.33	0/1541	0.68	0/2087
All	All	0.39	0/50270	0.71	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	U	0	1
10	J	0	2
10	X	0	2
All	All	0	5

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	100	ARG	NE-CZ-NH1	-11.40	110.10	121.50
10	J	149	ARG	NE-CZ-NH1	-11.40	110.10	121.50
7	U	68	ARG	NE-CZ-NH2	-11.37	108.97	119.20
12	L	100	ARG	NE-CZ-NH2	11.04	129.14	119.20
10	X	95	ARG	NE-CZ-NH1	-10.63	110.87	121.50
13	a	35	ARG	N-CA-C	10.50	122.72	111.28
7	U	68	ARG	CD-NE-CZ	10.30	138.82	124.40
10	J	95	ARG	NE-CZ-NH2	-10.25	109.98	119.20
10	J	149	ARG	NE-CZ-NH2	10.24	128.41	119.20
10	X	95	ARG	NE-CZ-NH2	10.01	128.21	119.20
10	J	95	ARG	CD-NE-CZ	9.88	138.23	124.40
10	X	149	ARG	NE-CZ-NH2	-9.85	110.34	119.20
10	J	149	ARG	CD-NE-CZ	9.71	138.00	124.40
12	Z	100	ARG	NE-CZ-NH2	-9.62	110.55	119.20
10	X	149	ARG	CD-NE-CZ	9.08	137.11	124.40
10	X	95	ARG	CD-NE-CZ	8.48	136.27	124.40
12	L	100	ARG	CD-NE-CZ	8.14	135.80	124.40
12	Z	100	ARG	CD-NE-CZ	8.02	135.62	124.40
7	U	68	ARG	NE-CZ-NH1	7.33	128.83	121.50
12	Z	100	ARG	NE-CZ-NH1	7.08	128.58	121.50
7	U	68	ARG	CG-CD-NE	-7.03	96.53	112.00
10	X	149	ARG	NE-CZ-NH1	6.29	127.78	121.50
11	K	99	SER	N-CA-C	5.85	118.30	109.23
3	C	201	VAL	N-CA-C	5.78	116.51	110.62
10	J	95	ARG	NE-CZ-NH1	5.69	127.19	121.50
3	Q	201	VAL	N-CA-C	5.68	116.42	110.62
12	Z	103	PHE	CA-C-N	5.05	125.32	119.92
12	Z	103	PHE	C-N-CA	5.05	125.32	119.92
12	L	103	PHE	CA-C-N	5.02	125.29	119.92
12	L	103	PHE	C-N-CA	5.02	125.29	119.92

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	149	ARG	Sidechain
10	J	95	ARG	Sidechain
7	U	68	ARG	Sidechain
10	X	149	ARG	Sidechain
10	X	95	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	2	0
1	O	1915	0	1929	5	0
2	B	1904	0	1904	15	0
2	P	1904	0	1904	9	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	5	0
5	E	1773	0	1775	2	0
5	S	1773	0	1775	4	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1719	0	1719	11	0
8	V	1719	0	1719	9	0
9	I	1581	0	1574	13	0
9	W	1581	0	1574	11	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	10	0
11	K	1640	0	1581	16	0
11	Y	1640	0	1581	14	0
12	L	1764	0	1716	6	0
12	Z	1764	0	1716	5	0
13	M	1824	0	1832	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	a	1824	0	1832	6	0
14	N	1512	0	1481	4	0
14	b	1512	0	1481	4	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
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	K	35	0	0	0	0
17	Y	35	0	0	1	0
18	A	20	0	0	0	0
18	B	13	0	0	0	0
18	C	12	0	0	0	0
18	D	12	0	0	0	0
18	E	8	0	0	0	0
18	F	14	0	0	0	0
18	G	18	0	0	0	0
18	H	22	0	0	0	0
18	I	17	0	0	0	0
18	J	18	0	0	0	0
18	K	15	0	0	0	0
18	L	15	0	0	0	0
18	M	25	0	0	1	0
18	N	19	0	0	0	0
18	O	18	0	0	0	0
18	P	16	0	0	1	0
18	Q	4	0	0	0	0
18	R	15	0	0	0	0
18	S	7	0	0	0	0
18	T	11	0	0	1	0
18	U	25	0	0	0	0
18	V	17	0	0	0	0
18	W	20	0	0	0	0
18	X	20	0	0	0	0
18	Y	11	0	0	0	0
18	Z	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	a	22	0	0	1	0
18	b	19	0	0	0	0
All	All	49899	0	49112	166	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 (166) 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)
2:B:93:HIS:NE2	2:B:113:ARG:HD3	1.60	1.15
11:K:35:ILE:HG22	11:K:45:MET:HE3	1.31	1.08
2:B:113:ARG:HH11	2:B:113:ARG:HG3	1.21	1.00
11:Y:35:ILE:HG22	11:Y:45:MET:HE3	1.48	0.93
11:K:44:THR:O	11:K:99:SER:OG	1.96	0.82
11:K:35:ILE:CG2	11:K:45:MET:HE3	2.12	0.75
11:Y:35:ILE:HG22	11:Y:45:MET:CE	2.17	0.74
10:J:55:GLN:CD	11:K:88:CYS:SG	2.76	0.69
10:J:3:ILE:HD11	10:J:168:LEU:HD13	1.75	0.68
10:X:3:ILE:HD11	10:X:168:LEU:HD13	1.75	0.68
2:B:93:HIS:CE1	2:B:113:ARG:HD3	2.28	0.67
10:J:23:ARG:NH2	11:K:119:THR:OG1	2.26	0.67
11:K:35:ILE:HG22	11:K:45:MET:CE	2.19	0.67
10:X:23:ARG:NH2	11:Y:119:THR:OG1	2.29	0.66
2:B:113:ARG:HG3	2:B:113:ARG:NH1	2.01	0.65
10:X:55:GLN:CD	11:Y:88:CYS:SG	2.80	0.64
2:B:113:ARG:HH11	2:B:113:ARG:CG	2.05	0.59
10:J:3:ILE:CD1	10:J:168:LEU:HD13	2.33	0.59
2:B:93:HIS:NE2	2:B:113:ARG:CD	2.53	0.58
10:J:55:GLN:NE2	11:K:88:CYS:SG	2.76	0.58
10:X:3:ILE:CD1	10:X:168:LEU:HD13	2.33	0.57
11:K:20:ALA:HB3	11:K:28:ALA:HB3	1.86	0.56
11:K:208:ASN:O	9:W:38:LYS:NZ	2.38	0.56
4:R:89:VAL:HG12	11:Y:61:LYS:HG3	1.87	0.56
11:Y:20:ALA:HB3	11:Y:28:ALA:HB3	1.87	0.56
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.36	0.55
14:b:152:VAL:HA	14:b:175:MET:HE1	1.88	0.55
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.42	0.54
10:X:55:GLN:NE2	11:Y:88:CYS:SG	2.81	0.54
2:P:93:HIS:HB3	18:P:301:HOH:O	2.07	0.54
11:K:144:LYS:HB2	11:K:147:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:89:VAL:HG12	11:K:61:LYS:HG3	1.89	0.53
14:N:152:VAL:HA	14:N:175:MET:HE1	1.88	0.53
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.74	0.53
11:Y:144:LYS:HB2	11:Y:147:LEU:HD13	1.90	0.53
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.91	0.52
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.91	0.52
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.74	0.52
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.42	0.52
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.51
12:L:100:ARG:HD2	12:L:105:TYR:CE2	2.46	0.51
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.41	0.51
2:B:113:ARG:NH1	2:B:113:ARG:CG	2.71	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.51
2:B:217:LYS:C	2:B:219:ALA:H	2.19	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.50
11:Y:35:ILE:CG2	11:Y:45:MET:CE	2.88	0.50
8:H:50:ALA:CB	9:I:126:ILE:CG2	2.90	0.50
11:K:35:ILE:CG2	11:K:45:MET:CE	2.86	0.50
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.42	0.49
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.12	0.49
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.77	0.49
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.27	0.49
2:P:50:LYS:O	2:P:51:VAL:C	2.55	0.49
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.95	0.49
2:P:217:LYS:C	2:P:219:ALA:H	2.20	0.49
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.95	0.49
3:C:51:LYS:O	3:C:52:LEU:HB2	2.12	0.48
8:V:50:ALA:CB	9:W:126:ILE:HG23	2.43	0.48
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.94	0.48
2:B:50:LYS:O	2:B:51:VAL:C	2.56	0.48
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.48	0.48
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.95	0.48
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.95	0.48
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.94	0.48
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.96	0.47
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.95	0.47
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.78	0.47
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.95	0.47
11:Y:49:ALA:HB2	17:Y:301:7DX:C32	2.44	0.47
10:J:3:ILE:HG22	10:J:18:SER:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:196:ARG:NH2	9:W:150:GLU:HG3	2.30	0.47
10:X:3:ILE:HG22	10:X:18:SER:CB	2.45	0.47
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.96	0.47
2:B:93:HIS:CD2	2:B:113:ARG:HG2	2.49	0.47
10:J:3:ILE:HG22	10:J:18:SER:HB3	1.95	0.47
13:M:96:LEU:O	13:M:100:MET:HG2	2.15	0.47
10:X:3:ILE:HG22	10:X:18:SER:HB3	1.96	0.47
11:K:18:SER:OG	11:K:30:ARG:HA	2.14	0.46
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.97	0.46
5:E:12:PHE:H	6:F:19:GLN:HE22	1.64	0.46
8:V:53:GLU:O	8:V:57:GLN:HG2	2.16	0.46
6:T:148:GLU:HG2	18:T:304:HOH:O	2.15	0.46
10:X:148:TYR:O	10:X:149:ARG:HD3	2.15	0.46
13:a:96:LEU:O	13:a:100:MET:HG2	2.15	0.46
11:Y:18:SER:OG	11:Y:30:ARG:HA	2.15	0.46
12:Z:138:ALA:HB3	12:Z:147:MET:HG2	1.98	0.46
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.97	0.45
8:H:196:ARG:NH2	9:I:150:GLU:O	2.49	0.45
8:V:50:ALA:CB	9:W:126:ILE:CG2	2.94	0.45
13:a:35:ARG:HG2	13:a:36:PHE:CE2	2.52	0.45
11:Y:104:TRP:CE2	11:Y:181:GLU:HB3	2.52	0.45
14:N:133:PHE:HA	14:b:132:THR:O	2.17	0.44
9:W:26:LEU:HD21	9:W:185:VAL:HG23	1.98	0.44
9:I:148:MET:HE2	9:I:172:ASN:HB2	1.99	0.44
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.17	0.44
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.00	0.44
9:I:26:LEU:HD21	9:I:185:VAL:HG23	1.98	0.44
9:W:148:MET:HE2	9:W:172:ASN:HB2	1.99	0.44
8:H:53:GLU:O	8:H:57:GLN:HG2	2.16	0.44
12:L:138:ALA:HB3	12:L:147:MET:HG2	1.98	0.44
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.53	0.44
3:C:35:LYS:HG2	3:C:158:SER:O	2.17	0.44
9:I:163:PHE:CE1	9:I:197:ARG:HD2	2.53	0.44
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.00	0.44
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.00	0.43
8:H:84:LYS:HA	8:H:113:ILE:HD11	2.01	0.43
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.53	0.43
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.00	0.43
11:K:104:TRP:CE2	11:K:181:GLU:HB3	2.52	0.43
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.99	0.43
2:B:93:HIS:CD2	2:B:113:ARG:HD3	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.54	0.43
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.00	0.43
3:C:201:VAL:O	3:C:202:GLN:HB3	2.18	0.43
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.99	0.43
5:S:98:PHE:O	13:a:91:TYR:HA	2.18	0.43
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.18	0.43
2:B:221:ASP:O	2:B:223:GLU:N	2.52	0.43
8:V:84:LYS:HA	8:V:113:ILE:HD11	2.01	0.43
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.84	0.42
2:P:221:ASP:O	2:P:223:GLU:N	2.52	0.42
9:W:163:PHE:CE1	9:W:197:ARG:HD2	2.54	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.01	0.42
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.50	0.42
13:a:2:GLN:NE2	18:a:301:HOH:O	2.52	0.42
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.50	0.42
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.02	0.42
11:K:45:MET:HG2	11:K:52:CYS:HB3	2.02	0.42
12:L:126:ASP:CG	12:L:130:SER:OG	2.63	0.42
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.02	0.42
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.55	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.41
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.02	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
5:S:12:PHE:H	6:T:19:GLN:HE22	1.68	0.41
13:a:27:LEU:HD21	13:a:34:LEU:HD22	2.02	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.56	0.41
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.50	0.41
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.03	0.41
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.03	0.41
8:H:102:GLY:HA2	8:H:178:MET:SD	2.61	0.41
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.86	0.41
8:H:50:ALA:HB3	9:I:126:ILE:CG2	2.51	0.41
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.03	0.41
12:Z:126:ASP:CG	12:Z:130:SER:OG	2.64	0.41
11:Y:125:MET:SD	11:Y:139:LEU:HB3	2.61	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.21	0.41
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.03	0.40
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:102:GLY:HA2	8:V:178:MET:SD	2.60	0.40
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.03	0.40
5:S:77:ALA:N	5:S:78:PRO:CD	2.85	0.40
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.02	0.40
6:F:202:ASP:OD1	6:F:202:ASP:N	2.55	0.40
5:E:77:ALA:N	5:E:78:PRO:CD	2.85	0.40
11:K:125:MET:SD	11:K:139:LEU:HB3	2.62	0.40
13:M:2:GLN:NE2	18:M:302:HOH:O	2.55	0.40
6:T:202:ASP:OD1	6:T:202:ASP:N	2.55	0.40
12:L:8:ASN:HA	12:L:30:ILE:O	2.22	0.40
13:M:17:ASP:OD1	13:M:18:ASN:N	2.55	0.40
1:O:12:PHE:H	2:P:20:GLN:HE22	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	30	54
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	30	54
2	B	242/258 (94%)	235 (97%)	4 (2%)	3 (1%)	10	27
2	P	242/258 (94%)	235 (97%)	4 (2%)	3 (1%)	10	27
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	37
3	Q	238/254 (94%)	233 (98%)	3 (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%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	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%)	204 (98%)	5 (2%)	0	100	100
11	Y	209/211 (99%)	203 (97%)	6 (3%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
13	a	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6282/6612 (95%)	6132 (98%)	138 (2%)	12 (0%)	43	68

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	222	GLY
3	C	202	GLN
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
3	C	205	ALA
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%)	205 (98%)	4 (2%)	50	77
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	77
2	B	203/216 (94%)	196 (97%)	7 (3%)	32	62
2	P	203/216 (94%)	196 (97%)	7 (3%)	32	62
3	C	212/226 (94%)	202 (95%)	10 (5%)	23	51
3	Q	212/226 (94%)	202 (95%)	10 (5%)	23	51
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%)	184 (97%)	6 (3%)	34	64
5	S	190/193 (98%)	184 (97%)	6 (3%)	34	64
6	F	201/239 (84%)	195 (97%)	6 (3%)	36	66
6	T	201/239 (84%)	195 (97%)	6 (3%)	36	66
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	62
7	U	206/210 (98%)	199 (97%)	7 (3%)	32	62
8	H	185/190 (97%)	181 (98%)	4 (2%)	45	74
8	V	185/190 (97%)	181 (98%)	4 (2%)	45	74
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	79
9	W	172/173 (99%)	169 (98%)	3 (2%)	53	79
10	J	173/175 (99%)	168 (97%)	5 (3%)	37	67
10	X	173/175 (99%)	168 (97%)	5 (3%)	37	67
11	K	170/170 (100%)	161 (95%)	9 (5%)	20	46
11	Y	170/170 (100%)	162 (95%)	8 (5%)	23	51
12	L	186/186 (100%)	181 (97%)	5 (3%)	39	69
12	Z	186/186 (100%)	181 (97%)	5 (3%)	39	69
13	M	199/208 (96%)	194 (98%)	5 (2%)	42	71
13	a	199/208 (96%)	194 (98%)	5 (2%)	42	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	156 (96%)	6 (4%)	30	59
14	b	162/162 (100%)	156 (96%)	6 (4%)	30	59
All	All	5324/5544 (96%)	5149 (97%)	175 (3%)	33	63

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
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	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	98	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	125	LEU
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

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Mol	Chain	Res	Type
5	E	55	LEU
5	E	71	LEU
5	E	188	LEU
5	E	231	LYS
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	221	ASN
6	F	240	GLN
7	G	26	THR
7	G	75	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	22	GLN
8	H	56	THR
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
10	J	1	MET
10	J	3	ILE
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	12	VAL
11	K	21	SER
11	K	35	ILE
11	K	62	GLU
11	K	88	CYS
11	K	99	SER
11	K	147	LEU
11	K	210	ILE
12	L	23	LEU
12	L	49	ASN
12	L	128	VAL
12	L	132	GLN

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Mol	Chain	Res	Type
12	L	150	LEU
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	35	THR
14	N	36	ARG
14	N	104	ASP
14	N	119	VAL
14	N	178	LEU
1	O	1	MET
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	79	LEU
2	P	102	ASN
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	98	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
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	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU

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Mol	Chain	Res	Type
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	231	LYS
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	221	ASN
6	T	240	GLN
7	U	26	THR
7	U	75	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	22	GLN
8	V	56	THR
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
10	X	1	MET
10	X	3	ILE
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	12	VAL
11	Y	21	SER
11	Y	35	ILE
11	Y	62	GLU
11	Y	88	CYS
11	Y	147	LEU
11	Y	210	ILE
12	Z	23	LEU

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Mol	Chain	Res	Type
12	Z	49	ASN
12	Z	128	VAL
12	Z	132	GLN
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	187	ARG
14	b	9	LYS
14	b	35	THR
14	b	36	ARG
14	b	104	ASP
14	b	119	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
3	C	17	GLN
3	C	115	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
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

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Mol	Chain	Res	Type
6	F	123	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
8	H	30	ASN
8	H	86	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
9	I	63	ASN
9	I	203	GLN
10	J	55	GLN
10	J	63	ASN
11	K	32	ASN
11	K	85	ASN
11	K	142	ASN
11	K	175	ASN
11	K	189	ASN
11	K	208	ASN
12	L	3	ASN
12	L	29	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	109	ASN
12	L	152	ASN
12	L	153	GLN
12	L	158	ASN
12	L	197	GLN
13	M	48	ASN
13	M	108	ASN
13	M	149	HIS
14	N	38	HIS
14	N	141	ASN
14	N	161	GLN
2	P	20	GLN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	176	GLN

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Mol	Chain	Res	Type
3	Q	17	GLN
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	100	ASN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	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
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	172	ASN
7	U	175	ASN
8	V	30	ASN
8	V	86	HIS
8	V	172	ASN
8	V	189	ASN
9	W	37	ASN
9	W	63	ASN
9	W	203	GLN
10	X	55	GLN
10	X	61	GLN
10	X	63	ASN
11	Y	32	ASN
11	Y	85	ASN
11	Y	142	ASN
11	Y	175	ASN
12	Z	3	ASN
12	Z	29	ASN
12	Z	36	ASN
12	Z	49	ASN

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Mol	Chain	Res	Type
12	Z	70	ASN
12	Z	109	ASN
12	Z	197	GLN
13	a	48	ASN
13	a	108	ASN
13	a	149	HIS
14	b	38	HIS
14	b	141	ASN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 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	7DX	K	301	-	39,39,39	3.54	11 (28%)	52,54,54	2.95	12 (23%)
17	7DX	Y	301	-	39,39,39	3.82	10 (25%)	52,54,54	3.36	14 (26%)

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	7DX	K	301	-	-	0/24/32/32	0/5/5/5
17	7DX	Y	301	-	-	0/24/32/32	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	301	7DX	C8-S33	-14.70	1.45	1.73
17	K	301	7DX	C8-S33	-11.54	1.51	1.73
17	K	301	7DX	C5-C6	-10.87	1.31	1.47
17	Y	301	7DX	C5-C6	-10.39	1.32	1.47
17	Y	301	7DX	C9-C8	-9.80	1.32	1.47
17	K	301	7DX	C9-C8	-9.46	1.33	1.47
17	Y	301	7DX	C34-S33	-7.12	1.54	1.71
17	K	301	7DX	C34-S33	-6.88	1.55	1.71
17	Y	301	7DX	C6-N7	-4.22	1.31	1.39
17	K	301	7DX	C34-C6	-4.01	1.31	1.36
17	Y	301	7DX	C34-C6	-3.99	1.31	1.36
17	K	301	7DX	C6-N7	-3.80	1.32	1.39
17	K	301	7DX	C15-N16	-3.66	1.32	1.40
17	K	301	7DX	C13-N14	-3.43	1.32	1.37
17	Y	301	7DX	C12-C13	-3.40	1.37	1.42
17	Y	301	7DX	C13-N14	-3.30	1.32	1.37
17	K	301	7DX	C12-C13	-3.30	1.37	1.42
17	Y	301	7DX	C15-N16	-3.29	1.32	1.40
17	Y	301	7DX	O27-C26	-2.42	1.22	1.30
17	K	301	7DX	O27-C26	-2.20	1.23	1.30
17	K	301	7DX	C32-C13	-2.18	1.38	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	301	7DX	C34-S33-C8	18.89	101.63	89.51
17	K	301	7DX	C34-S33-C8	16.55	100.13	89.51
17	Y	301	7DX	C9-C8-S33	6.34	128.50	122.30
17	K	301	7DX	C9-C8-S33	6.16	128.32	122.30
17	Y	301	7DX	S33-C8-N7	-5.81	108.48	114.22
17	K	301	7DX	S33-C8-N7	-5.72	108.57	114.22
17	Y	301	7DX	C6-C34-S33	-5.27	104.78	111.16
17	K	301	7DX	C6-C34-S33	-4.72	105.44	111.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	7DX	C15-N14-C13	4.34	123.46	117.32
17	Y	301	7DX	C15-N14-C13	4.16	123.21	117.32
17	Y	301	7DX	C22-C21-C20	-4.00	104.75	111.89
17	Y	301	7DX	C24-C25-C20	-3.57	105.53	111.89
17	Y	301	7DX	C19-C18-C17	3.54	120.03	111.65
17	K	301	7DX	C19-C18-C17	2.93	118.57	111.65
17	Y	301	7DX	C25-C20-C21	-2.70	104.82	109.43
17	Y	301	7DX	C21-C20-C19	2.66	115.93	112.03
17	Y	301	7DX	O28-C26-C19	-2.59	116.89	123.01
17	K	301	7DX	C15-N16-C17	-2.46	123.70	128.22
17	Y	301	7DX	C15-N16-C17	-2.46	123.71	128.22
17	K	301	7DX	O28-C26-C19	-2.32	117.53	123.01
17	Y	301	7DX	C12-C13-N14	-2.29	119.09	122.25
17	K	301	7DX	C24-C25-C20	-2.19	107.98	111.89
17	K	301	7DX	C12-C13-N14	-2.19	119.24	122.25
17	Y	301	7DX	C18-C17-N16	-2.13	111.99	114.62
17	K	301	7DX	C22-C21-C20	-2.06	108.21	111.89
17	K	301	7DX	C23-C22-C21	-2.03	107.24	111.42

There are no chirality outliers.

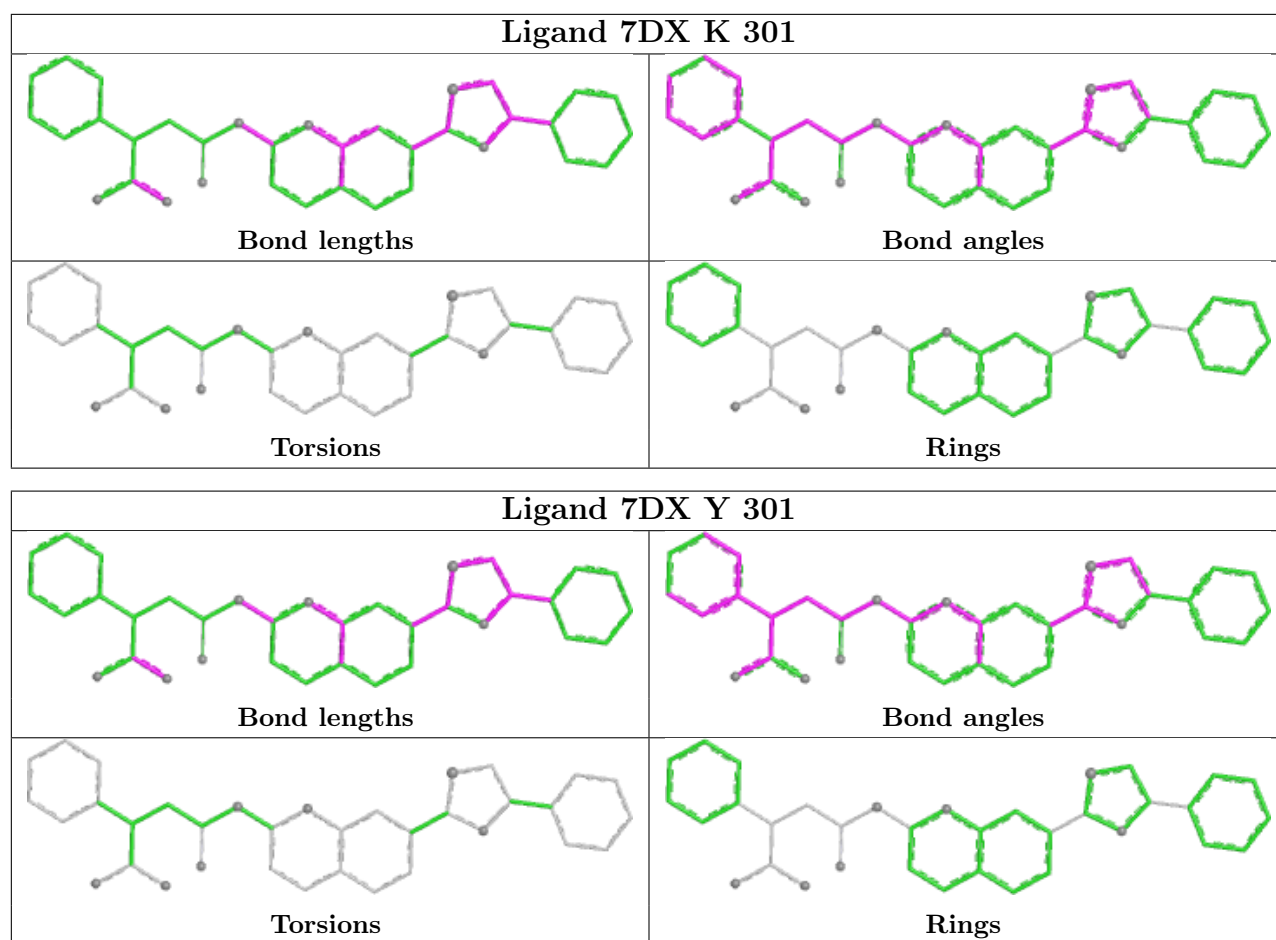
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	301	7DX	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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%)	-0.25	3 (1%) 76 75	33, 48, 84, 123	0
1	O	250/250 (100%)	-0.19	3 (1%) 76 75	36, 53, 99, 132	0
2	B	244/258 (94%)	0.05	9 (3%) 45 41	35, 55, 104, 155	0
2	P	244/258 (94%)	-0.02	6 (2%) 58 55	37, 57, 102, 151	0
3	C	240/254 (94%)	0.28	14 (5%) 29 25	33, 60, 132, 169	0
3	Q	240/254 (94%)	0.30	14 (5%) 29 25	26, 69, 147, 188	0
4	D	235/260 (90%)	-0.00	6 (2%) 57 54	41, 59, 92, 130	0
4	R	235/260 (90%)	0.38	15 (6%) 25 22	51, 71, 113, 144	0
5	E	231/234 (98%)	0.06	4 (1%) 69 67	40, 61, 101, 149	0
5	S	231/234 (98%)	0.22	8 (3%) 47 43	44, 67, 109, 146	0
6	F	243/288 (84%)	-0.14	4 (1%) 70 68	33, 53, 105, 130	0
6	T	243/288 (84%)	0.08	9 (3%) 45 41	39, 62, 119, 149	0
7	G	241/252 (95%)	-0.13	2 (0%) 82 81	32, 49, 88, 141	0
7	U	241/252 (95%)	-0.11	2 (0%) 82 81	34, 50, 86, 128	0
8	H	226/232 (97%)	-0.01	4 (1%) 67 65	33, 50, 86, 151	0
8	V	226/232 (97%)	0.00	5 (2%) 62 59	35, 51, 85, 157	0
9	I	204/205 (99%)	-0.34	1 (0%) 87 86	32, 46, 77, 96	0
9	W	204/205 (99%)	-0.32	1 (0%) 87 86	31, 46, 77, 99	0
10	J	195/198 (98%)	-0.15	2 (1%) 79 78	31, 49, 74, 122	0
10	X	195/198 (98%)	-0.16	6 (3%) 51 48	33, 50, 76, 135	0
11	K	211/211 (100%)	0.11	3 (1%) 73 72	38, 57, 88, 106	0
11	Y	211/211 (100%)	0.17	5 (2%) 59 56	39, 58, 90, 115	0
12	L	222/222 (100%)	-0.04	5 (2%) 61 58	37, 54, 99, 126	0
12	Z	222/222 (100%)	0.01	6 (2%) 56 53	34, 55, 98, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.24	4 (1%) 69 67	31, 49, 73, 93	0
13	a	233/246 (94%)	-0.23	2 (0%) 81 80	32, 50, 75, 93	0
14	N	196/196 (100%)	-0.28	1 (0%) 87 86	32, 44, 72, 102	0
14	b	196/196 (100%)	-0.30	0 100 100	32, 45, 74, 104	0
All	All	6342/6612 (95%)	-0.04	144 (2%) 61 58	26, 54, 100, 188	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	218	GLY	5.2
2	P	219	ALA	5.1
10	J	1	MET	4.9
2	P	218	GLY	4.8
10	X	1	MET	4.8
3	C	205	ALA	4.4
2	B	219	ALA	4.2
4	R	113	LEU	3.9
4	D	241	ALA	3.8
13	M	69	ASP	3.8
12	Z	174	TYR	3.7
2	B	51	VAL	3.6
2	B	220	ASN	3.6
8	V	224	GLN	3.6
10	J	2	ASP	3.6
4	R	112	ALA	3.5
9	W	1	SER	3.5
3	Q	205	ALA	3.5
12	L	166	GLY	3.4
2	P	51	VAL	3.4
8	V	223	ILE	3.3
3	C	51	LYS	3.3
3	Q	234	ILE	3.2
5	S	207	VAL	3.2
10	X	195	PHE	3.2
6	F	215	CYS	3.2
13	a	1	THR	3.2
3	Q	206	LYS	3.1
2	P	220	ASN	3.1
3	C	206	LYS	3.1
13	a	69	ASP	3.1
9	I	1	SER	3.1

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Mol	Chain	Res	Type	RSRZ
8	H	208	GLY	3.1
6	T	14	ASP	3.0
5	E	207	VAL	3.0
4	D	167	GLY	3.0
12	L	163	GLY	3.0
3	Q	50	LEU	2.9
3	C	186	VAL	2.9
4	R	116	GLY	2.9
4	R	125	LEU	2.9
11	Y	144	LYS	2.8
6	T	178	HIS	2.8
6	T	204	LYS	2.8
2	B	222	GLY	2.7
3	Q	175	LYS	2.7
2	P	52	THR	2.7
6	T	243	ILE	2.6
2	P	1	GLY	2.6
4	D	238	LYS	2.6
3	Q	51	LYS	2.6
3	Q	238	LYS	2.6
4	R	203	LYS	2.6
3	C	234	ILE	2.6
5	S	209	ASN	2.6
11	Y	145	TRP	2.6
10	X	174	MET	2.6
5	S	122	TYR	2.6
6	T	241	LYS	2.6
11	K	18	SER	2.5
2	B	1	GLY	2.5
4	R	217	GLN	2.5
5	E	209	ASN	2.5
10	X	2	ASP	2.5
12	Z	163	GLY	2.5
4	D	240	ALA	2.5
2	B	221	ASP	2.5
3	Q	3	ASP	2.5
10	X	11	ASP	2.5
13	M	47	ASP	2.5
7	G	3	TYR	2.5
4	R	240	ALA	2.5
4	R	241	ALA	2.5
4	R	233	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
6	T	206	LYS	2.5
12	L	165	ASN	2.5
4	R	1	ASP	2.5
7	U	168	GLU	2.5
4	R	114	ARG	2.4
3	C	3	ASP	2.4
11	K	146	ASP	2.4
8	H	224	GLN	2.4
4	D	112	ALA	2.4
5	S	3	ASN	2.4
3	C	240	GLU	2.4
12	L	174	TYR	2.4
3	C	50	LEU	2.4
11	K	145	TRP	2.4
6	T	244	ASN	2.3
5	E	122	TYR	2.3
2	B	52	THR	2.3
1	A	1	MET	2.3
8	V	208	GLY	2.3
1	O	249	ALA	2.3
4	R	225	ASN	2.3
3	C	204	GLY	2.3
3	Q	49	THR	2.2
13	M	1	THR	2.2
6	F	203	ASN	2.2
3	Q	141	ASP	2.2
11	Y	146	ASP	2.2
12	Z	166	GLY	2.2
12	Z	172	LEU	2.2
1	A	2	THR	2.2
3	Q	203	THR	2.2
5	S	173	ARG	2.2
3	C	216	ASP	2.2
6	T	39	ASN	2.2
8	V	9	ASN	2.2
12	Z	162	PRO	2.2
5	S	52	ALA	2.2
5	E	54	GLU	2.2
4	D	113	LEU	2.2
5	S	228	ALA	2.1
12	L	162	PRO	2.1
7	U	24	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	Q	239	GLN	2.1
6	F	244	ASN	2.1
6	T	201	GLU	2.1
1	O	2	THR	2.1
3	C	239	GLN	2.1
7	G	242	GLN	2.1
3	Q	186	VAL	2.1
8	H	212	VAL	2.1
14	N	103	ASP	2.1
1	O	53	SER	2.1
1	A	231	LYS	2.1
8	H	91	GLN	2.1
11	Y	68	LEU	2.1
13	M	37	ASN	2.1
5	S	53	ASP	2.0
10	X	194	ASP	2.0
2	B	204	ALA	2.0
3	C	99	GLU	2.0
3	Q	240	GLU	2.0
4	R	2	ARG	2.0
11	Y	88	CYS	2.0
12	Z	169	LYS	2.0
3	C	203	THR	2.0
4	R	111	LEU	2.0
4	R	204	LEU	2.0
6	F	243	ILE	2.0
3	C	220	VAL	2.0
8	V	212	VAL	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,

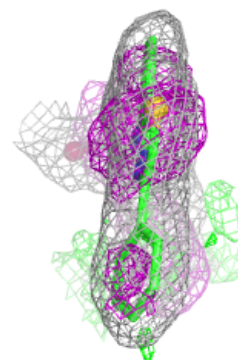
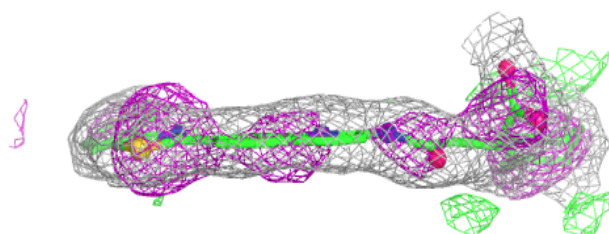
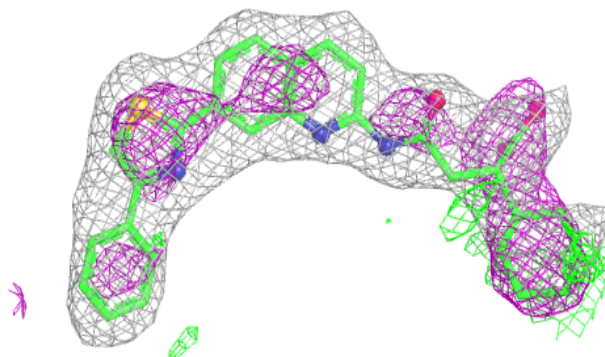
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

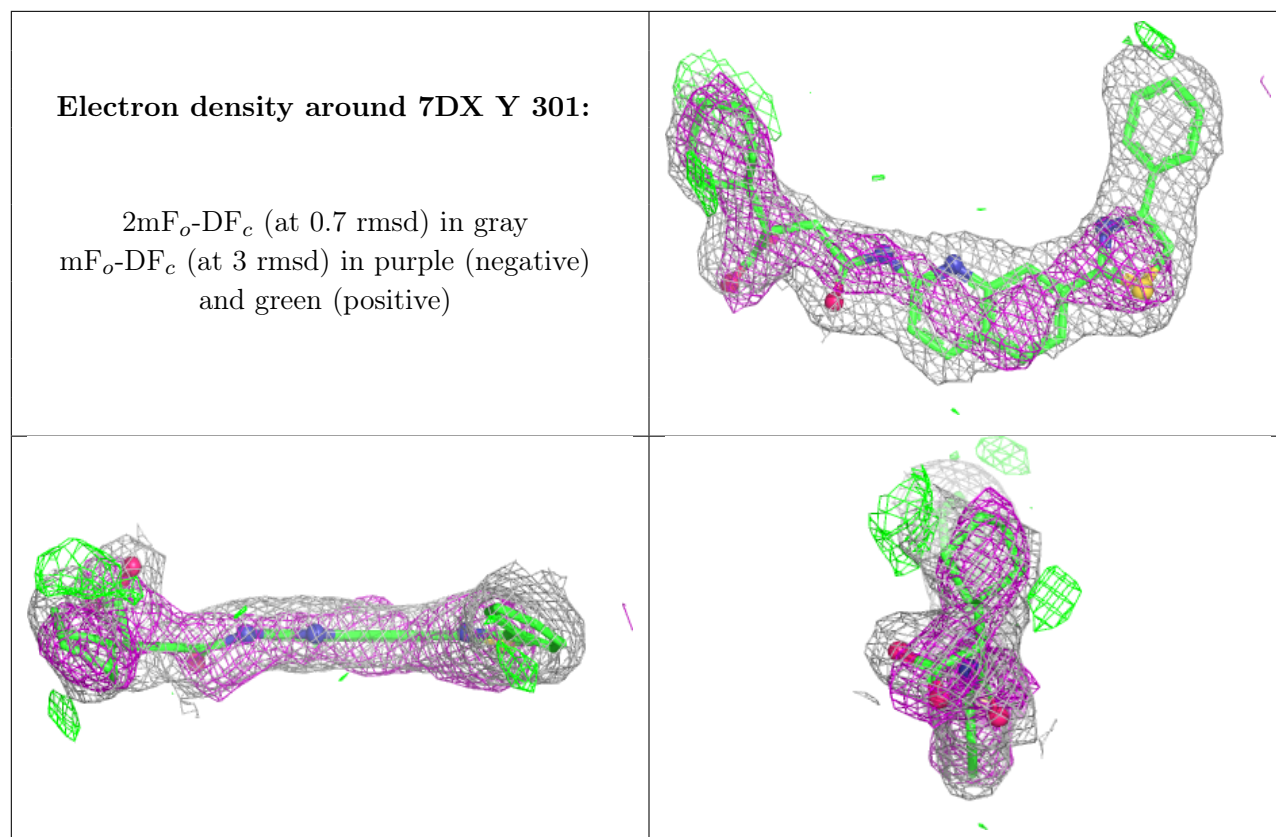
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	7DX	K	301	35/35	0.81	0.14	42,44,47,52	0
15	MG	I	301	1/1	0.83	0.16	59,59,59,59	0
17	7DX	Y	301	35/35	0.83	0.14	42,44,47,53	0
16	CL	b	201	1/1	0.88	0.10	61,61,61,61	0
15	MG	K	302	1/1	0.94	0.12	52,52,52,52	0
15	MG	N	201	1/1	0.95	0.06	42,42,42,42	0
15	MG	G	301	1/1	0.95	0.04	48,48,48,48	0
16	CL	G	302	1/1	0.96	0.11	30,30,30,30	0
15	MG	J	201	1/1	0.96	0.06	47,47,47,47	0
16	CL	N	202	1/1	0.97	0.10	53,53,53,53	0
15	MG	Z	301	1/1	0.97	0.04	49,49,49,49	0
15	MG	L	301	1/1	0.98	0.07	52,52,52,52	0
16	CL	U	301	1/1	0.99	0.17	30,30,30,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 7DX K 301:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.