



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2025 – 10:32 am BST

PDB ID : 9QB1 / pdb_00009qb1
Title : Yeast 20S proteasome mutant: beta5_T3M in complex with Bortezomib
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2025-02-28
Resolution : 2.80 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

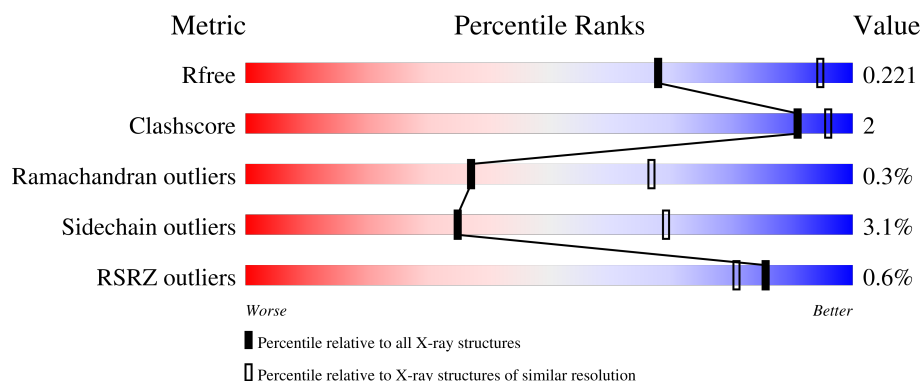
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

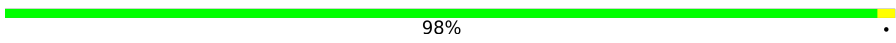
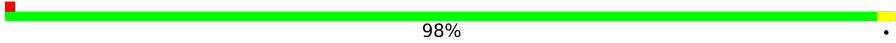



The reported resolution of this entry is 2.80 Å.

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.






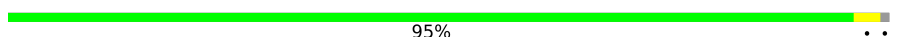


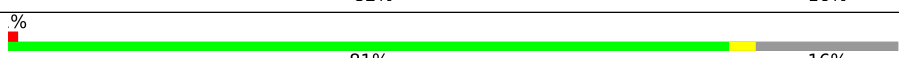



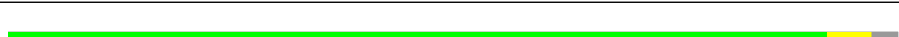


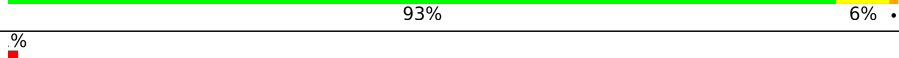
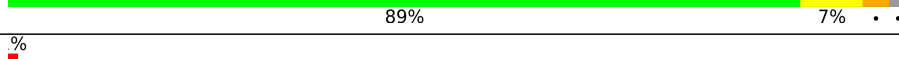



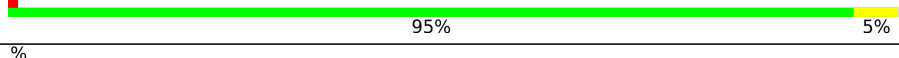
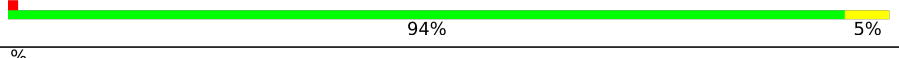
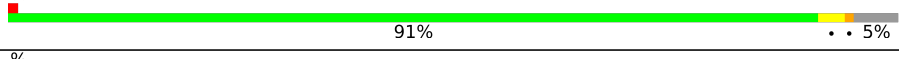

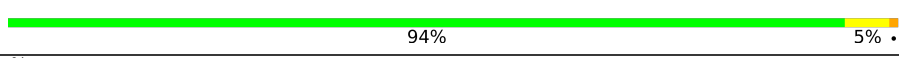
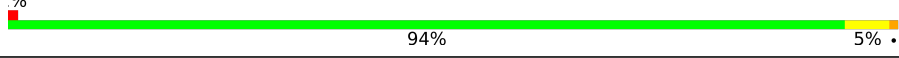

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	 98%
1	O	250	 98%
2	B	258	 88% 7% 5%
2	P	258	 87% 7% 5%
3	C	254	 88% 6%



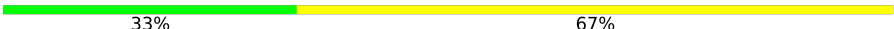
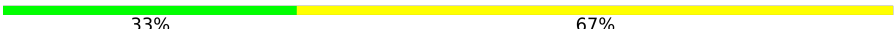
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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	231	
8	V	231	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	211	
11	Y	211	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	195	
14	b	195	
15	e	3	
15	f	3	

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Mol	Chain	Length	Quality of chain
15	g	3	 67% 33%
15	h	3	 33% 67%
15	i	3	 33% 67%
15	j	3	 33% 67%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49925 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	225	Total	C	N	O	S	0	0	0
			1712	1078	297	330	7			
8	V	225	Total	C	N	O	S	0	0	0
			1712	1078	297	330	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-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1638	1042	279	309	8			
11	Y	211	Total	C	N	O	S	0	0	0
			1638	1042	279	309	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	3	MET	THR	engineered mutation	UNP P30656
Y	3	MET	THR	engineered mutation	UNP P30656

- 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	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	195	Total	C	N	O	S	0	0	0
			1505	951	249	298	7			
14	b	195	Total	C	N	O	S	0	0	0
			1505	951	249	298	7			

- Molecule 15 is a protein called 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-C]PYRAZ

OLE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	3	Total	C	N	O	0	0	0
			35	24	5	6			
15	f	3	Total	C	N	O	0	0	0
			35	24	5	6			
15	g	3	Total	C	N	O	0	0	0
			35	24	5	6			
15	h	3	Total	C	N	O	0	0	0
			35	24	5	6			
15	i	3	Total	C	N	O	0	0	0
			35	24	5	6			
15	j	3	Total	C	N	O	0	0	0
			35	24	5	6			

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	b	1	Total	Cl	0	0
			1	1		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	16	Total	O	0	0
			16	16		
18	B	15	Total	O	0	0
			15	15		
18	C	13	Total	O	0	0
			13	13		
18	D	5	Total	O	0	0
			5	5		
18	E	5	Total	O	0	0
			5	5		
18	F	14	Total	O	0	0
			14	14		
18	G	19	Total	O	0	0
			19	19		
18	H	23	Total	O	0	0
			23	23		
18	I	12	Total	O	0	0
			12	12		
18	J	16	Total	O	0	0
			16	16		
18	K	8	Total	O	0	0
			8	8		
18	L	14	Total	O	0	0
			14	14		
18	M	21	Total	O	0	0
			21	21		
18	N	13	Total	O	0	0
			13	13		
18	O	5	Total	O	0	0
			5	5		
18	P	11	Total	O	0	0
			11	11		
18	Q	14	Total	O	0	0
			14	14		
18	R	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	S	7	Total 7	O 7	0	0
18	T	6	Total 6	O 6	0	0
18	U	18	Total 18	O 18	0	0
18	V	25	Total 25	O 25	0	0
18	W	12	Total 12	O 12	0	0
18	X	13	Total 13	O 13	0	0
18	Y	13	Total 13	O 13	0	0
18	Z	12	Total 12	O 12	0	0
18	a	21	Total 21	O 21	0	0
18	b	13	Total 13	O 13	0	0
18	e	1	Total 1	O 1	0	0
18	g	1	Total 1	O 1	0	0
18	i	2	Total 2	O 2	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.

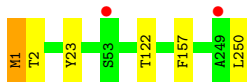
- Molecule 1: Proteasome subunit alpha type-2

Chain A:  98% .




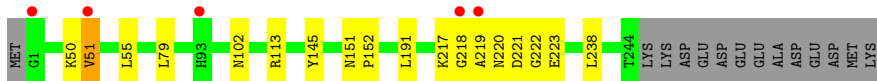
- Molecule 1: Proteasome subunit alpha type-2

Chain O:  98% .




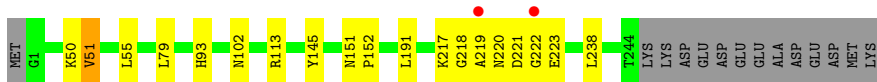
- Molecule 2: Proteasome subunit alpha type-3

Chain B:  88% 7% 5% 2%




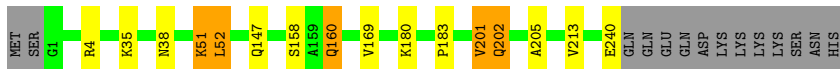
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  87% 7% 5% 2%

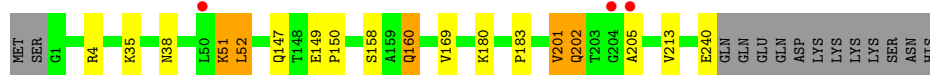
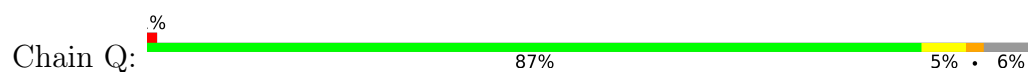


- Molecule 3: Proteasome subunit alpha type-4

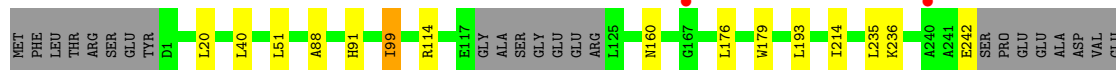
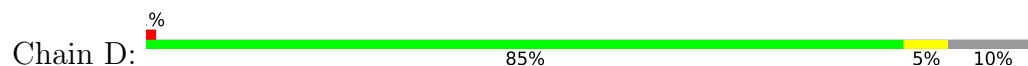
Chain C:  88% . . 6%



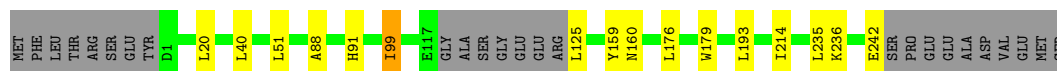
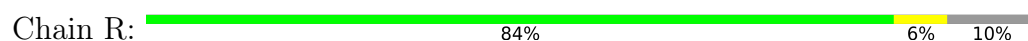
- Molecule 3: Proteasome subunit alpha type-4



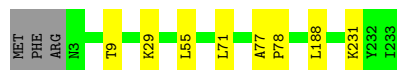
- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5



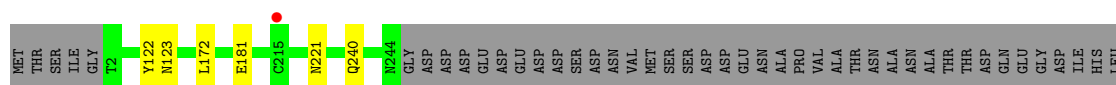
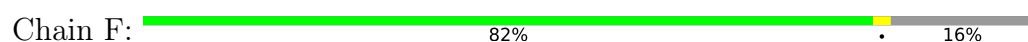
- Molecule 5: Proteasome subunit alpha type-6



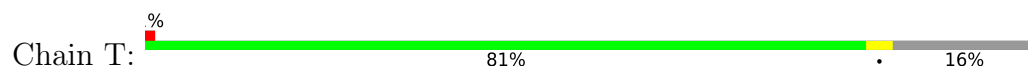
- Molecule 5: Proteasome subunit alpha type-6

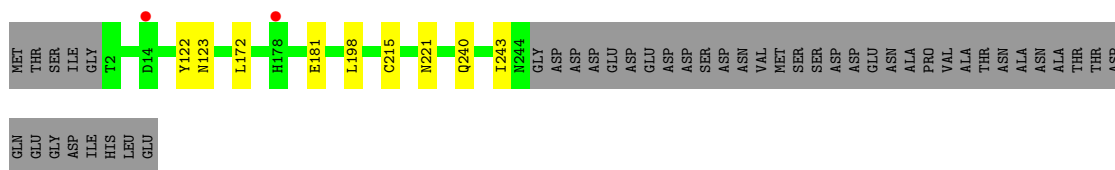


- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 6: Probable proteasome subunit alpha type-7





- Molecule 7: Proteasome subunit alpha type-1

Chain G: 90% 5% .



- Molecule 7: Proteasome subunit alpha type-1

Chain U: 90% 6% .



- Molecule 8: Proteasome subunit beta type-2

Chain H: 93% . .



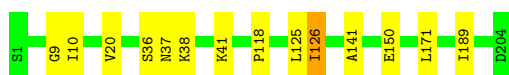
- Molecule 8: Proteasome subunit beta type-2

Chain V: 92% 5% .



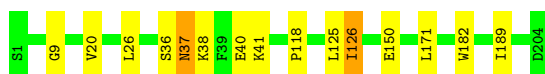
- Molecule 9: Proteasome subunit beta type-3

Chain I: 93% 6%

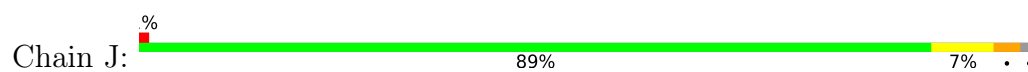


- Molecule 9: Proteasome subunit beta type-3

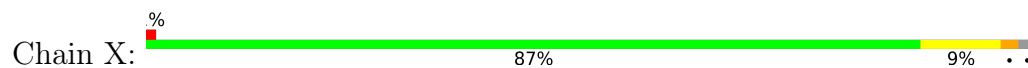
Chain W: 93% 6% .



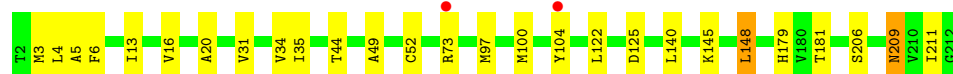
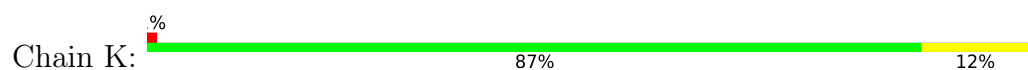
- Molecule 10: Proteasome subunit beta type-4



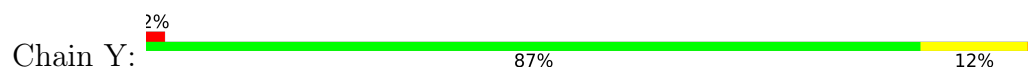
- Molecule 10: Proteasome subunit beta type-4



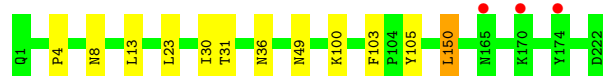
- Molecule 11: Proteasome subunit beta type-5



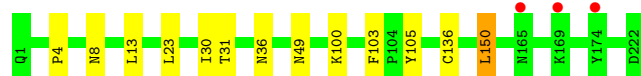
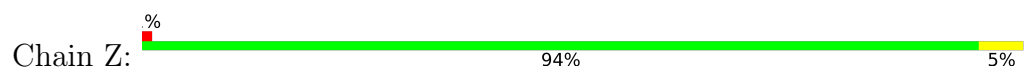
- Molecule 11: Proteasome subunit beta type-5



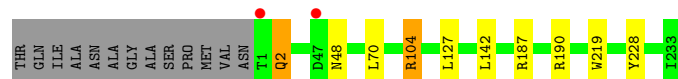
- Molecule 12: Proteasome subunit beta type-6



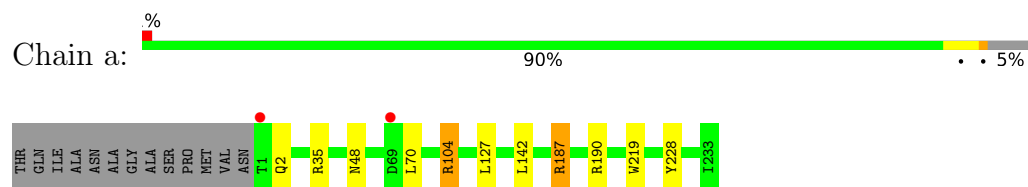
- Molecule 12: Proteasome subunit beta type-6



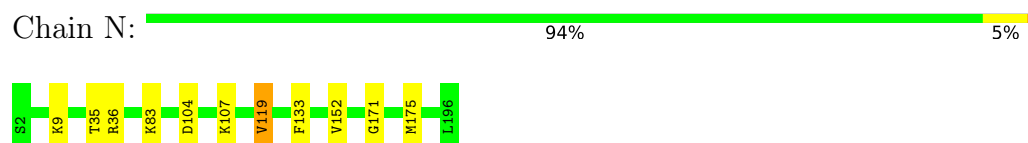
- Molecule 13: Proteasome subunit beta type-7



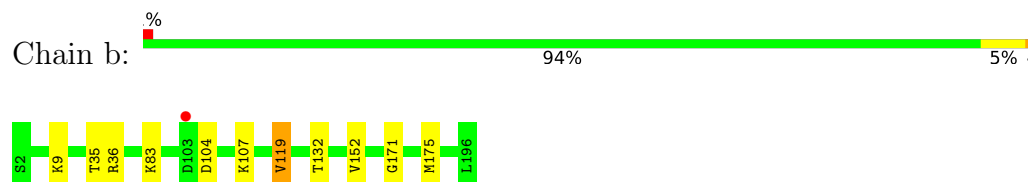
- Molecule 13: Proteasome subunit beta type-7



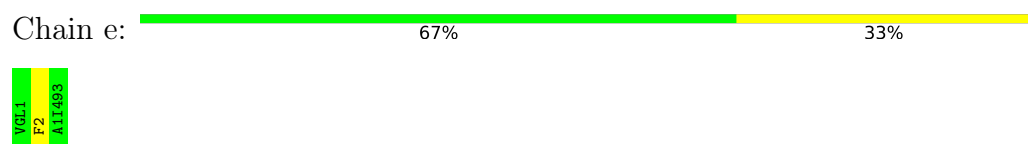
- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



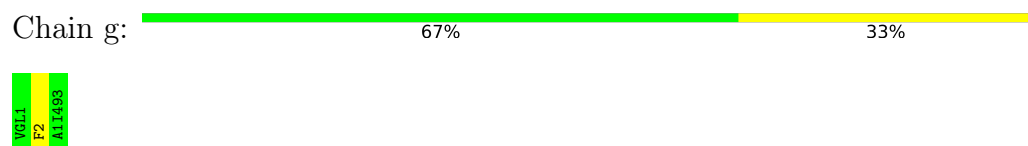
- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE



- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE



- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE



- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

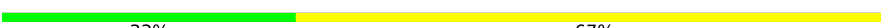


- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain i:  33% 67%

VCL1
F2
A11493

- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain j:  33% 67%

VCL1
F2
A11493

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.49Å 300.56Å 145.08Å 90.00° 112.95° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (15.00-2.80) 95.4 (15.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.193 , 0.215 0.200 , 0.221	Depositor DCC
R_{free} test set	12379 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49925	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: A1I49, VGL, CL, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/1952	0.67	0/2642
1	O	0.39	0/1952	0.68	0/2642
2	B	0.39	0/1934	0.66	0/2618
2	P	0.39	0/1934	0.67	0/2618
3	C	0.38	0/1910	0.68	1/2586 (0.0%)
3	Q	0.39	0/1910	0.68	1/2586 (0.0%)
4	D	0.38	0/1837	0.65	0/2475
4	R	0.38	0/1837	0.64	0/2475
5	E	0.39	0/1800	0.65	0/2433
5	S	0.38	0/1800	0.65	0/2433
6	F	0.39	0/1932	0.68	0/2609
6	T	0.38	0/1932	0.69	0/2609
7	G	0.38	0/1945	0.66	0/2634
7	U	0.38	0/1945	0.67	0/2634
8	H	0.33	0/1743	0.66	0/2363
8	V	0.33	0/1743	0.66	0/2363
9	I	0.34	0/1611	0.69	0/2174
9	W	0.36	0/1611	0.71	0/2174
10	J	0.45	0/1589	0.73	2/2142 (0.1%)
10	X	0.46	0/1589	0.74	0/2142
11	K	0.39	0/1675	0.72	0/2264
11	Y	0.34	0/1675	0.68	0/2264
12	L	0.33	0/1795	0.69	2/2420 (0.1%)
12	Z	0.33	0/1795	0.69	2/2420 (0.1%)
13	M	0.35	0/1855	0.69	0/2514
13	a	0.36	0/1855	0.70	1/2514 (0.0%)
14	N	0.34	0/1534	0.68	0/2077
14	b	0.33	0/1534	0.68	0/2077
15	e	1.35	0/11	1.91	1/13 (7.7%)
15	f	1.29	0/11	1.58	1/13 (7.7%)
15	g	1.32	0/11	1.89	1/13 (7.7%)
15	h	1.27	0/11	1.52	1/13 (7.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	i	1.33	0/11	1.74	1/13 (7.7%)
15	j	1.32	0/11	1.82	1/13 (7.7%)
All	All	0.38	0/50290	0.68	15/67980 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	35	ARG	N-CA-C	6.67	118.21	111.07
15	e	2	PHE	CA-CB-CG	-6.51	107.29	113.80
15	g	2	PHE	CA-CB-CG	-6.42	107.38	113.80
12	Z	103	PHE	CA-C-N	6.09	126.05	119.78
12	Z	103	PHE	C-N-CA	6.09	126.05	119.78
12	L	103	PHE	CA-C-N	6.00	125.96	119.78
12	L	103	PHE	C-N-CA	6.00	125.96	119.78
3	Q	201	VAL	N-CA-C	5.47	116.20	110.62
3	C	201	VAL	N-CA-C	5.41	116.14	110.62
15	j	2	PHE	CA-CB-CG	-5.39	108.41	113.80
15	f	2	PHE	CA-CB-CG	-5.30	108.50	113.80
10	J	147	HIS	CA-C-N	-5.29	115.70	123.00
10	J	147	HIS	C-N-CA	-5.29	115.70	123.00
15	i	2	PHE	CA-CB-CG	-5.20	108.61	113.80
15	h	2	PHE	CA-CB-CG	-5.16	108.64	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	1	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	6	0
2	P	1904	0	1904	7	0
3	C	1881	0	1895	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	5	0
8	H	1712	0	1709	10	0
8	V	1712	0	1709	10	0
9	I	1581	0	1574	9	0
9	W	1581	0	1574	8	0
10	J	1561	0	1569	20	0
10	X	1561	0	1569	15	0
11	K	1638	0	1587	14	0
11	Y	1638	0	1587	18	0
12	L	1757	0	1711	5	0
12	Z	1757	0	1711	5	0
13	M	1824	0	1832	5	0
13	a	1824	0	1832	5	0
14	N	1505	0	1471	5	0
14	b	1505	0	1471	5	0
15	e	35	0	11	0	0
15	f	35	0	11	1	0
15	g	35	0	11	0	0
15	h	35	0	11	1	0
15	i	35	0	11	1	0
15	j	35	0	11	1	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	J	1	0	0	0	0
16	K	1	0	0	0	0
16	N	1	0	0	0	0
16	V	1	0	0	0	0
16	Y	1	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	b	1	0	0	0	0
18	A	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	B	15	0	0	0	0
18	C	13	0	0	0	0
18	D	5	0	0	1	0
18	E	5	0	0	0	0
18	F	14	0	0	0	0
18	G	19	0	0	0	0
18	H	23	0	0	0	0
18	I	12	0	0	0	0
18	J	16	0	0	0	0
18	K	8	0	0	0	0
18	L	14	0	0	0	0
18	M	21	0	0	1	0
18	N	13	0	0	0	0
18	O	5	0	0	0	0
18	P	11	0	0	1	0
18	Q	14	0	0	0	0
18	R	9	0	0	0	0
18	S	7	0	0	0	0
18	T	6	0	0	1	0
18	U	18	0	0	0	0
18	V	25	0	0	0	0
18	W	12	0	0	0	0
18	X	13	0	0	1	0
18	Y	13	0	0	0	0
18	Z	12	0	0	0	0
18	a	21	0	0	0	0
18	b	13	0	0	0	0
18	e	1	0	0	0	0
18	g	1	0	0	0	0
18	i	2	0	0	0	0
All	All	49925	0	49140	159	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 (159) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:149:ARG:NE	11:Y:205:GLY:O	2.21	0.72
10:X:25:ILE:O	10:X:25:ILE:HG12	1.90	0.71
10:J:149:ARG:HH11	11:Y:206:SER:HA	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.25	0.68
10:J:139:TYR:HE1	10:J:171:ARG:HB3	1.59	0.68
11:K:73:ARG:NH2	11:K:104:TYR:O	2.26	0.67
9:I:38:LYS:NZ	11:Y:209:ASN:O	2.30	0.64
14:b:152:VAL:HA	14:b:175:MET:HE1	1.83	0.61
10:J:139:TYR:CE1	10:J:171:ARG:CB	2.84	0.60
10:J:139:TYR:CE1	10:J:171:ARG:HB3	2.37	0.60
14:N:152:VAL:HA	14:N:175:MET:HE1	1.84	0.60
2:P:93:HIS:HB3	18:P:301:HOH:O	2.03	0.59
11:K:52:CYS:HA	11:K:97:MET:HE3	1.84	0.58
10:X:152:MET:HE2	10:X:156:GLU:HB3	1.85	0.57
13:M:2:GLN:NE2	18:M:301:HOH:O	2.37	0.56
11:K:3:MET:SD	11:K:44:THR:HB	2.45	0.56
10:J:139:TYR:HE1	10:J:171:ARG:CB	2.18	0.56
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.88	0.55
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.88	0.55
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.89	0.55
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.88	0.55
6:T:215:CYS:HB3	18:T:303:HOH:O	2.06	0.55
9:I:125:LEU:HG	9:I:126:ILE:HG22	1.90	0.54
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.89	0.54
10:J:139:TYR:CE1	10:J:171:ARG:HB2	2.43	0.54
11:Y:3:MET:SD	11:Y:44:THR:HB	2.47	0.54
9:W:125:LEU:HG	9:W:126:ILE:HG22	1.89	0.53
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.91	0.53
11:K:49:ALA:HB3	15:f:1:VGL:H6	1.92	0.52
11:Y:49:ALA:HB3	15:h:1:VGL:H6	1.91	0.52
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.90	0.52
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.91	0.52
7:U:23:PHE:O	7:U:26:THR:HB	2.09	0.52
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.92	0.52
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.92	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.52
11:Y:209:ASN:OD1	11:Y:209:ASN:C	2.53	0.51
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.75	0.51
7:G:23:PHE:O	7:G:26:THR:HB	2.09	0.51
11:K:209:ASN:OD1	11:K:209:ASN:C	2.53	0.51
10:J:149:ARG:HH11	11:Y:206:SER:CA	2.21	0.50
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.76	0.50
2:P:50:LYS:O	2:P:51:VAL:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:LYS:O	2:B:51:VAL:C	2.55	0.49
2:B:217:LYS:C	2:B:219:ALA:H	2.21	0.49
8:H:114:HIS:CD2	15:i:1:VGL:H4	2.47	0.48
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.94	0.48
8:V:114:HIS:CD2	15:j:1:VGL:H4	2.48	0.48
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.94	0.48
10:J:147:HIS:HB2	10:J:160:LEU:HD13	1.95	0.48
14:N:35:THR:HG21	13:a:228:TYR:HE2	1.78	0.47
2:P:217:LYS:C	2:P:219:ALA:H	2.21	0.47
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.80	0.47
10:X:174:MET:HB2	18:X:207:HOH:O	2.15	0.47
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.96	0.47
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.97	0.47
8:H:35:HIS:CB	8:H:56:THR:HG21	2.44	0.47
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.79	0.47
8:V:35:HIS:CB	8:V:56:THR:HG21	2.45	0.47
9:W:26:LEU:CD2	9:W:40:GLU:HG3	2.44	0.47
8:H:196:ARG:NH2	9:I:150:GLU:O	2.49	0.46
10:J:139:TYR:OH	10:X:25:ILE:O	2.24	0.46
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.49	0.46
4:D:114:ARG:HD3	18:D:303:HOH:O	2.15	0.46
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.97	0.46
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.98	0.46
11:K:6:PHE:HA	11:K:125:ASP:O	2.16	0.46
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.97	0.46
3:C:51:LYS:O	3:C:52:LEU:HB2	2.15	0.46
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.97	0.46
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.51	0.46
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.51	0.46
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.16	0.46
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.97	0.46
10:J:25:ILE:HG12	10:J:25:ILE:O	2.15	0.46
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.15	0.45
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.17	0.45
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.52	0.45
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.51	0.45
8:H:139:GLU:OE1	13:a:187:ARG:NH1	2.45	0.45
10:X:147:HIS:HB2	10:X:160:LEU:HD13	1.98	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.97	0.45
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.17	0.45
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.47	0.45
11:K:206:SER:HA	10:X:149:ARG:HH22	1.81	0.45
3:C:201:VAL:O	3:C:202:GLN:HB3	2.17	0.45
11:K:3:MET:HB2	11:K:16:VAL:HG12	1.99	0.45
11:Y:179:HIS:CE1	11:Y:181:THR:HG23	2.52	0.44
2:B:145:TYR:OH	2:B:217:LYS:N	2.50	0.44
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.99	0.44
11:Y:3:MET:HB2	11:Y:16:VAL:HG12	1.99	0.44
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.47	0.44
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.00	0.44
3:C:35:LYS:HG2	3:C:158:SER:O	2.17	0.44
11:K:179:HIS:CE1	11:K:181:THR:HG23	2.53	0.43
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.85	0.43
2:P:145:TYR:OH	2:P:217:LYS:N	2.51	0.43
8:V:196:ARG:NH2	9:W:150:GLU:O	2.51	0.43
2:B:221:ASP:O	2:B:223:GLU:N	2.52	0.43
10:J:149:ARG:CG	10:J:149:ARG:HH21	2.32	0.43
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.01	0.43
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.01	0.43
2:P:221:ASP:O	2:P:223:GLU:N	2.52	0.43
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.00	0.43
10:X:147:HIS:N	10:X:147:HIS:ND1	2.66	0.43
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.54	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.00	0.43
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.01	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.43
11:Y:211:ILE:H	11:Y:211:ILE:HG13	1.73	0.43
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.01	0.42
10:X:163:LEU:HD12	10:X:163:LEU:HA	1.80	0.42
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.53	0.42
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.49	0.42
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.19	0.42
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.49	0.42
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.00	0.42
9:W:37:ASN:HB3	9:W:182:TRP:CE3	2.54	0.42
10:J:25:ILE:O	10:X:173:PRO:HD3	2.19	0.42
13:a:127:LEU:HG	13:a:142:LEU:HD12	2.01	0.42
7:U:73:VAL:HG12	7:U:133:THR:HB	2.01	0.42
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.50	0.42
11:K:5:ALA:HA	11:K:13:ILE:O	2.20	0.42
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.55	0.42
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.54	0.41
13:M:228:TYR:HE2	14:b:35:THR:HG21	1.84	0.41
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.02	0.41
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.50	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.41
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.50	0.41
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	2.02	0.41
7:G:73:VAL:HG12	7:G:133:THR:HB	2.02	0.41
12:L:4:PRO:O	13:M:104:ARG:NH1	2.49	0.41
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.20	0.41
10:J:23:ARG:NH1	10:J:50:ALA:CB	2.84	0.41
8:V:126:SER:O	8:V:127:LEU:HD12	2.21	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.41
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.56	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.03	0.41
12:Z:4:PRO:O	13:a:104:ARG:NH1	2.47	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.03	0.40
10:J:147:HIS:HB2	10:J:160:LEU:CD1	2.51	0.40
11:K:16:VAL:HG21	11:K:34:VAL:HG23	2.03	0.40
14:N:133:PHE:HA	14:b:132:THR:O	2.21	0.40
10:X:23:ARG:HD3	10:X:23:ARG:HA	1.54	0.40
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.21	0.40
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.36	0.40
2:B:217:LYS:C	2:B:219:ALA:N	2.79	0.40
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.51	0.40
6:T:198:LEU:HD12	6:T:243:ILE:HG22	2.04	0.40
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.04	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%)	238 (96%)	9 (4%)	1 (0%)	30	61
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	30	61
2	B	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	26
2	P	242/258 (94%)	232 (96%)	6 (2%)	4 (2%)	7	26
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	10	32
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	10	32
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
5	E	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	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	223/231 (96%)	216 (97%)	7 (3%)	0	100	100
8	V	223/231 (96%)	216 (97%)	7 (3%)	0	100	100
9	I	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
9	W	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	186 (96%)	7 (4%)	0	100	100
11	K	209/211 (99%)	205 (98%)	4 (2%)	0	100	100
11	Y	209/211 (99%)	205 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
14	N	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
14	b	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
All	All	6278/6606 (95%)	6104 (97%)	158 (2%)	16 (0%)	37	67

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
2	B	222	GLY
1	O	2	THR
2	P	218	GLY
2	P	222	GLY
2	B	220	ASN
2	P	220	ASN
3	C	205	ALA
3	Q	205	ALA
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	209/209 (100%)	205 (98%)	4 (2%)	52	82
1	O	209/209 (100%)	205 (98%)	4 (2%)	52	82
2	B	203/216 (94%)	197 (97%)	6 (3%)	36	70
2	P	203/216 (94%)	197 (97%)	6 (3%)	36	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	212/226 (94%)	202 (95%)	10 (5%)	22	54
3	Q	212/226 (94%)	202 (95%)	10 (5%)	22	54
4	D	194/215 (90%)	184 (95%)	10 (5%)	19	50
4	R	194/215 (90%)	183 (94%)	11 (6%)	17	46
5	E	190/193 (98%)	184 (97%)	6 (3%)	34	68
5	S	190/193 (98%)	184 (97%)	6 (3%)	34	68
6	F	201/239 (84%)	196 (98%)	5 (2%)	42	75
6	T	201/239 (84%)	196 (98%)	5 (2%)	42	75
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	66
7	U	206/210 (98%)	199 (97%)	7 (3%)	32	66
8	H	184/189 (97%)	182 (99%)	2 (1%)	70	90
8	V	184/189 (97%)	182 (99%)	2 (1%)	70	90
9	I	172/172 (100%)	169 (98%)	3 (2%)	56	84
9	W	172/172 (100%)	168 (98%)	4 (2%)	45	78
10	J	173/175 (99%)	166 (96%)	7 (4%)	27	60
10	X	173/175 (99%)	165 (95%)	8 (5%)	23	55
11	K	168/168 (100%)	161 (96%)	7 (4%)	25	58
11	Y	168/168 (100%)	161 (96%)	7 (4%)	25	58
12	L	185/185 (100%)	182 (98%)	3 (2%)	58	85
12	Z	185/185 (100%)	181 (98%)	4 (2%)	47	79
13	M	199/208 (96%)	193 (97%)	6 (3%)	36	70
13	a	199/208 (96%)	193 (97%)	6 (3%)	36	70
14	N	161/161 (100%)	156 (97%)	5 (3%)	35	69
14	b	161/161 (100%)	156 (97%)	5 (3%)	35	69
15	e	1/1 (100%)	1 (100%)	0	100	100
15	f	1/1 (100%)	1 (100%)	0	100	100
15	g	1/1 (100%)	1 (100%)	0	100	100
15	h	1/1 (100%)	1 (100%)	0	100	100
15	i	1/1 (100%)	1 (100%)	0	100	100
15	j	1/1 (100%)	1 (100%)	0	100	100
All	All	5320/5538 (96%)	5154 (97%)	166 (3%)	35	69

All (166) 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	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	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	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
5	E	188	LEU
5	E	231	LYS
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	221	ASN
6	F	240	GLN
7	G	26	THR

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Mol	Chain	Res	Type
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	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
10	J	3	ILE
10	J	23	ARG
10	J	25	ILE
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
10	J	149	ARG
11	K	4	LEU
11	K	35	ILE
11	K	100	MET
11	K	140	LEU
11	K	148	LEU
11	K	209	ASN
11	K	211	ILE
12	L	23	LEU
12	L	49	ASN
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	187	ARG
13	M	190	ARG
14	N	9	LYS
14	N	36	ARG
14	N	104	ASP
14	N	107	LYS
14	N	119	VAL
1	O	1	MET
1	O	122	THR
1	O	157	PHE

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Mol	Chain	Res	Type
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	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	52	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
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	221	ASN
6	T	240	GLN
7	U	26	THR
7	U	75	ASN
7	U	115	LEU

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Mol	Chain	Res	Type
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	38	LYS
9	W	126	ILE
9	W	171	LEU
10	X	3	ILE
10	X	23	ARG
10	X	25	ILE
10	X	28	LEU
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
10	X	147	HIS
11	Y	4	LEU
11	Y	35	ILE
11	Y	100	MET
11	Y	140	LEU
11	Y	148	LEU
11	Y	209	ASN
11	Y	211	ILE
12	Z	23	LEU
12	Z	49	ASN
12	Z	136	CYS
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	187	ARG
13	a	190	ARG
14	b	9	LYS
14	b	36	ARG
14	b	104	ASP
14	b	107	LYS
14	b	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	155	ASN
2	B	176	GLN
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
6	F	123	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
8	H	86	HIS
8	H	114	HIS
8	H	194	ASN
9	I	63	ASN
9	I	88	GLN
9	I	203	GLN
10	J	55	GLN
10	J	63	ASN
10	J	146	HIS
10	J	147	HIS
11	K	9	GLN
11	K	24	ASN
11	K	85	ASN

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Mol	Chain	Res	Type
11	K	143	ASN
11	K	176	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	79	HIS
12	L	80	ASN
12	L	155	ASN
12	L	158	ASN
12	L	197	GLN
13	M	26	ASN
13	M	48	ASN
13	M	108	ASN
13	M	149	HIS
13	M	194	ASN
13	M	213	GLN
14	N	38	HIS
14	N	141	ASN
2	P	93	HIS
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	176	GLN
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	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN

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Mol	Chain	Res	Type
6	T	86	ASN
6	T	123	ASN
7	U	30	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	175	ASN
8	V	86	HIS
8	V	114	HIS
8	V	194	ASN
9	W	37	ASN
9	W	63	ASN
9	W	88	GLN
9	W	203	GLN
10	X	55	GLN
10	X	63	ASN
10	X	147	HIS
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	29	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	79	HIS
12	Z	153	GLN
12	Z	155	ASN
12	Z	158	ASN
12	Z	197	GLN
13	a	48	ASN
13	a	62	HIS
13	a	108	ASN
13	a	149	HIS
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 [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 12 ligands modelled in this entry, 12 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 [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%)	-0.50	0 100 100	43, 58, 96, 136	0
1	O	250/250 (100%)	-0.48	2 (0%) 82 77	47, 67, 110, 147	0
2	B	244/258 (94%)	-0.33	5 (2%) 64 56	48, 69, 116, 168	0
2	P	244/258 (94%)	-0.34	2 (0%) 82 77	52, 71, 113, 157	0
3	C	240/254 (94%)	-0.26	0 100 100	46, 72, 133, 162	0
3	Q	240/254 (94%)	-0.15	3 (1%) 74 67	53, 83, 166, 186	0
4	D	235/260 (90%)	-0.37	2 (0%) 81 75	52, 73, 104, 147	0
4	R	235/260 (90%)	-0.22	0 100 100	60, 78, 120, 155	0
5	E	231/234 (98%)	-0.30	0 100 100	50, 74, 112, 154	0
5	S	231/234 (98%)	-0.16	1 (0%) 89 85	53, 80, 126, 160	0
6	F	243/288 (84%)	-0.36	1 (0%) 89 85	46, 69, 115, 144	0
6	T	243/288 (84%)	-0.22	2 (0%) 82 77	48, 76, 135, 164	0
7	G	241/252 (95%)	-0.50	0 100 100	42, 60, 98, 146	0
7	U	241/252 (95%)	-0.43	0 100 100	47, 63, 100, 149	0
8	H	225/231 (97%)	-0.50	1 (0%) 89 85	38, 56, 96, 156	0
8	V	225/231 (97%)	-0.51	1 (0%) 89 85	42, 59, 92, 173	0
9	I	204/204 (100%)	-0.64	0 100 100	41, 58, 86, 114	0
9	W	204/204 (100%)	-0.60	0 100 100	45, 61, 91, 114	0
10	J	195/198 (98%)	-0.50	1 (0%) 87 83	43, 60, 90, 128	0
10	X	195/198 (98%)	-0.50	1 (0%) 87 83	45, 63, 90, 140	0
11	K	211/211 (100%)	-0.17	2 (0%) 81 75	51, 68, 105, 122	0
11	Y	211/211 (100%)	-0.10	4 (1%) 66 58	52, 68, 110, 129	0
12	L	222/222 (100%)	-0.40	3 (1%) 73 66	44, 61, 111, 142	0
12	Z	222/222 (100%)	-0.39	3 (1%) 73 66	36, 62, 115, 147	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.63	2 (0%) 81 75	39, 57, 80, 99	0
13	a	233/246 (94%)	-0.59	2 (0%) 81 75	40, 57, 78, 100	0
14	N	195/195 (100%)	-0.59	0 100 100	39, 52, 81, 107	0
14	b	195/195 (100%)	-0.54	1 (0%) 87 83	40, 54, 83, 113	0
15	e	1/3 (33%)	-0.27	0 100 100	56, 56, 56, 56	0
15	f	1/3 (33%)	-0.08	0 100 100	60, 60, 60, 60	0
15	g	1/3 (33%)	0.01	0 100 100	60, 60, 60, 60	0
15	h	1/3 (33%)	0.20	0 100 100	65, 65, 65, 65	0
15	i	1/3 (33%)	1.75	0 100 100	55, 55, 55, 55	0
15	j	1/3 (33%)	0.76	0 100 100	57, 57, 57, 57	0
All	All	6344/6624 (95%)	-0.40	39 (0%) 85 81	36, 65, 113, 186	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	5.5
10	J	1	MET	4.2
3	Q	50	LEU	3.9
12	Z	174	TYR	3.9
2	B	219	ALA	3.8
8	V	223	ILE	3.5
12	L	174	TYR	3.5
2	P	219	ALA	3.3
12	L	165	ASN	3.2
11	Y	208	ASN	3.0
3	Q	204	GLY	2.9
2	B	51	VAL	2.9
13	a	1	THR	2.8
6	F	215	CYS	2.6
2	B	218	GLY	2.6
6	T	178	HIS	2.6
12	L	170	LYS	2.6
11	Y	148	LEU	2.5
14	b	103	ASP	2.4
8	H	223	ILE	2.4
12	Z	169	LYS	2.4
11	K	104	TYR	2.4
3	Q	205	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
12	Z	165	ASN	2.4
13	M	47	ASP	2.4
11	Y	46	ALA	2.4
13	M	1	THR	2.3
2	B	1	GLY	2.3
6	T	14	ASP	2.3
4	D	167	GLY	2.3
2	B	93	HIS	2.2
11	K	73	ARG	2.2
13	a	69	ASP	2.2
5	S	207	VAL	2.1
1	O	53	SER	2.0
1	O	249	ALA	2.0
4	D	240	ALA	2.0
11	Y	145	LYS	2.0
2	P	222	GLY	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
16	MG	Z	301	1/1	0.92	0.12	67,67,67,67	0
16	MG	Y	301	1/1	0.93	0.07	63,63,63,63	0
16	MG	I	301	1/1	0.94	0.16	75,75,75,75	0
16	MG	V	301	1/1	0.94	0.09	71,71,71,71	0
17	CL	b	201	1/1	0.97	0.11	50,50,50,50	0
16	MG	G	301	1/1	0.98	0.03	51,51,51,51	0
16	MG	J	201	1/1	0.98	0.13	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	MG	K	301	1/1	0.99	0.06	66,66,66,66	0
17	CL	G	302	1/1	0.99	0.09	40,40,40,40	0
17	CL	N	202	1/1	0.99	0.05	49,49,49,49	0
17	CL	U	301	1/1	0.99	0.08	46,46,46,46	0
16	MG	N	201	1/1	0.99	0.06	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.