



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 03:23 AM UTC

PDB ID : 9QB4 / pdb_00009qb4
Title : Yeast 20S proteasome mutant: beta5_T3M in complex with Carfilzomib
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2025-02-28
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

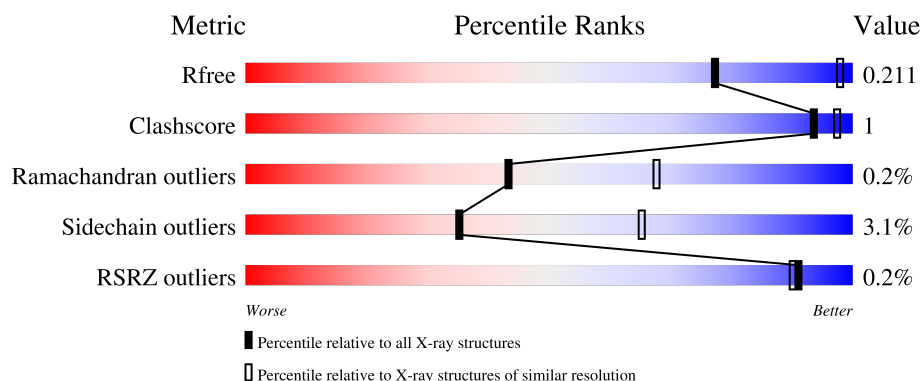
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



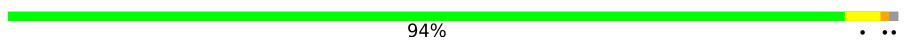
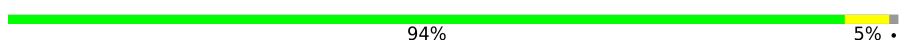
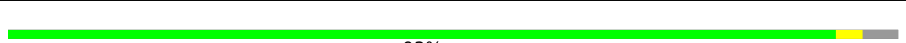
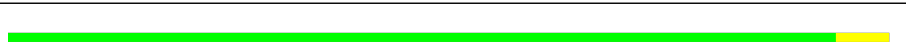
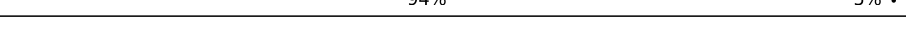
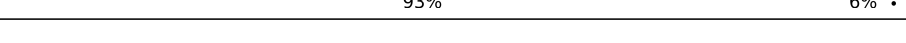
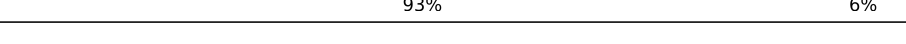
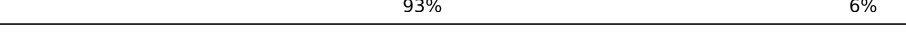
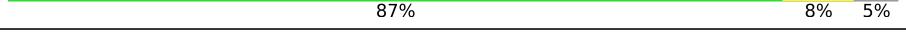
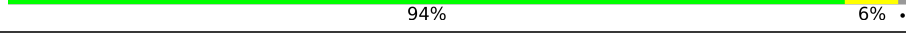
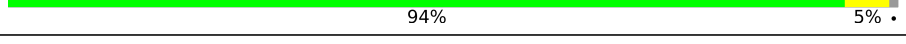
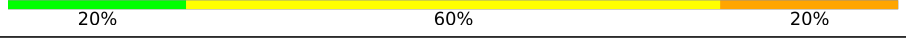
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	
1	O	250	
2	B	258	
2	P	258	
3	C	254	

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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	205	
9	W	205	
10	J	198	
10	X	198	
11	K	211	
11	Y	211	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	
15	e	5	
15	f	5	

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Mol	Chain	Length	Quality of chain
15	g	5	20%60%20%
15	h	5	20%40%40%
15	i	5	40%40%20%
15	j	5	40%40%20%

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49952 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	240	Total	C	N	O	S	0	0	0
			1903	1212	319	364	8			
7	U	240	Total	C	N	O	S	0	0	0
			1903	1212	319	364	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	7			
8	V	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	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 Carfilzomib.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	e	5	Total C N O 59 44 6 9	0	0	0
15	f	5	Total C N O 59 44 6 9	0	0	0
15	g	5	Total C N O 59 44 6 9	0	0	0
15	h	5	Total C N O 59 44 6 9	0	0	0
15	i	5	Total C N O 59 44 6 9	0	0	0
15	j	5	Total C N O 59 44 6 9	0	0	0

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

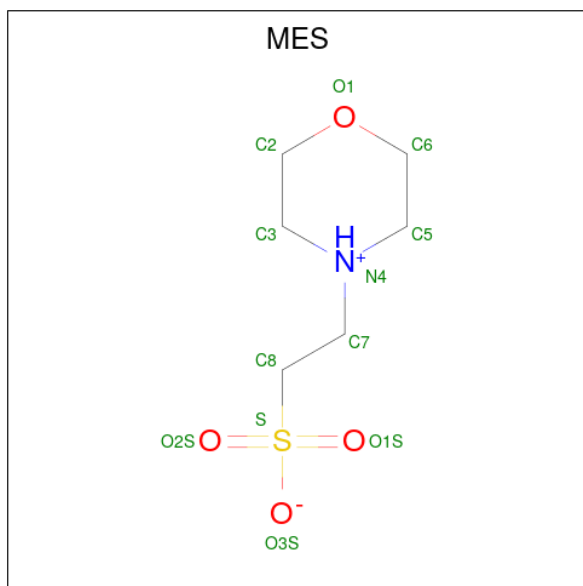
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Mg 1 1	0	0
16	I	1	Total Mg 1 1	0	0
16	K	1	Total Mg 1 1	0	0
16	N	1	Total Mg 1 1	0	0
16	V	1	Total Mg 1 1	0	0
16	Y	1	Total Mg 1 1	0	0
16	Z	1	Total Mg 1 1	0	0

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

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

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES)

(formula: C₆H₁₃NO₄S).



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	13	Total	O	0	0
			13	13		
19	B	16	Total	O	0	0
			16	16		
19	C	10	Total	O	0	0
			10	10		
19	D	4	Total	O	0	0
			4	4		
19	E	7	Total	O	0	0
			7	7		
19	F	11	Total	O	0	0
			11	11		
19	G	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	H	9	Total O 9 9	0	0
19	I	13	Total O 13 13	0	0
19	J	8	Total O 8 8	0	0
19	K	11	Total O 11 11	0	0
19	L	17	Total O 17 17	0	0
19	M	13	Total O 13 13	0	0
19	N	8	Total O 8 8	0	0
19	O	6	Total O 6 6	0	0
19	P	7	Total O 7 7	0	0
19	Q	4	Total O 4 4	0	0
19	R	3	Total O 3 3	0	0
19	S	3	Total O 3 3	0	0
19	T	12	Total O 12 12	0	0
19	U	13	Total O 13 13	0	0
19	V	9	Total O 9 9	0	0
19	W	7	Total O 7 7	0	0
19	X	14	Total O 14 14	0	0
19	Y	14	Total O 14 14	0	0
19	Z	18	Total O 18 18	0	0
19	a	14	Total O 14 14	0	0
19	b	12	Total O 12 12	0	0

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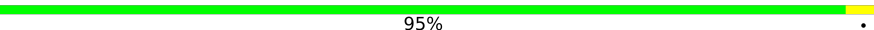
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	f	1	Total 1	O 1	0	0
19	h	1	Total 1	O 1	0	0
19	i	1	Total 1	O 1	0	0
19	j	3	Total 3	O 3	0	0

3 Residue-property plots [i](#)

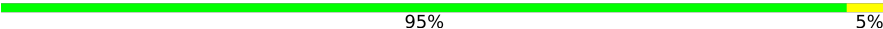
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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:  95% .



- Molecule 1: Proteasome subunit alpha type-2

Chain O:  95% 5%



- Molecule 2: Proteasome subunit alpha type-3

Chain B:  % 90% . . 5%



- Molecule 2: Proteasome subunit alpha type-3

Chain P:  % 89% 5% . 5%

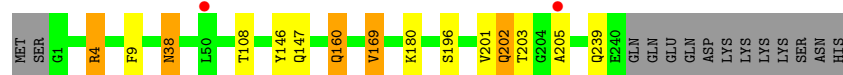
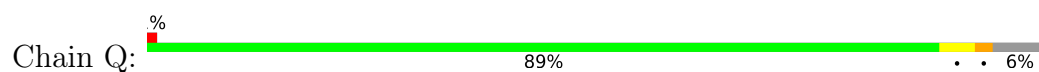


- Molecule 3: Proteasome subunit alpha type-4

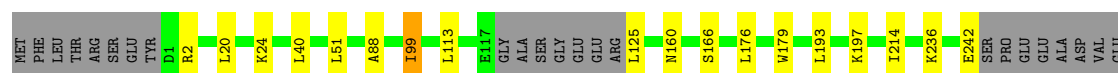
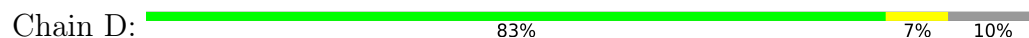
Chain C:  89% . . 6%



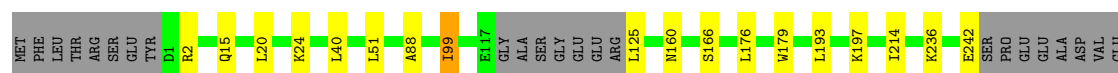
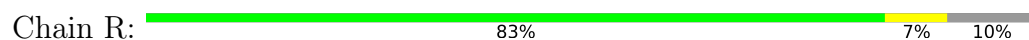
- Molecule 3: Proteasome subunit alpha type-4



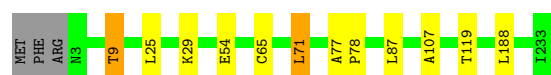
- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5



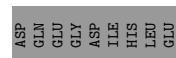
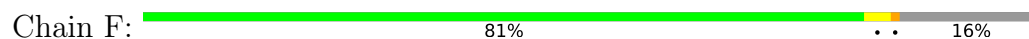
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 5: Proteasome subunit alpha type-6

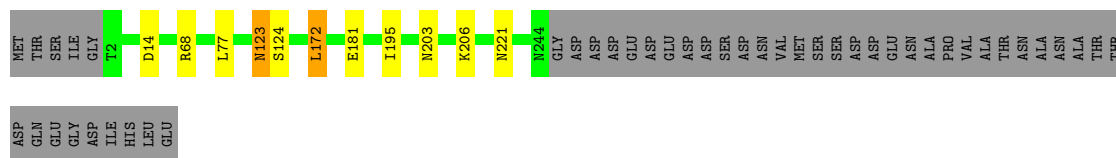


- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 6: Probable proteasome subunit alpha type-7

Chain T:  81% 16%



- Molecule 7: Proteasome subunit alpha type-1

Chain G:  90% 5% 5%



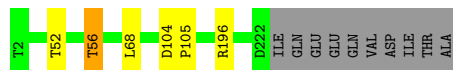
- Molecule 7: Proteasome subunit alpha type-1

Chain U:  90% 6% 5%



- Molecule 8: Proteasome subunit beta type-2

Chain H:  93% 1% 6%



- Molecule 8: Proteasome subunit beta type-2

Chain V:  93% 1% 6%



- Molecule 9: Proteasome subunit beta type-3

Chain I:  93% 6% 1%

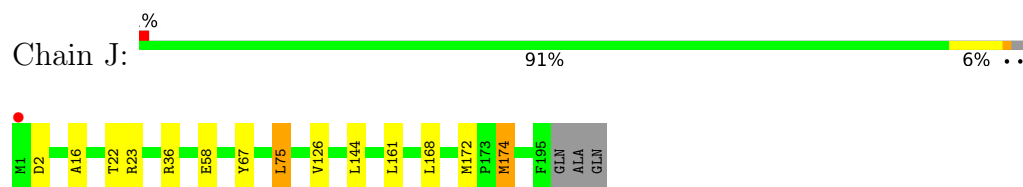


- Molecule 9: Proteasome subunit beta type-3

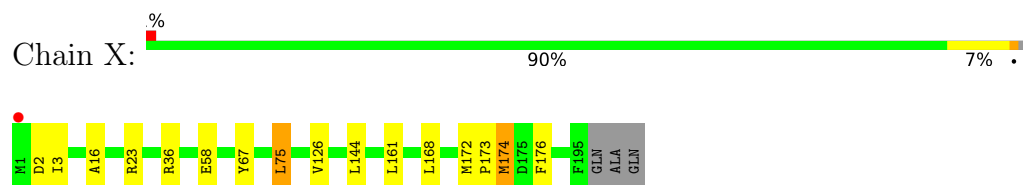
Chain W:  92% 7% 1%



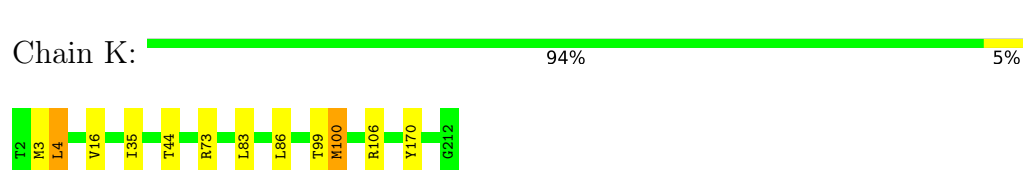
- Molecule 10: Proteasome subunit beta type-4



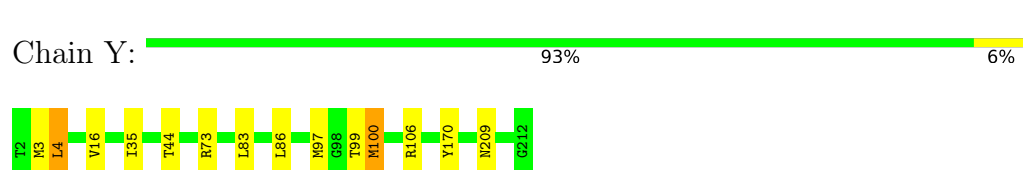
- Molecule 10: Proteasome subunit beta type-4



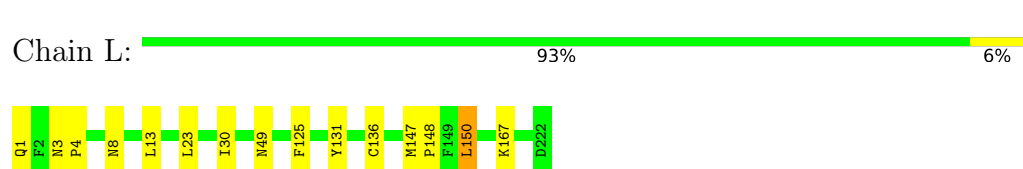
- Molecule 11: Proteasome subunit beta type-5



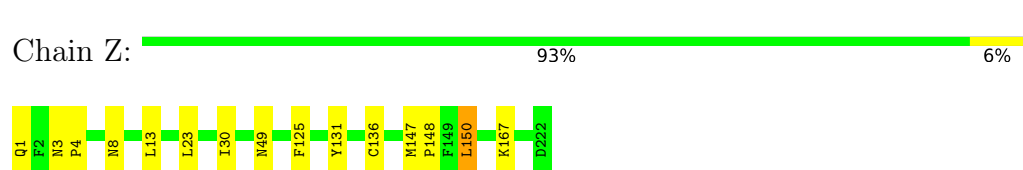
- Molecule 11: Proteasome subunit beta type-5



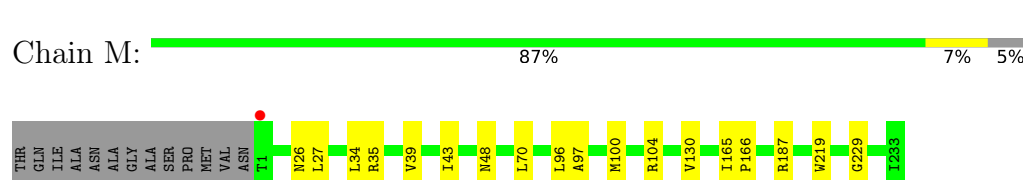
- Molecule 12: Proteasome subunit beta type-6



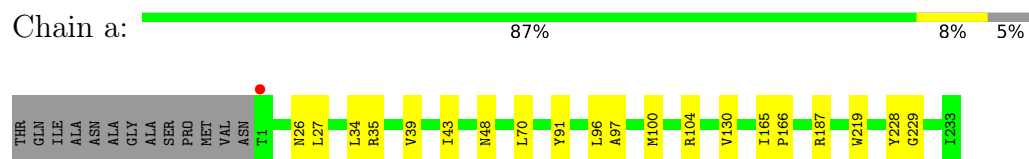
- Molecule 12: Proteasome subunit beta type-6



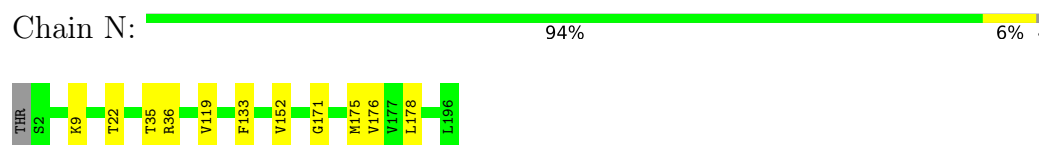
- Molecule 13: Proteasome subunit beta type-7



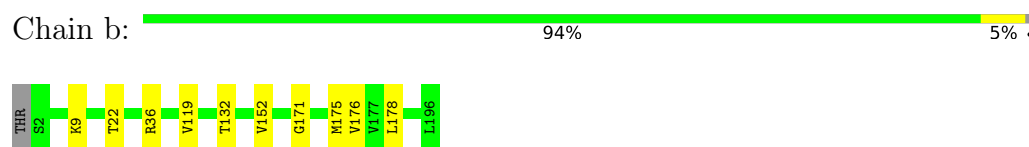
- Molecule 13: Proteasome subunit beta type-7



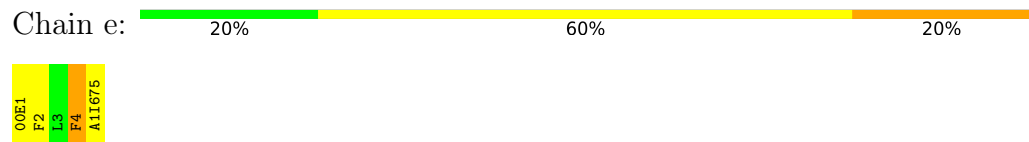
- Molecule 14: Proteasome subunit beta type-1



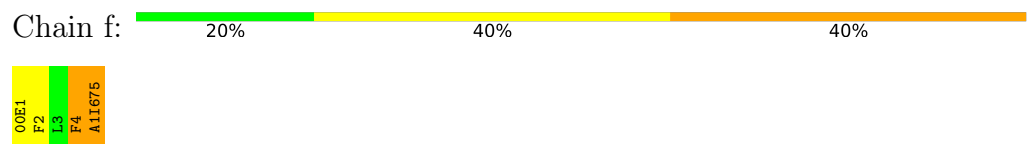
- Molecule 14: Proteasome subunit beta type-1



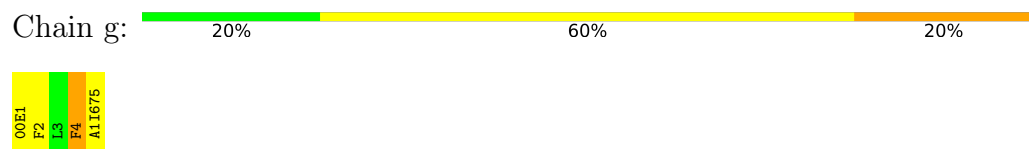
- Molecule 15: Carfilzomib



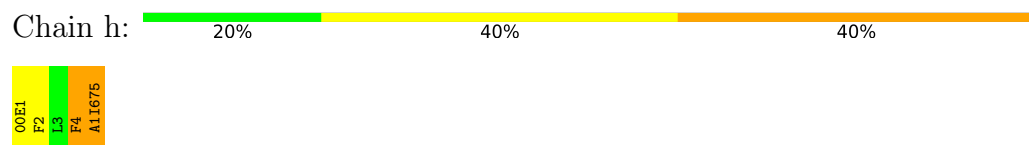
- Molecule 15: Carfilzomib



- Molecule 15: Carfilzomib

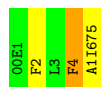


- Molecule 15: Carfilzomib



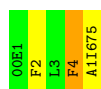
- Molecule 15: Carfilzomib

Chain i:  40% 40% 20%



● Molecule 15: Carfilzomib

Chain j:  40% 40% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.20Å 300.16Å 144.67Å 90.00° 112.84° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-2.70) 97.8 (15.00-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.173 , 0.207 0.172 , 0.211	Depositor DCC
R_{free} test set	14173 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	49952	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A1I67, MG, 00E, CL, MES, HPE

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	1.00	0/1952	1.39	0/2642
1	O	1.00	0/1952	1.39	0/2642
2	B	1.00	0/1934	1.40	0/2618
2	P	1.00	0/1934	1.40	0/2618
3	C	1.00	0/1910	1.43	0/2586
3	Q	1.01	0/1910	1.43	0/2586
4	D	1.00	0/1837	1.42	2/2475 (0.1%)
4	R	1.01	0/1837	1.42	2/2475 (0.1%)
5	E	1.01	0/1800	1.40	0/2433
5	S	1.01	0/1800	1.40	0/2433
6	F	0.99	0/1932	1.41	2/2609 (0.1%)
6	T	0.99	0/1932	1.41	2/2609 (0.1%)
7	G	0.98	0/1941	1.39	0/2629
7	U	0.99	0/1941	1.38	0/2629
8	H	0.99	0/1708	1.36	0/2316
8	V	0.99	0/1708	1.36	0/2316
9	I	0.96	0/1611	1.36	0/2174
9	W	0.96	0/1611	1.36	0/2174
10	J	0.97	0/1589	1.36	0/2142
10	X	0.97	0/1589	1.36	0/2142
11	K	0.97	0/1675	1.38	0/2264
11	Y	0.97	0/1675	1.38	0/2264
12	L	0.96	0/1795	1.33	0/2420
12	Z	0.96	0/1795	1.33	0/2420
13	M	0.97	0/1855	1.34	1/2514 (0.0%)
13	a	0.97	0/1855	1.34	1/2514 (0.0%)
14	N	0.97	0/1534	1.38	0/2077
14	b	0.98	0/1534	1.38	0/2077
15	e	1.18	0/19	1.34	1/24 (4.2%)
15	f	1.26	1/19 (5.3%)	2.01	1/24 (4.2%)
15	g	1.14	0/19	1.36	1/24 (4.2%)
15	h	1.20	0/19	1.92	1/24 (4.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	i	1.22	1/19 (5.3%)	1.29	1/24 (4.2%)
15	j	1.24	1/19 (5.3%)	1.39	1/24 (4.2%)
All	All	0.99	3/50260 (0.0%)	1.38	16/67942 (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
15	e	0	1
15	f	0	1
15	g	0	1
15	h	0	1
15	i	0	1
15	j	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	f	4	PHE	CB-CG	-5.19	1.38	1.50
15	j	4	PHE	CB-CG	-5.07	1.39	1.50
15	i	4	PHE	CB-CG	-5.04	1.39	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	f	4	PHE	CA-CB-CG	-8.71	105.09	113.80
15	h	4	PHE	CA-CB-CG	-8.39	105.41	113.80
13	M	35	ARG	N-CA-C	6.61	118.14	111.07
13	a	35	ARG	N-CA-C	6.44	117.97	111.07
15	j	4	PHE	CA-CB-CG	-5.82	107.98	113.80
15	g	4	PHE	CA-CB-CG	-5.69	108.11	113.80
15	e	4	PHE	CA-CB-CG	-5.55	108.25	113.80
15	i	4	PHE	CA-CB-CG	-5.35	108.45	113.80
6	F	77	LEU	CA-C-N	5.34	124.60	120.33
6	F	77	LEU	C-N-CA	5.34	124.60	120.33
6	T	77	LEU	CA-C-N	5.31	124.58	120.33
6	T	77	LEU	C-N-CA	5.31	124.58	120.33
4	R	2	ARG	CA-C-N	5.02	124.87	120.10
4	R	2	ARG	C-N-CA	5.02	124.87	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	ARG	CA-C-N	5.00	124.85	120.10
4	D	2	ARG	C-N-CA	5.00	124.85	120.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	e	4	PHE	Peptide
15	f	4	PHE	Peptide
15	g	4	PHE	Peptide
15	h	4	PHE	Peptide
15	i	4	PHE	Peptide
15	j	4	PHE	Peptide

5.2 Too-close contacts [i](#)

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	5	0
1	O	1915	0	1929	7	0
2	B	1904	0	1904	4	0
2	P	1904	0	1904	6	0
3	C	1881	0	1895	8	0
3	Q	1881	0	1895	9	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	5	0
5	S	1773	0	1775	4	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	3	0
7	G	1903	0	1898	4	0
7	U	1903	0	1898	5	0
8	H	1677	0	1678	2	0
8	V	1677	0	1678	3	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	X	1561	0	1569	8	0
11	K	1638	0	1587	9	0
11	Y	1638	0	1587	11	0
12	L	1757	0	1711	6	0
12	Z	1757	0	1711	6	0
13	M	1824	0	1832	6	0
13	a	1824	0	1832	8	0
14	N	1505	0	1471	5	0
14	b	1505	0	1471	4	0
15	e	59	0	40	0	0
15	f	59	0	40	1	0
15	g	59	0	40	0	0
15	h	59	0	40	1	0
15	i	59	0	40	0	0
15	j	59	0	40	0	0
16	G	1	0	0	0	0
16	I	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	H	12	0	13	0	0
18	K	12	0	13	0	0
18	V	12	0	13	0	0
18	h	12	0	13	0	0
19	A	13	0	0	0	0
19	B	16	0	0	0	0
19	C	10	0	0	0	0
19	D	4	0	0	0	0
19	E	7	0	0	0	0
19	F	11	0	0	0	0
19	G	9	0	0	0	0
19	H	9	0	0	0	0
19	I	13	0	0	0	0
19	J	8	0	0	0	0
19	K	11	0	0	0	0
19	L	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	M	13	0	0	0	0
19	N	8	0	0	0	0
19	O	6	0	0	0	0
19	P	7	0	0	0	0
19	Q	4	0	0	0	0
19	R	3	0	0	0	0
19	S	3	0	0	0	0
19	T	12	0	0	0	0
19	U	13	0	0	0	0
19	V	9	0	0	0	0
19	W	7	0	0	0	0
19	X	14	0	0	0	0
19	Y	14	0	0	0	0
19	Z	18	0	0	0	0
19	a	14	0	0	0	0
19	b	12	0	0	0	0
19	f	1	0	0	0	0
19	h	1	0	0	0	0
19	i	1	0	0	0	0
19	j	3	0	0	0	0
All	All	49952	0	49298	139	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (139) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.50	0.76
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.50	0.76
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.72	0.72
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.72	0.71
14:b:152:VAL:HA	14:b:175:MET:HE1	1.74	0.69
14:N:152:VAL:HA	14:N:175:MET:HE1	1.74	0.67
11:Y:83:LEU:CD2	11:Y:99:THR:HG21	2.34	0.57
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.39	0.57
7:U:23:PHE:O	7:U:26:THR:HB	2.05	0.57
7:G:23:PHE:O	7:G:26:THR:HB	2.05	0.56
11:K:83:LEU:CD2	11:K:99:THR:HG21	2.35	0.56
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.40	0.56
11:K:3:MET:HB2	11:K:16:VAL:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:170:TYR:O	15:h:5:A1I67:C58	2.54	0.55
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.88	0.55
11:Y:3:MET:HB2	11:Y:16:VAL:HG12	1.89	0.55
11:K:170:TYR:O	15:f:5:A1I67:C58	2.55	0.55
10:J:174:MET:HA	10:X:174:MET:HA	1.88	0.55
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.89	0.54
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.89	0.54
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.90	0.54
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.07	0.54
11:K:4:LEU:HD22	11:K:4:LEU:C	2.33	0.53
12:L:8:ASN:HA	12:L:30:ILE:O	2.09	0.53
6:T:123:ASN:C	6:T:123:ASN:HD22	2.17	0.53
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.90	0.53
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.34	0.53
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.91	0.53
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.38	0.53
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.90	0.52
1:O:119:GLN:O	1:O:122:THR:HB	2.10	0.52
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.39	0.51
6:F:123:ASN:C	6:F:123:ASN:HD22	2.19	0.50
3:C:38:ASN:C	3:C:38:ASN:HD22	2.20	0.50
11:Y:3:MET:HE3	11:Y:100:MET:HE2	1.93	0.50
1:A:119:GLN:O	1:A:122:THR:HB	2.11	0.49
7:G:78:ILE:N	7:G:79:PRO:CD	2.76	0.49
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.94	0.49
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.95	0.49
12:L:147:MET:N	12:L:148:PRO:HD2	2.27	0.49
7:U:78:ILE:N	7:U:79:PRO:CD	2.76	0.48
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.49	0.48
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.48	0.48
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.28	0.48
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.95	0.48
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.94	0.48
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.95	0.48
11:K:3:MET:HE3	11:K:100:MET:HE2	1.94	0.48
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.48	0.48
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.44	0.48
3:Q:38:ASN:HD22	3:Q:38:ASN:C	2.22	0.48
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.44	0.47
11:Y:83:LEU:HD21	11:Y:99:THR:HG21	1.95	0.47
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:6:ASP:OD2	3:Q:4:ARG:HG3	2.14	0.47
3:C:108:THR:HG21	3:C:146:TYR:HB3	1.97	0.47
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.97	0.46
14:N:133:PHE:HA	14:b:132:THR:O	2.15	0.46
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	1.97	0.46
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.50	0.46
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.96	0.46
9:I:7:ASN:HA	9:I:29:GLY:O	2.16	0.45
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.98	0.45
9:W:7:ASN:HA	9:W:29:GLY:O	2.16	0.45
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.99	0.45
5:S:98:PHE:O	13:a:91:TYR:HA	2.15	0.45
13:a:165:ILE:HB	13:a:166:PRO:HD3	1.99	0.45
6:T:123:ASN:HD22	6:T:124:SER:N	2.15	0.45
7:G:34:LEU:C	7:G:34:LEU:HD23	2.42	0.45
13:M:165:ILE:HB	13:M:166:PRO:HD3	1.99	0.45
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.99	0.45
6:F:123:ASN:HD22	6:F:124:SER:N	2.15	0.44
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.00	0.44
13:a:96:LEU:O	13:a:100:MET:HG2	2.16	0.44
10:J:168:LEU:O	10:J:172:MET:HB2	2.17	0.44
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.82	0.44
10:X:168:LEU:O	10:X:172:MET:HB2	2.17	0.44
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.00	0.44
13:M:96:LEU:O	13:M:100:MET:HG2	2.18	0.44
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.66	0.44
5:S:9:THR:HG21	5:S:119:THR:HA	2.00	0.44
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.32	0.44
5:S:77:ALA:N	5:S:78:PRO:CD	2.81	0.44
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.53	0.44
3:C:201:VAL:HG13	3:C:202:GLN:N	2.32	0.43
5:E:9:THR:HG21	5:E:119:THR:HA	2.00	0.43
2:P:50:LYS:O	2:P:51:VAL:C	2.61	0.43
3:C:201:VAL:O	3:C:202:GLN:CB	2.66	0.43
7:U:34:LEU:HD23	7:U:34:LEU:C	2.42	0.43
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.51	0.43
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.00	0.43
4:D:113:LEU:HD12	5:E:78:PRO:HB2	2.01	0.43
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.51	0.43
1:O:149:GLN:O	1:O:156:TYR:HA	2.19	0.43
5:E:77:ALA:N	5:E:78:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.54	0.43
8:H:52:THR:O	8:H:56:THR:HB	2.19	0.43
4:R:24:LYS:O	4:R:166:SER:HA	2.18	0.43
2:B:50:LYS:O	2:B:51:VAL:C	2.62	0.43
11:K:83:LEU:HD21	11:K:99:THR:HG21	2.00	0.43
4:D:24:LYS:O	4:D:166:SER:HA	2.19	0.42
1:A:149:GLN:O	1:A:156:TYR:HA	2.19	0.42
8:V:52:THR:O	8:V:56:THR:HB	2.19	0.42
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.67	0.42
11:Y:97:MET:HE2	11:Y:97:MET:HB3	1.85	0.42
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.45	0.42
11:K:86:LEU:C	11:K:86:LEU:HD13	2.45	0.42
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.84	0.42
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.55	0.42
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.52	0.42
5:E:65:CYS:SG	5:E:71:LEU:CD1	3.08	0.41
1:O:12:PHE:H	2:P:20:GLN:HE22	1.68	0.41
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.01	0.41
11:Y:44:THR:HG1	11:Y:100:MET:H	1.67	0.41
10:J:22:THR:HG21	10:X:173:PRO:HB3	2.02	0.41
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.01	0.41
7:G:26:THR:HG21	7:G:131:ILE:HD12	2.02	0.41
2:P:134:PHE:O	2:P:149:THR:HA	2.21	0.41
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.03	0.41
13:a:26:ASN:HA	13:a:39:VAL:O	2.20	0.41
9:I:14:MET:HB3	9:I:162:LEU:HD11	2.03	0.41
13:M:26:ASN:HA	13:M:39:VAL:O	2.20	0.41
11:K:4:LEU:C	11:K:4:LEU:CD2	2.94	0.41
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.56	0.41
1:O:55:LEU:HB3	7:U:159:ALA:O	2.20	0.41
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.01	0.41
8:V:210:THR:HG21	9:W:167:SER:HB3	2.03	0.41
1:A:64:VAL:HG11	1:A:212:ALA:HB3	2.03	0.41
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.85	0.41
14:N:35:THR:HG21	13:a:228:TYR:HE2	1.85	0.41
11:Y:100:MET:HE3	11:Y:100:MET:HB2	1.85	0.41
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.24	0.40
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.56	0.40
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.86	0.40
2:B:6:ASP:OD2	3:C:4:ARG:HG3	2.21	0.40
11:K:44:THR:HG1	11:K:100:MET:H	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ALA:HB1	1:A:154:GLY:O	2.21	0.40
1:O:115:ALA:HB1	1:O:154:GLY:O	2.20	0.40
9:W:14:MET:HB3	9:W:162:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	240 (97%)	8 (3%)	0	100	100
1	O	248/250 (99%)	240 (97%)	8 (3%)	0	100	100
2	B	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	30	54
2	P	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	30	54
3	C	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	9	25
3	Q	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	9	25
4	D	231/260 (89%)	223 (96%)	8 (4%)	0	100	100
4	R	231/260 (89%)	223 (96%)	8 (4%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
6	T	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
7	G	238/252 (94%)	233 (98%)	5 (2%)	0	100	100
7	U	238/252 (94%)	233 (98%)	5 (2%)	0	100	100
8	H	219/231 (95%)	213 (97%)	6 (3%)	0	100	100
8	V	219/231 (95%)	213 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	24	48
10	X	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	24	48
11	K	209/211 (99%)	204 (98%)	5 (2%)	0	100	100
11	Y	209/211 (99%)	204 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	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%)	9 (4%)	1 (0%)	30	54
13	a	231/246 (94%)	222 (96%)	8 (4%)	1 (0%)	30	54
14	N	193/196 (98%)	186 (96%)	7 (4%)	0	100	100
14	b	193/196 (98%)	186 (96%)	7 (4%)	0	100	100
15	e	2/5 (40%)	2 (100%)	0	0	100	100
15	f	2/5 (40%)	2 (100%)	0	0	100	100
15	g	2/5 (40%)	2 (100%)	0	0	100	100
15	h	2/5 (40%)	2 (100%)	0	0	100	100
15	i	2/5 (40%)	2 (100%)	0	0	100	100
15	j	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6280/6640 (95%)	6093 (97%)	175 (3%)	12 (0%)	43	68

All (12) 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
3	C	205	ALA
3	Q	205	ALA
3	C	239	GLN
3	Q	239	GLN
10	J	2	ASP
10	X	2	ASP
13	M	229	GLY
13	a	229	GLY

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%)	204 (98%)	5 (2%)	43	72
1	O	209/209 (100%)	204 (98%)	5 (2%)	43	72
2	B	203/216 (94%)	195 (96%)	8 (4%)	28	57
2	P	203/216 (94%)	195 (96%)	8 (4%)	28	57
3	C	212/226 (94%)	205 (97%)	7 (3%)	33	63
3	Q	212/226 (94%)	205 (97%)	7 (3%)	33	63
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%)	193 (96%)	8 (4%)	28	56
6	T	201/239 (84%)	193 (96%)	8 (4%)	28	56
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	62
7	U	206/210 (98%)	199 (97%)	7 (3%)	32	62
8	H	180/189 (95%)	177 (98%)	3 (2%)	53	79
8	V	180/189 (95%)	177 (98%)	3 (2%)	53	79
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%)	169 (98%)	4 (2%)	44	73
10	X	173/175 (99%)	169 (98%)	4 (2%)	44	73
11	K	168/168 (100%)	163 (97%)	5 (3%)	36	66
11	Y	168/168 (100%)	163 (97%)	5 (3%)	36	66
12	L	185/185 (100%)	179 (97%)	6 (3%)	34	64
12	Z	185/185 (100%)	179 (97%)	6 (3%)	34	64
13	M	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	161/162 (99%)	157 (98%)	4 (2%)	42	71
14	b	161/162 (99%)	157 (98%)	4 (2%)	42	71
15	e	2/2 (100%)	2 (100%)	0	100	100
15	f	2/2 (100%)	2 (100%)	0	100	100
15	g	2/2 (100%)	2 (100%)	0	100	100
15	h	2/2 (100%)	2 (100%)	0	100	100
15	i	2/2 (100%)	2 (100%)	0	100	100
15	j	2/2 (100%)	2 (100%)	0	100	100
All	All	5318/5548 (96%)	5154 (97%)	164 (3%)	35	65

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	29	LYS
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
2	B	50	LYS
2	B	52	THR
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	114	LEU
2	B	184	LYS
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	203	THR
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU

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Mol	Chain	Res	Type
4	D	193	LEU
4	D	197	LYS
4	D	214	ILE
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	188	LEU
6	F	14	ASP
6	F	68	ARG
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	221	ASN
7	G	83	ASN
7	G	115	LEU
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	56	THR
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	23	ARG
10	J	75	LEU
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	35	ILE
11	K	73	ARG
11	K	100	MET
11	K	106	ARG
12	L	1	GLN

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Mol	Chain	Res	Type
12	L	23	LEU
12	L	49	ASN
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	187	ARG
14	N	9	LYS
14	N	22	THR
14	N	36	ARG
14	N	119	VAL
1	O	17	LYS
1	O	29	LYS
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
2	P	50	LYS
2	P	52	THR
2	P	55	LEU
2	P	58	GLN
2	P	79	LEU
2	P	114	LEU
2	P	184	LYS
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	203	THR
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	197	LYS

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Mol	Chain	Res	Type
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	188	LEU
6	T	14	ASP
6	T	68	ARG
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	221	ASN
7	U	83	ASN
7	U	115	LEU
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	56	THR
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	23	ARG
10	X	75	LEU
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	35	ILE
11	Y	73	ARG
11	Y	100	MET
11	Y	106	ARG
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN

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Mol	Chain	Res	Type
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	187	ARG
14	b	9	LYS
14	b	22	THR
14	b	36	ARG
14	b	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (143) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	155	ASN
2	B	176	GLN
2	B	232	GLN
3	C	38	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	233	GLN
4	D	15	GLN
4	D	91	HIS
4	D	106	GLN
4	D	160	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

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Mol	Chain	Res	Type
5	E	120	GLN
5	E	147	GLN
5	E	151	ASN
5	E	184	ASN
6	F	86	ASN
6	F	123	ASN
6	F	178	HIS
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	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	88	GLN
10	J	37	GLN
10	J	55	GLN
10	J	63	ASN
10	J	146	HIS
10	J	147	HIS
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	143	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	153	GLN
12	L	158	ASN
13	M	26	ASN
13	M	48	ASN
13	M	62	HIS
13	M	102	GLN

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Mol	Chain	Res	Type
14	N	38	HIS
14	N	141	ASN
14	N	161	GLN
1	O	30	GLN
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	176	GLN
2	P	232	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	233	GLN
4	R	15	GLN
4	R	91	HIS
4	R	106	GLN
4	R	160	ASN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	147	GLN
5	S	151	ASN
5	S	184	ASN
6	T	86	ASN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	175	ASN

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Mol	Chain	Res	Type
8	V	30	ASN
8	V	86	HIS
8	V	172	ASN
8	V	189	ASN
8	V	200	GLN
9	W	44	HIS
9	W	63	ASN
9	W	88	GLN
10	X	37	GLN
10	X	55	GLN
10	X	63	ASN
10	X	146	HIS
11	Y	9	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	153	GLN
12	Z	158	ASN
12	Z	165	ASN
13	a	48	ASN
13	a	62	HIS
13	a	102	GLN
13	a	108	ASN
13	a	149	HIS
14	b	38	HIS
14	b	141	ASN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
15	00E	f	1	15	9,9,10	0.85	0	10,10,12	2.69	3 (30%)
15	A1I67	i	5	15,14	13,19,20	1.10	1 (7%)	11,29,31	1.08	1 (9%)
15	A1I67	j	5	15,14	13,19,20	1.13	1 (7%)	11,29,31	1.03	1 (9%)
15	A1I67	f	5	15,11	13,19,20	1.05	1 (7%)	11,29,31	1.09	1 (9%)
15	A1I67	e	5	15,8	13,19,20	1.17	1 (7%)	11,29,31	1.04	0
15	A1I67	g	5	15,8	13,19,20	1.16	1 (7%)	11,29,31	1.16	1 (9%)
15	00E	j	1	15	9,9,10	0.64	0	10,10,12	1.06	0
15	00E	h	1	15	9,9,10	0.86	0	10,10,12	2.62	2 (20%)
15	A1I67	h	5	15,11	13,19,20	1.13	1 (7%)	11,29,31	1.05	1 (9%)
15	00E	i	1	15	9,9,10	0.67	0	10,10,12	1.03	0
15	HPE	e	2	15	11,12,13	1.30	1 (9%)	9,14,16	0.43	0
15	00E	e	1	15	9,9,10	0.76	0	10,10,12	1.10	1 (10%)
15	00E	g	1	15	9,9,10	0.79	0	10,10,12	1.12	1 (10%)
15	HPE	h	2	15	11,12,13	1.51	1 (9%)	9,14,16	0.91	0
15	HPE	i	2	15	11,12,13	1.36	1 (9%)	9,14,16	0.69	0
15	HPE	j	2	15	11,12,13	1.38	1 (9%)	9,14,16	0.69	0
15	HPE	f	2	15	11,12,13	1.48	1 (9%)	9,14,16	0.87	0
15	HPE	g	2	15	11,12,13	1.29	1 (9%)	9,14,16	0.40	0

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
15	00E	f	1	15	-	2/2/11/12	0/1/1/1
15	A1I67	i	5	15,14	-	3/4/36/38	0/0/1/1
15	A1I67	j	5	15,14	-	3/4/36/38	0/0/1/1
15	A1I67	f	5	15,11	-	3/4/36/38	0/0/1/1
15	A1I67	e	5	15,8	-	4/4/36/38	0/0/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	A1I67	g	5	15,8	-	4/4/36/38	0/0/1/1
15	00E	j	1	15	-	2/2/11/12	0/1/1/1
15	00E	h	1	15	-	2/2/11/12	0/1/1/1
15	A1I67	h	5	15,11	-	3/4/36/38	0/0/1/1
15	00E	i	1	15	-	2/2/11/12	0/1/1/1
15	HPE	e	2	15	-	3/6/7/9	0/1/1/1
15	00E	e	1	15	-	2/2/11/12	0/1/1/1
15	00E	g	1	15	-	2/2/11/12	0/1/1/1
15	HPE	h	2	15	-	2/6/7/9	0/1/1/1
15	HPE	i	2	15	-	0/6/7/9	0/1/1/1
15	HPE	j	2	15	-	0/6/7/9	0/1/1/1
15	HPE	f	2	15	-	2/6/7/9	0/1/1/1
15	HPE	g	2	15	-	3/6/7/9	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	h	2	HPE	CG-CD	-4.68	1.38	1.51
15	f	2	HPE	CG-CD	-4.58	1.38	1.51
15	j	2	HPE	CG-CD	-4.11	1.40	1.51
15	i	2	HPE	CG-CD	-4.03	1.40	1.51
15	e	2	HPE	CG-CD	-3.86	1.40	1.51
15	g	2	HPE	CG-CD	-3.80	1.41	1.51
15	j	5	A1I67	O48-C47	3.14	1.44	1.39
15	i	5	A1I67	O48-C47	3.09	1.44	1.39
15	h	5	A1I67	O48-C47	3.07	1.44	1.39
15	e	5	A1I67	O48-C47	2.91	1.44	1.39
15	g	5	A1I67	O48-C47	2.77	1.44	1.39
15	f	5	A1I67	O48-C47	2.74	1.44	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	f	1	00E	CA-NB-CD2	7.17	117.96	110.49
15	h	1	00E	CA-NB-CD2	7.02	117.81	110.49
15	f	1	00E	CE2-CD2-NB	-3.17	105.31	110.12
15	h	1	00E	CE2-CD2-NB	-2.99	105.58	110.12
15	i	5	A1I67	C59-C51-C47	2.68	115.33	110.91
15	j	5	A1I67	C59-C51-C47	2.50	115.04	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	f	5	A1I67	C59-C51-C47	2.44	114.93	110.91
15	h	5	A1I67	C59-C51-C47	2.33	114.76	110.91
15	g	1	00E	CD2-NB-CD1	2.13	113.43	108.84
15	e	1	00E	CD2-NB-CD1	2.09	113.34	108.84
15	f	1	00E	CA-NB-CD1	-2.07	108.33	110.49
15	g	5	A1I67	C59-C51-C47	2.00	114.22	110.91

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	e	1	00E	C-CA-NB-CD2
15	f	1	00E	C-CA-NB-CD1
15	f	1	00E	C-CA-NB-CD2
15	g	1	00E	C-CA-NB-CD1
15	h	1	00E	C-CA-NB-CD1
15	h	1	00E	C-CA-NB-CD2
15	e	2	HPE	C-CA-CB-CG
15	f	2	HPE	N-CA-CB-CG
15	f	2	HPE	C-CA-CB-CG
15	g	2	HPE	C-CA-CB-CG
15	h	2	HPE	N-CA-CB-CG
15	h	2	HPE	C-CA-CB-CG
15	e	5	A1I67	N-C42-C43-C44
15	f	5	A1I67	N-C42-C43-C44
15	g	5	A1I67	N-C42-C43-C44
15	h	5	A1I67	N-C42-C43-C44
15	i	5	A1I67	N-C42-C43-C44
15	j	5	A1I67	N-C42-C43-C44
15	e	5	A1I67	C42-C43-C44-C46
15	g	5	A1I67	C42-C43-C44-C46
15	e	5	A1I67	C42-C43-C44-C45
15	g	5	A1I67	C42-C43-C44-C45
15	i	5	A1I67	C42-C43-C44-C46
15	j	5	A1I67	C42-C43-C44-C46
15	f	5	A1I67	C42-C43-C44-C46
15	h	5	A1I67	C42-C43-C44-C46
15	e	5	A1I67	C47-C42-C43-C44
15	g	5	A1I67	C47-C42-C43-C44
15	i	5	A1I67	C47-C42-C43-C44
15	j	5	A1I67	C47-C42-C43-C44
15	e	1	00E	C-CA-NB-CD1

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Mol	Chain	Res	Type	Atoms
15	f	5	A1I67	C47-C42-C43-C44
15	h	5	A1I67	C47-C42-C43-C44
15	e	2	HPE	CE1-CD-CG-CB
15	g	2	HPE	CE1-CD-CG-CB
15	e	2	HPE	CE2-CD-CG-CB
15	g	2	HPE	CE2-CD-CG-CB
15	g	1	00E	C-CA-NB-CD2
15	i	1	00E	C-CA-NB-CD1
15	i	1	00E	C-CA-NB-CD2
15	j	1	00E	C-CA-NB-CD1
15	j	1	00E	C-CA-NB-CD2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	f	5	A1I67	1	0
15	h	5	A1I67	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 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	$\# Z > 2$
18	MES	h	101	-	12,12,12	0.68	0	15,16,16	0.30	0
18	MES	K	302	-	12,12,12	0.72	0	15,16,16	0.34	0
18	MES	H	301	-	12,12,12	0.72	0	15,16,16	0.28	0
18	MES	V	302	-	12,12,12	0.70	0	15,16,16	0.31	0

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
18	MES	h	101	-	-	0/6/14/14	0/1/1/1
18	MES	K	302	-	-	0/6/14/14	0/1/1/1
18	MES	H	301	-	-	5/6/14/14	0/1/1/1
18	MES	V	302	-	-	2/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	H	301	MES	C7-C8-S-O1S
18	H	301	MES	C7-C8-S-O2S
18	H	301	MES	C7-C8-S-O3S
18	H	301	MES	C8-C7-N4-C3
18	H	301	MES	C8-C7-N4-C5
18	V	302	MES	C8-C7-N4-C5
18	V	302	MES	C8-C7-N4-C3

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%)	-0.63	1 (0%) 88 87	49, 64, 97, 161	0
1	O	250/250 (100%)	-0.62	1 (0%) 88 87	53, 71, 109, 158	0
2	B	244/258 (94%)	-0.52	3 (1%) 76 75	52, 70, 114, 171	0
2	P	244/258 (94%)	-0.50	2 (0%) 82 81	55, 73, 118, 162	0
3	C	240/254 (94%)	-0.49	0 100 100	49, 74, 135, 147	0
3	Q	240/254 (94%)	-0.47	2 (0%) 82 81	56, 86, 153, 165	0
4	D	235/260 (90%)	-0.58	0 100 100	54, 76, 103, 143	0
4	R	235/260 (90%)	-0.54	0 100 100	55, 77, 110, 148	0
5	E	231/234 (98%)	-0.59	0 100 100	57, 78, 110, 135	0
5	S	231/234 (98%)	-0.50	0 100 100	56, 81, 118, 137	0
6	F	243/288 (84%)	-0.56	0 100 100	51, 72, 112, 145	0
6	T	243/288 (84%)	-0.57	0 100 100	51, 76, 122, 142	0
7	G	240/252 (95%)	-0.64	0 100 100	48, 65, 98, 143	0
7	U	240/252 (95%)	-0.65	0 100 100	51, 66, 98, 125	0
8	H	221/231 (95%)	-0.69	0 100 100	49, 60, 87, 121	0
8	V	221/231 (95%)	-0.67	0 100 100	50, 63, 90, 121	0
9	I	204/205 (99%)	-0.81	0 100 100	46, 59, 86, 112	0
9	W	204/205 (99%)	-0.79	0 100 100	45, 63, 85, 108	0
10	J	195/198 (98%)	-0.73	1 (0%) 87 86	46, 62, 87, 127	0
10	X	195/198 (98%)	-0.75	1 (0%) 87 86	50, 64, 89, 133	0
11	K	211/211 (100%)	-0.72	0 100 100	49, 63, 86, 117	0
11	Y	211/211 (100%)	-0.67	0 100 100	52, 63, 88, 115	0
12	L	222/222 (100%)	-0.75	0 100 100	46, 65, 88, 104	0
12	Z	222/222 (100%)	-0.73	0 100 100	47, 62, 89, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.74	1 (0%) 88 87	46, 61, 82, 94	0
13	a	233/246 (94%)	-0.75	1 (0%) 88 87	44, 60, 79, 89	0
14	N	195/196 (99%)	-0.77	0 100 100	46, 56, 82, 107	0
14	b	195/196 (99%)	-0.74	0 100 100	44, 58, 84, 109	0
15	e	2/5 (40%)	-0.88	0 100 100	59, 59, 59, 61	0
15	f	2/5 (40%)	-0.89	0 100 100	59, 59, 59, 61	0
15	g	2/5 (40%)	-0.40	0 100 100	61, 61, 61, 66	0
15	h	2/5 (40%)	-1.09	0 100 100	57, 57, 57, 60	0
15	i	2/5 (40%)	-0.53	0 100 100	57, 57, 57, 60	0
15	j	2/5 (40%)	-0.86	0 100 100	59, 59, 59, 62	0
All	All	6340/6640 (95%)	-0.64	13 (0%) 91 90	44, 67, 108, 171	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	205	ALA	3.7
10	X	1	MET	3.5
3	Q	50	LEU	3.3
1	A	1	MET	3.3
2	B	51	VAL	3.0
2	B	219	ALA	2.9
10	J	1	MET	2.8
1	O	1	MET	2.7
13	a	1	THR	2.5
2	B	218	GLY	2.5
2	P	51	VAL	2.4
13	M	1	THR	2.3
2	P	219	ALA	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	00E	i	1	9/10	0.73	0.13	98,128,133,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	00E	j	1	9/10	0.74	0.13	109,137,142,143	0
15	00E	e	1	9/10	0.86	0.13	83,113,121,121	0
15	00E	g	1	9/10	0.89	0.14	69,108,118,122	0
15	00E	h	1	9/10	0.91	0.10	79,99,105,106	0
15	HPE	i	2	12/13	0.91	0.12	73,100,118,119	0
15	HPE	j	2	12/13	0.92	0.13	76,96,114,115	0
15	HPE	g	2	12/13	0.94	0.08	66,69,74,75	0
15	HPE	h	2	12/13	0.94	0.09	69,70,72,72	0
15	00E	f	1	9/10	0.95	0.08	74,102,109,110	0
15	A1I67	e	5	19/20	0.96	0.09	57,64,73,74	0
15	HPE	f	2	12/13	0.97	0.07	61,76,80,80	0
15	HPE	e	2	12/13	0.97	0.06	61,73,76,76	0
15	A1I67	g	5	19/20	0.97	0.08	56,64,72,75	0
15	A1I67	h	5	19/20	0.97	0.08	51,55,59,59	0
15	A1I67	i	5	19/20	0.97	0.07	49,50,58,63	0
15	A1I67	f	5	19/20	0.98	0.06	52,55,58,59	0
15	A1I67	j	5	19/20	0.98	0.06	50,52,59,65	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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($\text{\AA}^2$)	Q<0.9
18	MES	V	302	12/12	0.87	0.14	102,122,126,129	0
18	MES	H	301	12/12	0.92	0.11	92,111,114,115	0
16	MG	I	301	1/1	0.94	0.18	91,91,91,91	0
16	MG	Y	301	1/1	0.95	0.06	82,82,82,82	0
16	MG	Z	301	1/1	0.95	0.07	79,79,79,79	0
18	MES	h	101	12/12	0.95	0.10	71,77,81,81	0
18	MES	K	302	12/12	0.96	0.09	76,80,84,87	0
17	CL	b	201	1/1	0.96	0.06	80,80,80,80	0
16	MG	V	301	1/1	0.96	0.09	93,93,93,93	0
17	CL	U	301	1/1	0.99	0.03	58,58,58,58	0
16	MG	G	301	1/1	0.99	0.04	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	MG	K	301	1/1	0.99	0.04	71,71,71,71	0
16	MG	N	201	1/1	0.99	0.04	60,60,60,60	0
17	CL	G	302	1/1	0.99	0.04	55,55,55,55	0
17	CL	N	202	1/1	0.99	0.02	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.