



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:10 AM UTC

PDB ID : 4QBY / pdb_00004qby
Title : yCP in complex with BOC-ALA-ALA-ALA-CHO
Authors : Arciniega, M.; Beck, P.; Lange, O.; Groll, M.; Huber, R.
Deposited on : 2014-05-09
Resolution : 3.00 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

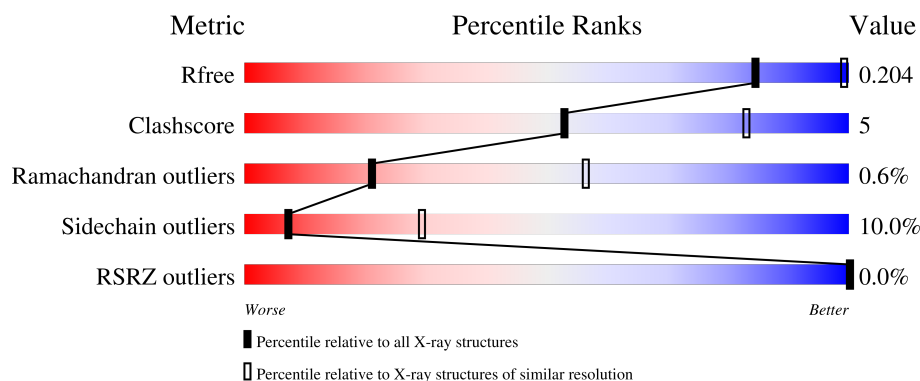
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	 89% 10% .
1	O	250	 87% 11% .
2	B	258	 72% 21% . 5%
2	P	258	 72% 21% . 5%
3	C	254	 77% 13% . 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	 78%12% • 6%
4	D	260	 71%17% • 10%
4	R	260	 71%17% • 10%
5	E	234	 73%21% • •
5	S	234	 73%23% • •
6	F	288	 72%11% • 16%
6	T	288	 71%13% • 16%
7	G	252	 79%14% • •
7	U	252	 77%16% • •
8	H	232	 77%18% • •
8	V	232	 78%17% • •
9	I	205	 78%20% •
9	W	205	 78%20% •
10	J	198	 %81%15% • •
10	X	198	 %81%15% • •
11	K	212	 83%17%
11	Y	212	 86%13% •
12	L	222	 82%17% •
12	Z	222	 82%16% •
13	M	246	 84%9% • 5%
13	a	246	 83%10% • 5%
14	N	196	 84%15% •
14	b	196	 83%15% •
15	1	4	 75%25%
15	2	4	 75%25%

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Mol	Chain	Length	Quality of chain	
15	3	4		25%
15	4	4		25%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49645 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

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

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

- Molecule 15 is a protein called BOC-ALA-ALA-ALA-CHO.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	1	4	Total	C	N	O	0	0	0
			22	14	3	5			
15	2	4	Total	C	N	O	0	0	0
			22	14	3	5			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	3	4	Total	C	N	O	0	0	0
			22	14	3	5			
15	4	4	Total	C	N	O	0	0	0
			22	14	3	5			

- 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	H	1	Total	Mg	0	0
			1	1		
16	I	2	Total	Mg	0	0
			2	2		
16	J	1	Total	Mg	0	0
			1	1		
16	K	2	Total	Mg	0	0
			2	2		
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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	7	Total	O	0	0
			7	7		
17	B	6	Total	O	0	0
			6	6		
17	C	5	Total	O	0	0
			5	5		
17	D	5	Total	O	0	0
			5	5		
17	E	5	Total	O	0	0
			5	5		
17	F	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	G	10	Total O 10 10	0	0
17	H	8	Total O 8 8	0	0
17	I	4	Total O 4 4	0	0
17	J	8	Total O 8 8	0	0
17	K	3	Total O 3 3	0	0
17	L	7	Total O 7 7	0	0
17	M	10	Total O 10 10	0	0
17	N	6	Total O 6 6	0	0
17	O	5	Total O 5 5	0	0
17	P	8	Total O 8 8	0	0
17	Q	6	Total O 6 6	0	0
17	R	3	Total O 3 3	0	0
17	S	1	Total O 1 1	0	0
17	T	7	Total O 7 7	0	0
17	U	5	Total O 5 5	0	0
17	V	11	Total O 11 11	0	0
17	W	3	Total O 3 3	0	0
17	X	7	Total O 7 7	0	0
17	Y	5	Total O 5 5	0	0
17	Z	4	Total O 4 4	0	0
17	2	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	a	16	Total 16	O 16	0	0
17	3	2	Total 2	O 2	0	0
17	b	5	Total 5	O 5	0	0
17	4	1	Total 1	O 1	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.

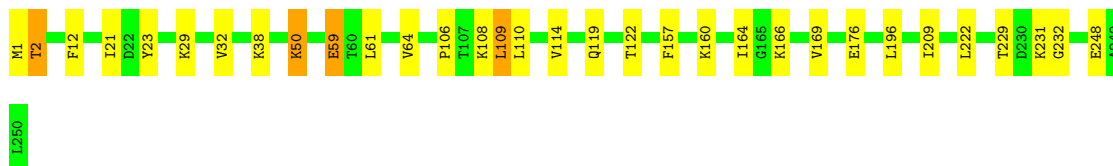
- Molecule 1: Proteasome subunit alpha type-2

Chain A: 



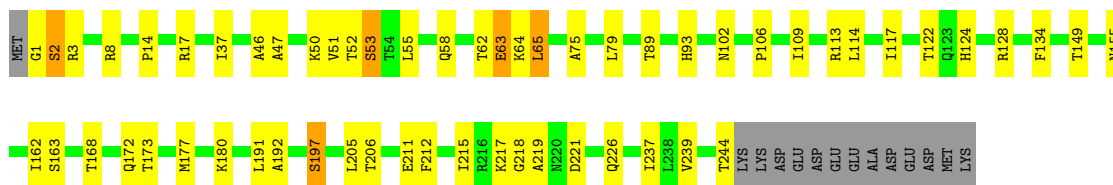
- Molecule 1: Proteasome subunit alpha type-2

Chain O: 



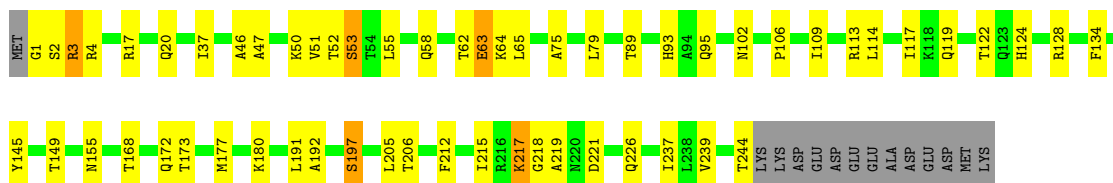
- Molecule 2: Proteasome subunit alpha type-3

Chain B: 



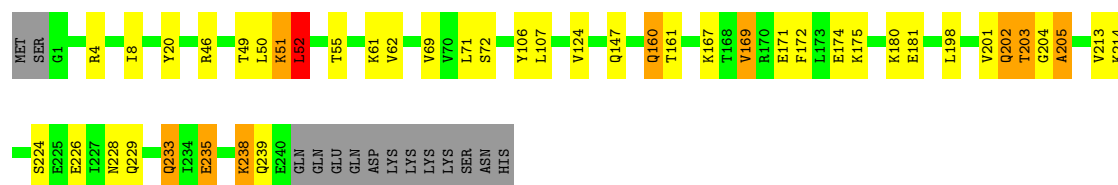
- Molecule 2: Proteasome subunit alpha type-3

Chain P: 



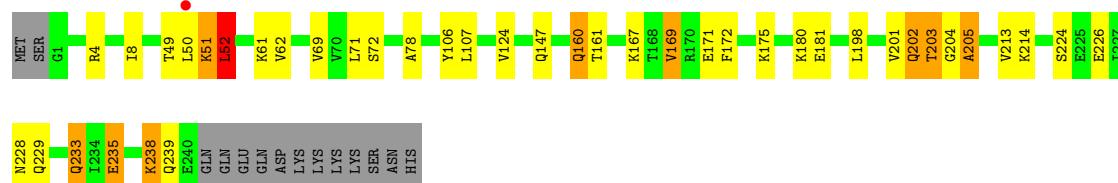
- Molecule 3: Proteasome subunit alpha type-4

Chain C:  77% 13% 6%



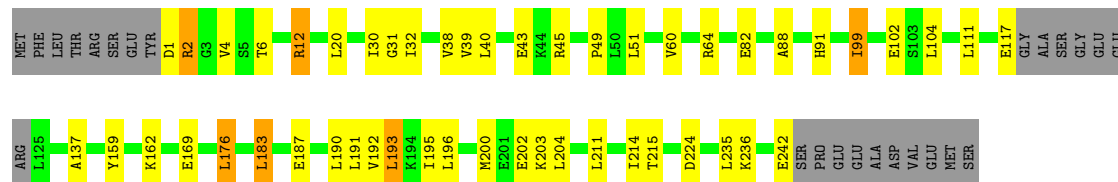
- Molecule 3: Proteasome subunit alpha type-4

Chain Q:  78% 12% 6%



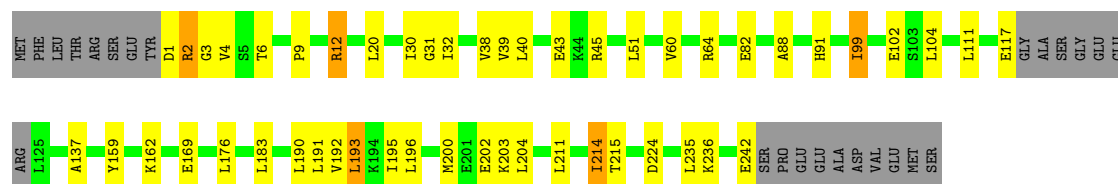
- Molecule 4: Proteasome subunit alpha type-5

Chain D:  71% 17% 10%



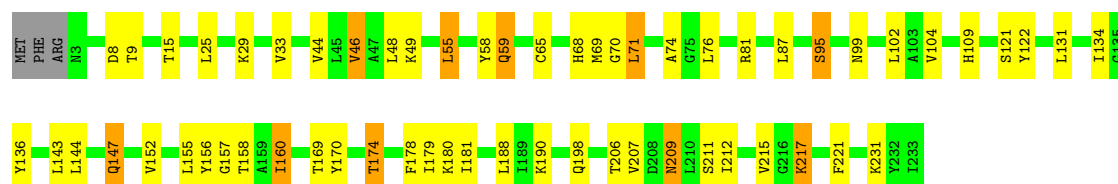
- Molecule 4: Proteasome subunit alpha type-5

Chain R:  71% 17% 10%

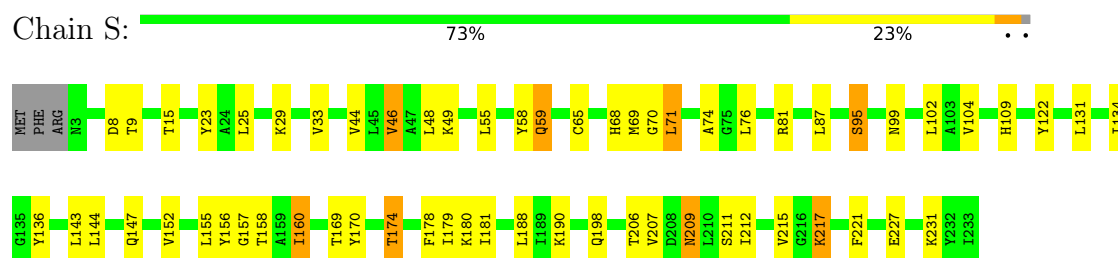


- Molecule 5: Proteasome subunit alpha type-6

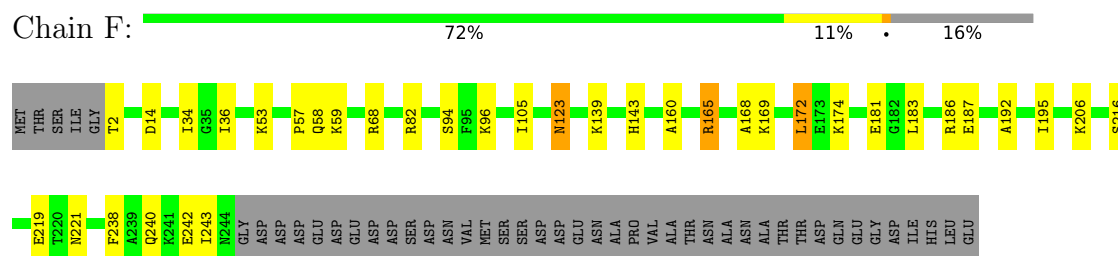
Chain E:  73% 21% 6%



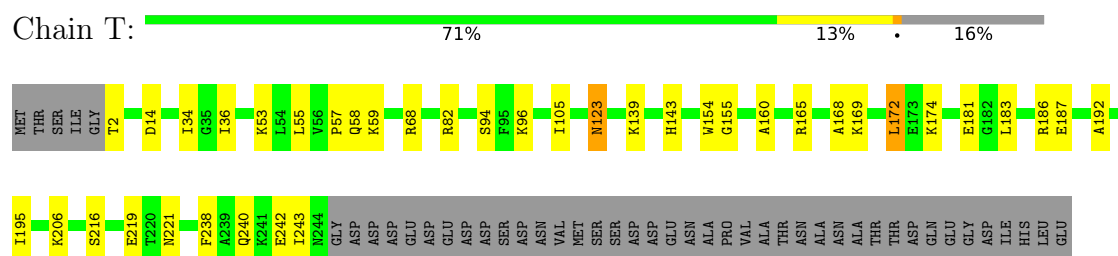
- Molecule 5: Proteasome subunit alpha type-6



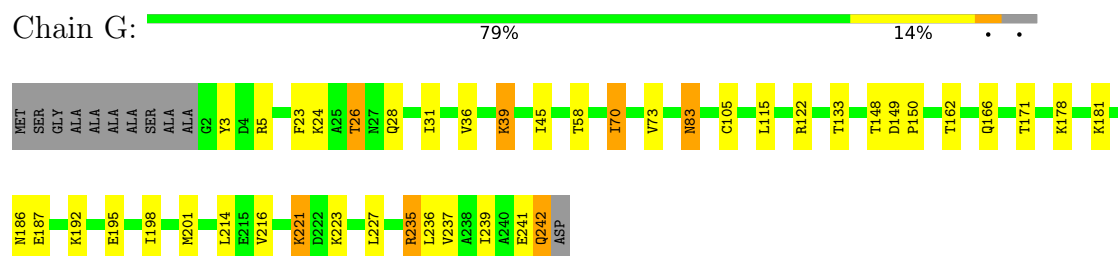
- Molecule 6: Probable proteasome subunit alpha type-7



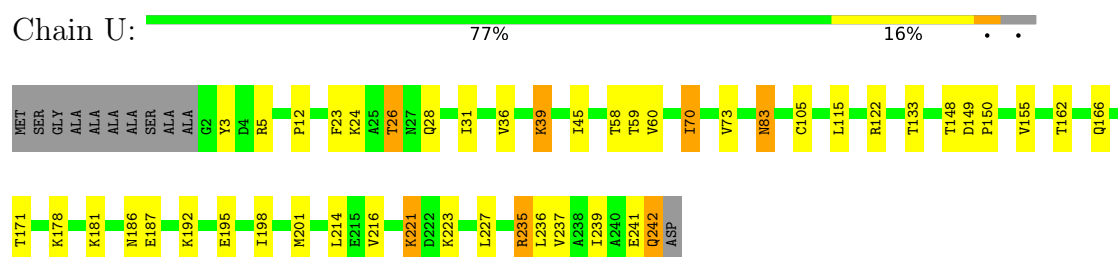
- Molecule 6: Probable proteasome subunit alpha type-7



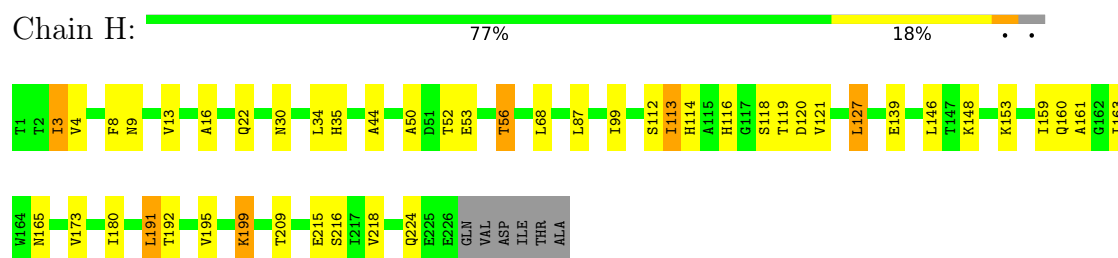
- Molecule 7: Proteasome subunit alpha type-1



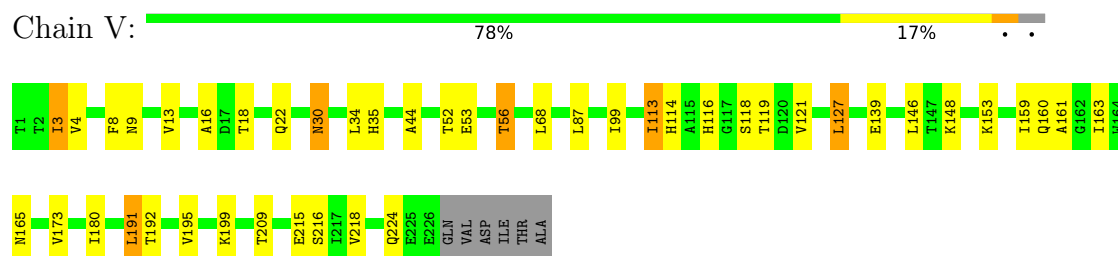
- Molecule 7: Proteasome subunit alpha type-1



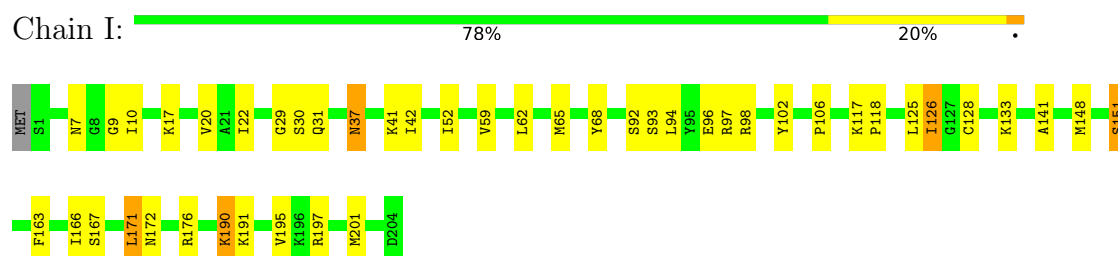
- Molecule 8: Proteasome subunit beta type-2



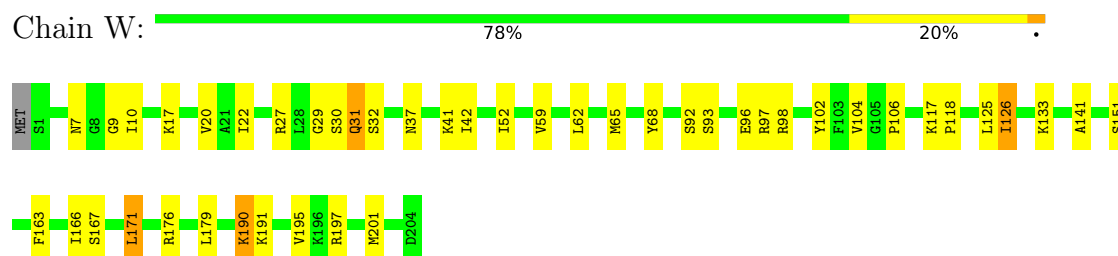
- Molecule 8: Proteasome subunit beta type-2



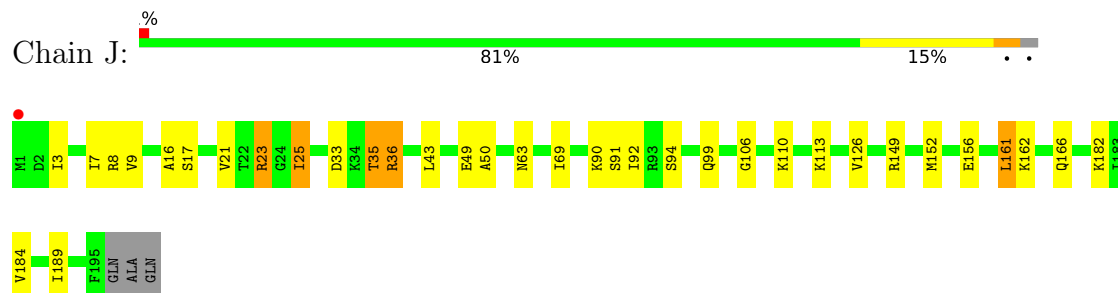
- Molecule 9: Proteasome subunit beta type-3



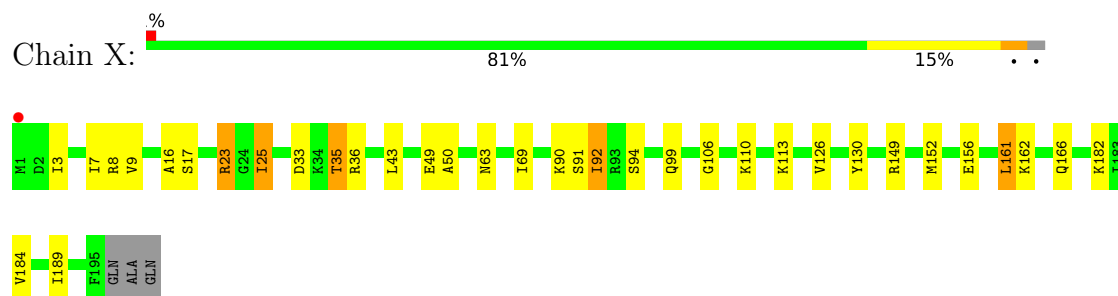
- Molecule 9: Proteasome subunit beta type-3



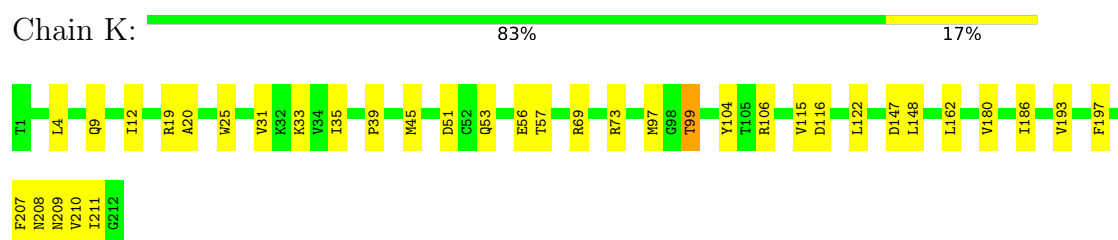
- Molecule 10: Proteasome subunit beta type-4



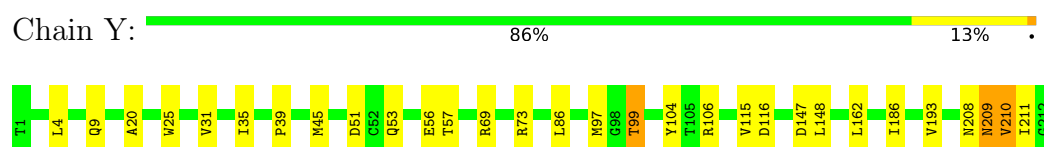
- Molecule 10: Proteasome subunit beta type-4



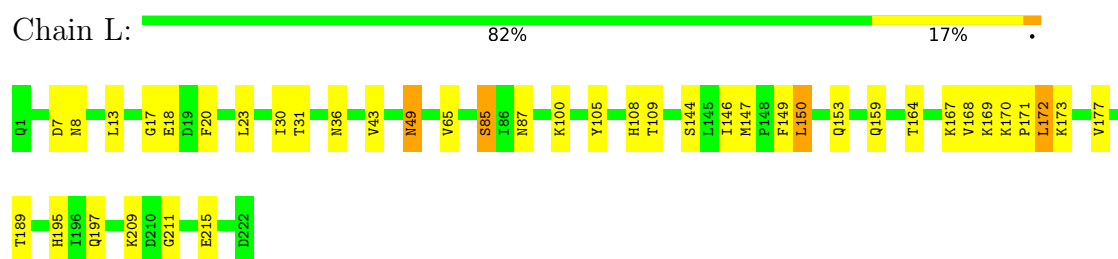
- Molecule 11: Proteasome subunit beta type-5



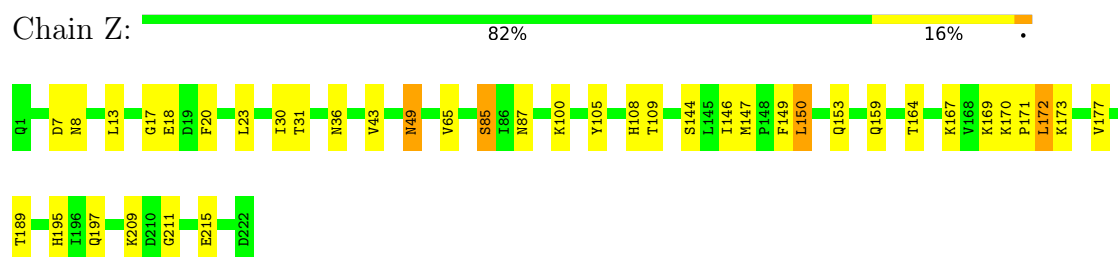
- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-6



- Molecule 12: Proteasome subunit beta type-6



- Molecule 13: Proteasome subunit beta type-7

Chain M:  84% 9% • 5%



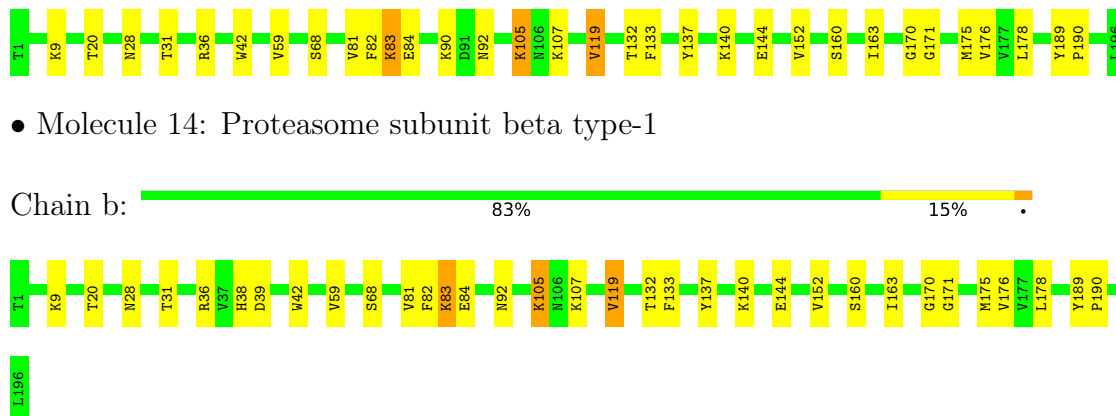
- Molecule 13: Proteasome subunit beta type-7

Chain a:  83% 10% • 5%



- Molecule 14: Proteasome subunit beta type-1

Chain N:  84% 15% •



- Molecule 15: BOC-ALA-ALA-ALA-CHO

Chain 1:  75% 25%



- Molecule 15: BOC-ALA-ALA-ALA-CHO

Chain 2:  75% 25%



- Molecule 15: BOC-ALA-ALA-ALA-CHO

Chain 3:  75% 25%



• Molecule 15: BOC-ALA-ALA-ALA-CHO

Chain 4:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.99Å 300.13Å 144.80Å 90.00° 112.51° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.1 (15.00-3.00) 91.4 (15.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.178 , 0.207 0.179 , 0.204	Depositor DCC
R_{free} test set	9676 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.0	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	49645	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: BOC, MG, 2A1

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	0.43	0/1952	0.79	0/2642
1	O	0.43	0/1952	0.79	0/2642
2	B	0.42	0/1934	0.77	0/2618
2	P	0.42	0/1934	0.77	0/2618
3	C	0.45	0/1910	0.83	0/2586
3	Q	0.45	0/1910	0.83	1/2586 (0.0%)
4	D	0.43	0/1837	0.75	0/2475
4	R	0.43	0/1837	0.75	0/2475
5	E	0.42	0/1800	0.76	2/2433 (0.1%)
5	S	0.42	0/1800	0.76	0/2433
6	F	0.42	0/1932	0.79	0/2609
6	T	0.43	0/1932	0.79	0/2609
7	G	0.41	0/1945	0.78	0/2634
7	U	0.41	0/1945	0.78	0/2634
8	H	0.41	0/1750	0.76	0/2373
8	V	0.41	0/1750	0.76	0/2373
9	I	0.41	0/1611	0.75	0/2174
9	W	0.41	0/1611	0.75	0/2174
10	J	0.43	0/1589	0.76	0/2142
10	X	0.43	0/1589	0.75	0/2142
11	K	0.42	0/1681	0.78	0/2274
11	Y	0.42	0/1681	0.78	0/2274
12	L	0.41	0/1795	0.76	0/2420
12	Z	0.40	0/1795	0.75	0/2420
13	M	0.42	0/1855	0.77	0/2514
13	a	0.42	0/1855	0.77	0/2514
14	N	0.40	0/1541	0.75	0/2087
14	b	0.41	0/1541	0.75	0/2087
15	1	0.87	0/9	0.40	0/11
15	2	0.49	0/9	0.63	0/11
15	3	0.86	0/9	0.38	0/11
15	4	0.51	0/9	0.68	0/11

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.42	0/50300	0.77	3/68006 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	E	147	GLN	CA-C-N	5.13	124.85	119.82
5	E	147	GLN	C-N-CA	5.13	124.85	119.82
3	Q	4	ARG	N-CA-C	5.06	117.81	110.42

There are no chirality outliers.

There are no planarity outliers.

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	11	0
1	O	1915	0	1929	14	0
2	B	1904	0	1904	24	0
2	P	1904	0	1904	24	0
3	C	1881	0	1895	21	0
3	Q	1881	0	1895	17	0
4	D	1813	0	1797	21	0
4	R	1813	0	1797	21	0
5	E	1773	0	1775	27	0
5	S	1773	0	1775	27	0
6	F	1892	0	1883	17	0
6	T	1892	0	1883	20	0
7	G	1907	0	1901	15	0
7	U	1907	0	1901	20	0
8	H	1719	0	1718	26	0
8	V	1719	0	1718	25	0
9	I	1581	0	1574	25	0
9	W	1581	0	1574	22	0
10	J	1561	0	1569	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	X	1561	0	1569	14	0
11	K	1644	0	1594	18	0
11	Y	1644	0	1594	16	0
12	L	1757	0	1711	23	0
12	Z	1757	0	1711	22	0
13	M	1824	0	1832	13	0
13	a	1824	0	1832	13	0
14	N	1512	0	1481	19	0
14	b	1512	0	1481	19	0
15	1	22	0	19	3	0
15	2	22	0	19	1	0
15	3	22	0	19	2	0
15	4	22	0	19	1	0
16	G	1	0	0	0	0
16	H	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	K	2	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	2	1	0	0	0	0
17	3	2	0	0	0	0
17	4	1	0	0	0	0
17	A	7	0	0	0	0
17	B	6	0	0	0	0
17	C	5	0	0	0	0
17	D	5	0	0	0	0
17	E	5	0	0	0	0
17	F	6	0	0	0	0
17	G	10	0	0	0	0
17	H	8	0	0	1	0
17	I	4	0	0	0	0
17	J	8	0	0	1	0
17	K	3	0	0	0	0
17	L	7	0	0	0	0
17	M	10	0	0	0	0
17	N	6	0	0	0	0
17	O	5	0	0	0	0
17	P	8	0	0	0	0
17	Q	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	R	3	0	0	0	0
17	S	1	0	0	0	0
17	T	7	0	0	0	0
17	U	5	0	0	0	0
17	V	11	0	0	1	0
17	W	3	0	0	0	0
17	X	7	0	0	0	0
17	Y	5	0	0	0	0
17	Z	4	0	0	0	0
17	a	16	0	0	1	0
17	b	5	0	0	0	0
All	All	49645	0	49202	495	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 5.

All (495) 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)
11:K:209:ASN:ND2	10:X:130:TYR:OH	1.93	0.99
3:C:201:VAL:O	3:C:202:GLN:HB3	1.79	0.82
3:Q:201:VAL:O	3:Q:202:GLN:HB3	1.80	0.82
12:L:172:LEU:H	12:L:172:LEU:HD23	1.46	0.81
12:Z:172:LEU:HD23	12:Z:172:LEU:H	1.46	0.79
8:V:114:HIS:HB2	17:V:401:HOH:O	1.81	0.79
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.86	0.74
11:K:53:GLN:O	11:K:57:THR:HG23	1.87	0.74
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.70	0.73
6:T:68:ARG:NH1	13:a:72:THR:OG1	2.23	0.72
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.54	0.72
10:J:149:ARG:O	10:J:152:MET:HG3	1.89	0.72
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.54	0.72
10:X:149:ARG:O	10:X:152:MET:HG3	1.89	0.71
12:L:159:GLN:HG2	8:V:209:THR:HG21	1.72	0.71
3:C:51:LYS:O	3:C:52:LEU:HB2	1.90	0.71
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.55	0.71
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.55	0.71
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.89	0.70
14:b:152:VAL:HA	14:b:175:MET:HE1	1.73	0.70
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.72	0.70
14:N:152:VAL:HA	14:N:175:MET:HE1	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:34:ILE:HG22	6:T:160:ALA:HB2	1.75	0.69
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.74	0.69
6:F:34:ILE:HG22	6:F:160:ALA:HB2	1.75	0.68
7:U:23:PHE:O	7:U:26:THR:HB	1.93	0.68
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.74	0.68
6:F:68:ARG:NH1	13:M:72:THR:OG1	2.26	0.68
7:G:23:PHE:O	7:G:26:THR:HB	1.93	0.67
11:K:51:ASP:HB3	11:K:97:MET:HE2	1.76	0.67
7:U:45:ILE:HG22	7:U:216:VAL:HG22	1.76	0.67
7:G:45:ILE:HG22	7:G:216:VAL:HG22	1.76	0.67
11:Y:51:ASP:HB3	11:Y:97:MET:HE2	1.76	0.66
8:V:192:THR:HG22	8:V:192:THR:O	1.97	0.65
1:A:119:GLN:O	1:A:122:THR:HB	1.97	0.64
3:C:161:THR:HG21	3:C:169:VAL:HG22	1.79	0.64
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.62	0.64
8:H:192:THR:O	8:H:192:THR:HG22	1.97	0.64
3:Q:161:THR:HG21	3:Q:169:VAL:HG22	1.80	0.64
8:H:209:THR:HG21	12:Z:159:GLN:HG2	1.81	0.63
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.64	0.62
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.64	0.62
1:O:119:GLN:O	1:O:122:THR:HB	1.98	0.62
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.83	0.61
13:a:174:GLU:O	13:a:178:VAL:HG23	2.01	0.61
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.83	0.60
13:M:174:GLU:O	13:M:178:VAL:HG23	2.01	0.60
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.67	0.60
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.37	0.59
10:X:23:ARG:NH2	10:X:50:ALA:HB2	2.16	0.59
9:W:22:ILE:HG23	9:W:42:ILE:HD13	1.85	0.59
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.84	0.59
10:J:23:ARG:NH2	10:J:50:ALA:HB2	2.17	0.59
8:V:3:ILE:HG21	8:V:44:ALA:HB1	1.84	0.59
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.85	0.59
8:V:52:THR:O	8:V:56:THR:HB	2.03	0.59
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.38	0.59
8:H:3:ILE:HG21	8:H:44:ALA:HB1	1.84	0.58
9:I:22:ILE:HG23	9:I:42:ILE:HD13	1.85	0.58
10:J:35:THR:HG23	10:J:43:LEU:HD11	1.85	0.58
5:S:134:ILE:HD12	5:S:215:VAL:HG12	1.85	0.58
10:X:35:THR:HG23	10:X:43:LEU:HD11	1.85	0.58
5:E:134:ILE:HD12	5:E:215:VAL:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:208:ASN:C	11:K:210:VAL:H	2.11	0.58
10:J:23:ARG:HH22	10:J:50:ALA:CB	2.17	0.58
2:B:93:HIS:HB3	2:B:113:ARG:NH2	2.19	0.58
8:H:52:THR:O	8:H:56:THR:HB	2.03	0.58
3:C:201:VAL:O	3:C:202:GLN:CB	2.50	0.57
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.86	0.57
10:X:23:ARG:HH22	10:X:50:ALA:CB	2.17	0.57
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.86	0.57
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.85	0.57
6:T:123:ASN:C	6:T:123:ASN:HD22	2.11	0.57
2:P:93:HIS:HB3	2:P:113:ARG:NH2	2.19	0.57
6:F:123:ASN:C	6:F:123:ASN:HD22	2.12	0.57
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.86	0.57
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.87	0.57
8:V:4:VAL:HG22	8:V:159:ILE:HD11	1.86	0.57
14:b:105:LYS:C	14:b:105:LYS:HD2	2.30	0.57
4:D:45:ARG:HG2	4:D:45:ARG:O	2.04	0.56
10:J:23:ARG:NH2	10:J:50:ALA:CB	2.68	0.56
5:S:109:HIS:HB3	6:T:82:ARG:NH2	2.20	0.56
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.51	0.56
4:R:45:ARG:O	4:R:45:ARG:HG2	2.06	0.56
8:V:3:ILE:HG22	8:V:16:ALA:HB2	1.88	0.55
7:G:195:GLU:HG3	7:G:235:ARG:HG3	1.88	0.55
10:X:23:ARG:NH2	10:X:50:ALA:CB	2.69	0.55
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.88	0.55
5:S:71:LEU:HD23	5:S:131:LEU:HD22	1.89	0.55
6:T:240:GLN:HE21	6:T:240:GLN:HA	1.71	0.55
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.88	0.55
6:F:240:GLN:HE21	6:F:240:GLN:HA	1.72	0.55
8:H:3:ILE:HG22	8:H:16:ALA:HB2	1.89	0.55
12:L:147:MET:HE2	9:W:176:ARG:NH2	2.22	0.55
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.89	0.55
5:E:71:LEU:HD23	5:E:131:LEU:HD22	1.89	0.55
9:I:52:ILE:HB	9:I:59:VAL:HG13	1.89	0.55
12:L:8:ASN:HA	12:L:30:ILE:O	2.07	0.55
12:L:17:GLY:HA3	12:L:20:PHE:CE1	2.42	0.55
4:R:12:ARG:HH11	4:R:12:ARG:HB2	1.72	0.54
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.88	0.54
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.88	0.54
12:Z:17:GLY:HA3	12:Z:20:PHE:CE1	2.42	0.54
6:T:59:LYS:HE2	6:T:59:LYS:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.87	0.54
9:I:98:ARG:O	9:I:126:ILE:HD11	2.08	0.54
14:N:105:LYS:HD2	14:N:105:LYS:C	2.32	0.54
9:I:176:ARG:NH2	12:Z:147:MET:HE2	2.22	0.54
8:V:215:GLU:HG2	9:W:197:ARG:HG2	1.89	0.54
7:U:83:ASN:C	7:U:83:ASN:HD22	2.16	0.54
9:W:167:SER:O	9:W:171:LEU:HB2	2.08	0.54
3:C:235:GLU:O	3:C:238:LYS:HB2	2.08	0.54
6:F:59:LYS:HE2	6:F:59:LYS:HA	1.89	0.53
11:K:25:TRP:CH2	12:L:144:SER:HA	2.43	0.53
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.08	0.53
4:D:12:ARG:HH11	4:D:12:ARG:HB2	1.72	0.53
7:G:73:VAL:HG12	7:G:133:THR:HB	1.90	0.53
7:G:83:ASN:C	7:G:83:ASN:HD22	2.16	0.53
4:R:32:ILE:CD1	4:R:192:VAL:HG23	2.39	0.53
9:I:167:SER:O	9:I:171:LEU:HB2	2.09	0.53
3:Q:235:GLU:O	3:Q:238:LYS:HB2	2.08	0.53
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.24	0.53
5:E:49:LYS:HE2	5:E:211:SER:HB2	1.91	0.53
4:D:32:ILE:CD1	4:D:192:VAL:HG23	2.39	0.53
4:D:38:VAL:HG11	4:D:137:ALA:HB1	1.91	0.53
12:L:159:GLN:HG2	8:V:209:THR:CG2	2.38	0.52
4:R:38:VAL:HG11	4:R:137:ALA:HB1	1.90	0.52
9:W:98:ARG:O	9:W:126:ILE:HD11	2.10	0.52
3:C:204:GLY:O	3:C:205:ALA:O	2.27	0.52
3:Q:204:GLY:O	3:Q:205:ALA:O	2.27	0.52
7:U:73:VAL:HG12	7:U:133:THR:HB	1.90	0.52
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.90	0.52
13:a:161:ARG:HG3	13:a:161:ARG:HH11	1.75	0.52
5:E:155:LEU:HD13	5:E:158:THR:HB	1.92	0.52
10:J:91:SER:O	10:J:94:SER:HB2	2.09	0.52
4:R:82:GLU:OE2	11:Y:69:ARG:NH1	2.43	0.52
10:X:91:SER:O	10:X:94:SER:HB2	2.10	0.52
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.45	0.52
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.75	0.51
14:N:20:THR:HG22	14:N:31:THR:OG1	2.10	0.51
14:b:20:THR:HG22	14:b:31:THR:OG1	2.11	0.51
11:Y:25:TRP:CH2	12:Z:144:SER:HA	2.44	0.51
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.57	0.51
6:T:240:GLN:HA	6:T:240:GLN:NE2	2.26	0.51
4:D:1:ASP:O	4:D:2:ARG:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:183:LEU:HD11	6:F:187:GLU:HB3	1.93	0.51
8:H:113:ILE:HB	8:H:119:THR:HG22	1.93	0.51
11:K:162:LEU:CD1	11:K:193:VAL:HG13	2.41	0.51
5:S:68:HIS:HE1	5:S:102:LEU:O	1.93	0.51
1:A:1:MET:HE2	5:E:121:SER:HB2	1.91	0.51
12:L:172:LEU:H	12:L:172:LEU:CD2	2.22	0.51
11:Y:208:ASN:C	11:Y:210:VAL:H	2.18	0.51
4:D:1:ASP:O	4:D:2:ARG:CB	2.59	0.51
8:H:139:GLU:OE1	13:a:187:ARG:NH1	2.44	0.51
8:V:113:ILE:HB	8:V:119:THR:HG22	1.93	0.51
5:E:33:VAL:HG12	5:E:48:LEU:HD23	1.93	0.50
12:L:195:HIS:HD2	12:L:197:GLN:H	1.58	0.50
4:R:1:ASP:O	4:R:2:ARG:CB	2.59	0.50
12:Z:172:LEU:H	12:Z:172:LEU:CD2	2.22	0.50
5:E:65:CYS:SG	5:E:71:LEU:HD12	2.52	0.50
5:S:49:LYS:HE2	5:S:211:SER:HB2	1.92	0.50
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.42	0.50
6:T:183:LEU:HD11	6:T:187:GLU:HB3	1.93	0.50
8:H:3:ILE:HD12	8:H:99:ILE:HD12	1.93	0.50
4:R:1:ASP:O	4:R:2:ARG:HB2	2.10	0.50
8:V:87:LEU:HD12	8:V:113:ILE:HD11	1.93	0.50
2:P:89:THR:HG21	2:P:117:ILE:CD1	2.42	0.50
5:S:155:LEU:HD13	5:S:158:THR:HB	1.93	0.50
9:W:65:MET:HE1	9:W:93:SER:HB3	1.94	0.50
10:X:33:ASP:OD2	10:X:182:LYS:NZ	2.45	0.50
2:B:37:ILE:HD12	2:B:192:ALA:HB2	1.94	0.49
15:3:1:BOC:H23	15:3:1:BOC:O1	2.11	0.49
1:A:106:PRO:HG2	1:A:109:LEU:HB2	1.95	0.49
6:F:240:GLN:HA	6:F:240:GLN:NE2	2.26	0.49
9:I:65:MET:HE1	9:I:93:SER:HB3	1.94	0.49
8:V:99:ILE:HG13	8:V:127:LEU:HD22	1.93	0.49
8:V:192:THR:O	8:V:192:THR:CG2	2.61	0.49
8:H:99:ILE:HG13	8:H:127:LEU:HD22	1.94	0.49
2:P:197:SER:HA	2:P:205:LEU:HD22	1.95	0.49
4:D:193:LEU:HD22	4:D:211:LEU:HD11	1.94	0.49
5:E:68:HIS:HE1	5:E:102:LEU:O	1.94	0.49
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.41	0.49
2:P:37:ILE:HD12	2:P:192:ALA:HB2	1.95	0.49
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.47	0.49
15:1:1:BOC:O1	15:1:1:BOC:H23	2.11	0.49
11:K:99:THR:HG22	11:K:115:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:3:ILE:HD12	8:V:99:ILE:HD12	1.92	0.49
11:Y:162:LEU:CD1	11:Y:193:VAL:HG13	2.42	0.49
12:Z:170:LYS:HG3	12:Z:171:PRO:HD2	1.95	0.49
13:a:190:ARG:HD2	17:a:305:HOH:O	2.13	0.49
12:L:170:LYS:HG3	12:L:171:PRO:HD2	1.95	0.49
9:W:7:ASN:HA	9:W:29:GLY:O	2.13	0.49
3:Q:62:VAL:HG22	3:Q:72:SER:HB3	1.95	0.49
11:Y:56:GLU:OE2	11:Y:99:THR:OG1	2.27	0.49
2:B:89:THR:HG21	2:B:117:ILE:CD1	2.43	0.48
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.42	0.48
1:O:106:PRO:HG2	1:O:109:LEU:HB2	1.95	0.48
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.48	0.48
4:D:82:GLU:OE2	11:K:69:ARG:NH1	2.47	0.48
1:A:122:THR:HG22	2:B:128:ARG:NH2	2.27	0.48
2:B:215:ILE:HG12	2:B:226:GLN:HG3	1.95	0.48
8:H:215:GLU:HG2	9:I:197:ARG:HG2	1.95	0.48
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.95	0.48
14:N:140:LYS:HG3	14:b:137:TYR:CE2	2.49	0.48
5:S:33:VAL:HG12	5:S:48:LEU:HD23	1.93	0.48
8:H:87:LEU:HD12	8:H:113:ILE:HD11	1.94	0.48
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.48	0.48
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.47	0.48
1:A:59:GLU:CD	1:A:59:GLU:H	2.22	0.48
10:J:33:ASP:OD2	10:J:182:LYS:NZ	2.45	0.48
4:R:193:LEU:HD22	4:R:211:LEU:HD11	1.94	0.48
5:S:46:VAL:HG13	5:S:212:ILE:HG12	1.95	0.48
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.62	0.48
6:T:57:PRO:O	6:T:58:GLN:HB2	2.13	0.48
7:U:83:ASN:C	7:U:83:ASN:ND2	2.72	0.48
12:Z:149:PHE:CE1	12:Z:153:GLN:HG3	2.49	0.48
4:D:176:LEU:HD22	5:E:55:LEU:HD22	1.96	0.48
8:H:114:HIS:HB2	17:H:403:HOH:O	2.13	0.48
9:I:125:LEU:HD21	15:1:1:BOC:H12	1.95	0.48
11:Y:99:THR:HG22	11:Y:115:VAL:O	2.14	0.48
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	1.96	0.48
3:C:198:LEU:HA	3:C:201:VAL:HG12	1.96	0.48
5:E:109:HIS:HB3	6:F:82:ARG:NH2	2.28	0.48
11:K:197:PHE:HE1	11:K:207:PHE:CE1	2.32	0.48
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.95	0.48
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.95	0.47
5:E:70:GLY:HA3	5:E:221:PHE:CE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:215:ILE:HG12	2:P:226:GLN:HG3	1.96	0.47
2:B:1:GLY:HA3	5:E:122:TYR:CE1	2.50	0.47
2:B:63:GLU:HG2	2:B:64:LYS:HG2	1.97	0.47
3:C:62:VAL:HG22	3:C:72:SER:HB3	1.95	0.47
8:H:192:THR:O	8:H:192:THR:CG2	2.61	0.47
9:I:171:LEU:HD11	9:I:201:MET:HB3	1.95	0.47
2:B:52:THR:HG22	2:B:53:SER:O	2.15	0.47
12:L:146:ILE:HG22	12:L:150:LEU:HD22	1.95	0.47
1:O:12:PHE:H	2:P:20:GLN:HE22	1.62	0.47
13:a:17:ASP:OD1	13:a:18:ASN:N	2.47	0.47
6:F:57:PRO:O	6:F:58:GLN:HB2	2.13	0.47
3:Q:202:GLN:HG3	3:Q:203:THR:N	2.30	0.47
3:C:172:PHE:CD1	3:C:172:PHE:C	2.93	0.47
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.96	0.47
11:K:208:ASN:C	11:K:210:VAL:N	2.72	0.47
1:O:59:GLU:CD	1:O:59:GLU:H	2.22	0.47
2:P:63:GLU:HG2	2:P:64:LYS:HG2	1.96	0.47
11:Y:208:ASN:C	11:Y:210:VAL:N	2.72	0.47
5:E:136:TYR:CE2	5:E:217:LYS:HA	2.50	0.47
10:J:25:ILE:HG12	10:J:25:ILE:O	2.14	0.47
5:S:136:TYR:CE2	5:S:217:LYS:HA	2.49	0.47
14:b:20:THR:CG2	14:b:28:ASN:HB3	2.44	0.47
11:K:73:ARG:NH2	11:K:104:TYR:O	2.47	0.47
4:R:9:PRO:HA	5:S:23:TYR:CG	2.50	0.47
6:T:168:ALA:O	6:T:172:LEU:HD22	2.15	0.47
14:N:20:THR:CG2	14:N:28:ASN:HB3	2.45	0.47
1:O:122:THR:HG22	2:P:128:ARG:NH2	2.29	0.47
5:S:65:CYS:SG	5:S:71:LEU:HD12	2.54	0.47
10:X:25:ILE:HG12	10:X:25:ILE:O	2.14	0.47
9:I:7:ASN:HA	9:I:29:GLY:O	2.14	0.46
13:M:17:ASP:OD1	13:M:18:ASN:N	2.47	0.46
2:P:119:GLN:CG	3:Q:78:ALA:HB1	2.45	0.46
14:b:163:ILE:HG23	14:b:170:GLY:HA2	1.97	0.46
2:B:197:SER:HA	2:B:205:LEU:HD22	1.97	0.46
3:C:202:GLN:HG3	3:C:203:THR:N	2.30	0.46
5:E:46:VAL:HG13	5:E:212:ILE:HG12	1.95	0.46
6:F:168:ALA:O	6:F:172:LEU:HD22	2.15	0.46
12:L:149:PHE:CE1	12:L:153:GLN:HG3	2.50	0.46
5:E:95:SER:O	5:E:99:ASN:HA	2.16	0.46
7:G:83:ASN:C	7:G:83:ASN:ND2	2.72	0.46
3:Q:172:PHE:CD1	3:Q:172:PHE:C	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:137:TYR:CE2	14:b:140:LYS:HG3	2.50	0.46
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.96	0.46
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.98	0.46
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.98	0.46
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.97	0.46
2:P:52:THR:HG22	2:P:53:SER:O	2.16	0.46
13:a:179:ASN:HD22	13:a:182:ARG:HH11	1.62	0.46
14:N:59:VAL:HG22	14:N:81:VAL:HG12	1.98	0.46
5:S:170:TYR:HB2	5:S:198:GLN:HG3	1.97	0.45
7:U:242:GLN:HA	7:U:242:GLN:NE2	2.31	0.45
5:S:95:SER:O	5:S:99:ASN:HA	2.16	0.45
8:V:3:ILE:CG2	8:V:44:ALA:HB1	2.46	0.45
9:W:171:LEU:HD11	9:W:201:MET:HB3	1.96	0.45
8:H:165:ASN:HD22	13:a:156:ARG:HH11	1.63	0.45
7:U:3:TYR:C	7:U:5:ARG:H	2.24	0.45
10:X:152:MET:HE2	10:X:156:GLU:HB3	1.98	0.45
11:Y:208:ASN:O	11:Y:210:VAL:N	2.49	0.45
5:E:170:TYR:HB2	5:E:198:GLN:HG3	1.97	0.45
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.51	0.45
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.99	0.45
8:H:8:PHE:CE2	8:H:148:LYS:HB2	2.52	0.45
4:R:159:TYR:CG	4:R:162:LYS:HB2	2.52	0.45
6:T:123:ASN:C	6:T:123:ASN:ND2	2.74	0.45
7:G:242:GLN:NE2	7:G:242:GLN:HA	2.32	0.45
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.47	0.45
4:D:43:GLU:HG3	4:D:200:MET:HE3	1.98	0.45
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.52	0.45
4:R:43:GLU:HG3	4:R:200:MET:HE3	1.98	0.45
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.47	0.45
8:H:3:ILE:CG2	8:H:44:ALA:HB1	2.46	0.45
6:F:105:ILE:HG21	6:F:143:HIS:HB2	1.98	0.45
13:a:95:TYR:O	13:a:99:VAL:HG23	2.16	0.45
14:b:59:VAL:HG22	14:b:81:VAL:HG12	1.98	0.45
5:E:143:LEU:CD2	5:E:157:GLY:HA2	2.47	0.45
6:F:123:ASN:C	6:F:123:ASN:ND2	2.75	0.45
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.99	0.45
2:P:1:GLY:HA3	5:S:122:TYR:CE1	2.51	0.45
5:S:69:MET:HE2	5:S:104:VAL:HA	1.98	0.45
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.99	0.45
5:E:74:ALA:HB3	5:E:160:ILE:HD12	2.00	0.44
11:K:56:GLU:OE2	11:K:99:THR:OG1	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:168:THR:O	2:P:172:GLN:HB2	2.17	0.44
13:M:95:TYR:O	13:M:99:VAL:HG23	2.16	0.44
4:R:191:LEU:O	4:R:195:ILE:HG13	2.17	0.44
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.99	0.44
4:D:159:TYR:CG	4:D:162:LYS:HB2	2.53	0.44
7:G:70:ILE:HD13	7:G:105:CYS:HA	1.99	0.44
3:Q:229:GLN:O	3:Q:233:GLN:HB2	2.17	0.44
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.99	0.44
5:S:143:LEU:CD2	5:S:157:GLY:HA2	2.47	0.44
9:W:125:LEU:HD21	15:3:1:BOC:H12	1.98	0.44
3:C:229:GLN:O	3:C:233:GLN:HB2	2.17	0.44
8:V:8:PHE:CE2	8:V:148:LYS:HB2	2.52	0.44
9:W:31:GLN:HB3	9:W:32:SER:H	1.65	0.44
6:F:36:ILE:HD12	6:F:192:ALA:HB2	2.00	0.44
1:O:196:LEU:HD23	1:O:209:ILE:HD12	2.00	0.44
5:S:178:PHE:HA	5:S:181:ILE:CD1	2.48	0.44
6:T:36:ILE:HD12	6:T:192:ALA:HB2	2.00	0.44
9:W:62:LEU:HD21	9:W:102:TYR:CD2	2.53	0.44
10:X:106:GLY:HA2	10:X:184:VAL:HG11	1.99	0.44
11:Y:116:ASP:OD1	11:Y:116:ASP:C	2.61	0.44
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.83	0.44
9:I:62:LEU:HD21	9:I:102:TYR:CD2	2.53	0.44
7:U:70:ILE:HD13	7:U:105:CYS:HA	1.99	0.44
8:V:8:PHE:HB2	8:V:146:LEU:O	2.18	0.44
8:H:8:PHE:HB2	8:H:146:LEU:O	2.18	0.44
8:H:173:VAL:HB	8:H:191:LEU:HB2	2.00	0.44
12:Z:100:LYS:HD3	12:Z:105:TYR:CZ	2.53	0.44
9:I:125:LEU:CD2	15:1:1:BOC:H12	2.48	0.43
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.53	0.43
5:E:69:MET:HE2	5:E:104:VAL:HA	1.99	0.43
9:I:126:ILE:HD12	9:I:126:ILE:HA	1.85	0.43
10:J:35:THR:CG2	10:J:43:LEU:HD11	2.47	0.43
10:J:152:MET:HE2	10:J:156:GLU:HB3	1.99	0.43
13:M:2:GLN:HG2	14:N:90:LYS:HD2	2.00	0.43
5:S:74:ALA:HB3	5:S:160:ILE:HD12	2.00	0.43
2:B:168:THR:O	2:B:172:GLN:HB2	2.17	0.43
8:H:199:LYS:HE3	9:I:151:SER:O	2.17	0.43
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.54	0.43
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	2.00	0.43
1:A:196:LEU:HD23	1:A:209:ILE:HD12	2.00	0.43
7:G:3:TYR:C	7:G:5:ARG:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:209:THR:CG2	12:Z:159:GLN:HG2	2.47	0.43
3:Q:106:TYR:CD1	3:Q:106:TYR:C	2.96	0.43
11:Y:97:MET:HE3	11:Y:97:MET:HB2	1.95	0.43
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.00	0.43
11:K:116:ASP:OD1	11:K:116:ASP:C	2.61	0.43
12:L:172:LEU:HD23	12:L:172:LEU:N	2.25	0.43
14:N:83:LYS:HG3	14:N:119:VAL:HG22	2.01	0.43
9:W:163:PHE:CE1	9:W:197:ARG:HD2	2.54	0.43
2:B:46:ALA:HB2	2:B:212:PHE:CE1	2.54	0.43
9:I:163:PHE:CE1	9:I:197:ARG:HD2	2.53	0.43
14:N:133:PHE:HA	14:b:132:THR:O	2.19	0.43
7:U:187:GLU:CG	7:U:192:LYS:HB2	2.48	0.43
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.84	0.43
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.44	0.43
6:F:238:PHE:O	6:F:242:GLU:HG2	2.19	0.43
7:G:187:GLU:CG	7:G:192:LYS:HB2	2.47	0.43
9:I:190:LYS:O	9:I:191:LYS:C	2.62	0.43
14:N:132:THR:O	14:b:133:PHE:HA	2.19	0.43
14:N:189:TYR:HB3	14:N:190:PRO:HD2	2.01	0.43
6:T:105:ILE:HG21	6:T:143:HIS:HB2	2.00	0.43
8:V:173:VAL:HB	8:V:191:LEU:HB2	2.01	0.43
3:C:106:TYR:CD1	3:C:106:TYR:C	2.96	0.42
3:C:202:GLN:HG3	3:C:203:THR:H	1.84	0.42
4:D:191:LEU:O	4:D:195:ILE:HG13	2.18	0.42
2:P:46:ALA:HB2	2:P:212:PHE:CE1	2.54	0.42
2:B:14:PRO:HA	3:C:20:TYR:CG	2.55	0.42
12:L:13:LEU:HD13	12:L:150:LEU:HD21	2.00	0.42
8:V:114:HIS:CD2	8:V:116:HIS:H	2.37	0.42
13:a:127:LEU:HG	13:a:142:LEU:HD12	2.01	0.42
2:P:95:GLN:HB3	9:W:68:TYR:CD2	2.54	0.42
5:E:178:PHE:HA	5:E:181:ILE:CD1	2.49	0.42
9:I:98:ARG:HD2	9:I:126:ILE:CG1	2.49	0.42
14:N:20:THR:CG2	14:N:31:THR:OG1	2.67	0.42
12:Z:172:LEU:HD23	12:Z:172:LEU:N	2.25	0.42
5:E:71:LEU:CD2	5:E:131:LEU:HD22	2.49	0.42
8:H:160:GLN:O	8:H:161:ALA:C	2.63	0.42
10:J:106:GLY:HA2	10:J:184:VAL:HG11	2.00	0.42
11:K:19:ARG:O	11:K:33:LYS:NZ	2.50	0.42
10:X:92:ILE:HD12	10:X:92:ILE:HA	1.86	0.42
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.02	0.42
1:O:61:LEU:HB2	7:U:155:VAL:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:238:PHE:O	6:T:242:GLU:HG2	2.20	0.42
9:W:68:TYR:CD1	9:W:68:TYR:C	2.98	0.42
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.49	0.42
2:P:64:LYS:O	2:P:75:ALA:HA	2.20	0.42
6:T:34:ILE:HG22	6:T:160:ALA:CB	2.47	0.42
8:V:160:GLN:O	8:V:161:ALA:C	2.62	0.42
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.01	0.42
10:X:35:THR:CG2	10:X:43:LEU:HD11	2.48	0.42
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.01	0.42
2:P:3:ARG:NH2	4:R:3:GLY:HA2	2.34	0.42
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.50	0.42
5:S:206:THR:H	5:S:209:ASN:ND2	2.18	0.42
14:b:20:THR:CG2	14:b:31:THR:OG1	2.68	0.42
2:B:106:PRO:HG2	2:B:109:ILE:HD12	2.02	0.41
3:C:174:GLU:HG2	4:D:49:PRO:HG2	2.02	0.41
7:G:39:LYS:HD2	7:G:186:ASN:ND2	2.35	0.41
13:M:35:ARG:HD2	13:M:35:ARG:O	2.20	0.41
5:S:71:LEU:HD22	5:S:71:LEU:C	2.45	0.41
9:W:190:LYS:O	9:W:191:LYS:C	2.63	0.41
8:H:114:HIS:CD2	8:H:116:HIS:H	2.38	0.41
2:P:134:PHE:O	2:P:149:THR:HA	2.20	0.41
5:S:71:LEU:CD2	5:S:131:LEU:HD22	2.49	0.41
5:S:81:ARG:HH11	5:S:81:ARG:HG3	1.85	0.41
14:b:189:TYR:HB3	14:b:190:PRO:HD2	2.01	0.41
2:B:134:PHE:O	2:B:149:THR:HA	2.21	0.41
5:S:155:LEU:CD2	6:T:55:LEU:HD23	2.50	0.41
5:S:156:TYR:CD1	5:S:179:ILE:HD11	2.55	0.41
1:A:110:LEU:O	1:A:114:VAL:HG23	2.21	0.41
7:G:198:ILE:HG23	7:G:214:LEU:HD11	2.03	0.41
10:J:23:ARG:NE	17:J:302:HOH:O	2.53	0.41
11:K:97:MET:HE3	11:K:97:MET:HB2	1.96	0.41
1:O:50:LYS:HG3	1:O:50:LYS:O	2.21	0.41
5:S:58:TYR:O	5:S:59:GLN:C	2.63	0.41
12:Z:85:SER:HB2	12:Z:87:ASN:OD1	2.20	0.41
5:E:156:TYR:CD1	5:E:179:ILE:HD11	2.56	0.41
6:F:165:ARG:HE	6:F:165:ARG:HB3	1.69	0.41
14:N:83:LYS:HE2	14:N:83:LYS:HB3	1.90	0.41
5:S:170:TYR:O	5:S:174:THR:OG1	2.38	0.41
7:U:216:VAL:HB	7:U:227:LEU:HD12	2.02	0.41
13:a:35:ARG:HD2	13:a:35:ARG:O	2.20	0.41
15:4:1:BOC:O1	15:4:1:BOC:H23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:LYS:O	2:B:75:ALA:HA	2.19	0.41
10:J:36:ARG:HA	10:J:36:ARG:HD3	1.90	0.41
1:O:110:LEU:O	1:O:114:VAL:HG23	2.21	0.41
2:P:106:PRO:HG2	2:P:109:ILE:HD12	2.02	0.41
7:U:39:LYS:HD2	7:U:186:ASN:ND2	2.35	0.41
13:a:182:ARG:HA	13:a:214:VAL:HG21	2.03	0.41
14:b:83:LYS:HG3	14:b:119:VAL:HG22	2.01	0.41
3:C:46:ARG:HH12	3:C:55:THR:HG22	1.86	0.41
8:H:112:SER:OG	8:H:120:ASP:HB2	2.21	0.41
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.03	0.41
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.84	0.41
9:W:98:ARG:HD2	9:W:126:ILE:CG1	2.51	0.41
2:B:8:ARG:HD2	3:C:4:ARG:HH21	1.85	0.41
8:H:50:ALA:HB2	9:I:128:CYS:HB2	2.02	0.41
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.01	0.41
12:L:164:THR:O	12:L:167:LYS:HD2	2.20	0.41
14:N:59:VAL:HG11	14:N:82:PHE:CE2	2.56	0.41
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.03	0.41
12:Z:164:THR:O	12:Z:167:LYS:HD2	2.20	0.41
14:b:59:VAL:HG11	14:b:82:PHE:CE2	2.56	0.41
2:B:65:LEU:HD22	2:B:211:GLU:HB3	2.03	0.41
4:D:31:GLY:HA2	4:D:39:VAL:O	2.20	0.41
5:E:81:ARG:HG3	5:E:81:ARG:HH11	1.85	0.41
5:E:206:THR:H	5:E:209:ASN:ND2	2.18	0.41
9:I:68:TYR:CD1	9:I:68:TYR:C	2.99	0.41
9:I:94:LEU:HD11	9:I:106:PRO:HG2	2.03	0.41
12:L:85:SER:HB2	12:L:87:ASN:OD1	2.21	0.41
13:M:182:ARG:HA	13:M:214:VAL:HG21	2.02	0.41
4:R:31:GLY:HA2	4:R:39:VAL:O	2.21	0.41
4:R:204:LEU:C	4:R:204:LEU:HD23	2.46	0.41
12:Z:7:ASP:OD1	12:Z:7:ASP:C	2.64	0.41
14:b:38:HIS:O	14:b:39:ASP:C	2.64	0.41
14:b:83:LYS:HE3	14:b:84:GLU:N	2.36	0.41
5:E:170:TYR:O	5:E:174:THR:OG1	2.39	0.41
12:L:7:ASP:OD1	12:L:7:ASP:C	2.62	0.41
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.66	0.41
4:D:183:LEU:HD23	4:D:187:GLU:HB3	2.03	0.40
5:E:71:LEU:C	5:E:71:LEU:HD22	2.46	0.40
11:K:12:ILE:HB	11:K:180:VAL:HB	2.04	0.40
14:N:83:LYS:HE3	14:N:84:GLU:N	2.36	0.40
4:R:214:ILE:O	4:R:214:ILE:HG13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:27:ARG:HD3	9:W:179:LEU:O	2.21	0.40
1:A:2:THR:HB	1:A:3:ASP:H	1.64	0.40
1:A:4:ARG:HB2	2:B:2:SER:OG	2.21	0.40
12:L:164:THR:HG21	12:L:168:VAL:HB	2.03	0.40
1:O:38:LYS:HB2	1:O:160:LYS:O	2.21	0.40
7:U:198:ILE:HG23	7:U:214:LEU:HD11	2.03	0.40
15:2:1:BOC:H23	15:2:1:BOC:O1	2.21	0.40
3:C:71:LEU:C	3:C:71:LEU:HD23	2.46	0.40
7:G:216:VAL:HB	7:G:227:LEU:HD12	2.03	0.40
2:P:145:TYR:OH	2:P:217:LYS:N	2.54	0.40
9:I:148:MET:HE2	9:I:172:ASN:HB2	2.04	0.40
1:O:21:ILE:HD11	1:O:122:THR:HG23	2.03	0.40
3:Q:71:LEU:HD23	3:Q:71:LEU:C	2.46	0.40
11:Y:86:LEU:HD13	11:Y:86:LEU:C	2.46	0.40
2:B:162:ILE:HG13	2:B:163:SER:N	2.37	0.40
4:D:204:LEU:HD23	4:D:204:LEU:C	2.47	0.40
5:E:58:TYR:O	5:E:59:GLN:C	2.64	0.40
2:P:4:ARG:HG2	7:U:3:TYR:CZ	2.57	0.40
8:V:18:THR:HB	8:V:30:ASN:HA	2.03	0.40
8:V:209:THR:O	8:V:209:THR:HG22	2.22	0.40
9:W:104:VAL:HG23	9:W:106:PRO:HD3	2.03	0.40
14:b:83:LYS:HE2	14:b:83:LYS:HB3	1.90	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%)	6 (2%)	2 (1%)	16	50
1	O	248/250 (99%)	240 (97%)	6 (2%)	2 (1%)	16	50
2	B	242/258 (94%)	226 (93%)	12 (5%)	4 (2%)	7	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	242/258 (94%)	226 (93%)	12 (5%)	4 (2%)	7	32
3	C	238/254 (94%)	226 (95%)	9 (4%)	3 (1%)	9	38
3	Q	238/254 (94%)	226 (95%)	9 (4%)	3 (1%)	9	38
4	D	231/260 (89%)	222 (96%)	8 (4%)	1 (0%)	30	65
4	R	231/260 (89%)	223 (96%)	7 (3%)	1 (0%)	30	65
5	E	229/234 (98%)	217 (95%)	10 (4%)	2 (1%)	14	48
5	S	229/234 (98%)	217 (95%)	10 (4%)	2 (1%)	14	48
6	F	241/288 (84%)	229 (95%)	11 (5%)	1 (0%)	30	65
6	T	241/288 (84%)	229 (95%)	11 (5%)	1 (0%)	30	65
7	G	239/252 (95%)	228 (95%)	10 (4%)	1 (0%)	30	65
7	U	239/252 (95%)	228 (95%)	10 (4%)	1 (0%)	30	65
8	H	224/232 (97%)	216 (96%)	8 (4%)	0	100	100
8	V	224/232 (97%)	216 (96%)	8 (4%)	0	100	100
9	I	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
9	W	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
10	J	193/198 (98%)	180 (93%)	12 (6%)	1 (0%)	24	60
10	X	193/198 (98%)	181 (94%)	11 (6%)	1 (0%)	24	60
11	K	210/212 (99%)	199 (95%)	9 (4%)	2 (1%)	12	45
11	Y	210/212 (99%)	199 (95%)	8 (4%)	3 (1%)	9	36
12	L	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
12	Z	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
13	M	231/246 (94%)	218 (94%)	13 (6%)	0	100	100
13	a	231/246 (94%)	218 (94%)	13 (6%)	0	100	100
14	N	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
14	b	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
15	1	2/4 (50%)	2 (100%)	0	0	100	100
15	2	2/4 (50%)	2 (100%)	0	0	100	100
15	3	2/4 (50%)	2 (100%)	0	0	100	100
15	4	2/4 (50%)	2 (100%)	0	0	100	100
All	All	6292/6630 (95%)	5990 (95%)	267 (4%)	35 (1%)	21	56

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	51	VAL
3	C	202	GLN
3	C	205	ALA
4	D	2	ARG
5	E	231	LYS
1	O	2	THR
2	P	51	VAL
3	Q	202	GLN
3	Q	205	ALA
4	R	2	ARG
5	S	231	LYS
1	A	166	LYS
2	B	219	ALA
5	E	59	GLN
11	K	39	PRO
1	O	166	LYS
2	P	219	ALA
5	S	59	GLN
11	Y	39	PRO
11	Y	209	ASN
2	B	221	ASP
3	C	52	LEU
2	P	221	ASP
3	Q	52	LEU
11	Y	106	ARG
2	B	218	GLY
7	G	221	LYS
11	K	106	ARG
2	P	218	GLY
6	F	243	ILE
6	T	243	ILE
7	U	221	LYS
10	J	9	VAL
10	X	9	VAL

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%)	193 (92%)	16 (8%)	12	40
1	O	209/209 (100%)	193 (92%)	16 (8%)	12	40
2	B	203/216 (94%)	178 (88%)	25 (12%)	4	21
2	P	203/216 (94%)	178 (88%)	25 (12%)	4	21
3	C	212/226 (94%)	186 (88%)	26 (12%)	4	21
3	Q	212/226 (94%)	186 (88%)	26 (12%)	4	21
4	D	194/215 (90%)	169 (87%)	25 (13%)	4	19
4	R	194/215 (90%)	169 (87%)	25 (13%)	4	19
5	E	190/193 (98%)	166 (87%)	24 (13%)	4	20
5	S	190/193 (98%)	165 (87%)	25 (13%)	4	18
6	F	201/239 (84%)	186 (92%)	15 (8%)	12	41
6	T	201/239 (84%)	186 (92%)	15 (8%)	12	41
7	G	206/210 (98%)	180 (87%)	26 (13%)	4	20
7	U	206/210 (98%)	180 (87%)	26 (13%)	4	20
8	H	185/190 (97%)	163 (88%)	22 (12%)	5	22
8	V	185/190 (97%)	163 (88%)	22 (12%)	5	22
9	I	172/173 (99%)	157 (91%)	15 (9%)	9	35
9	W	172/173 (99%)	157 (91%)	15 (9%)	9	35
10	J	173/175 (99%)	152 (88%)	21 (12%)	5	21
10	X	173/175 (99%)	152 (88%)	21 (12%)	5	21
11	K	169/169 (100%)	160 (95%)	9 (5%)	20	54
11	Y	169/169 (100%)	159 (94%)	10 (6%)	18	50
12	L	185/185 (100%)	169 (91%)	16 (9%)	10	36
12	Z	185/185 (100%)	169 (91%)	16 (9%)	10	36
13	M	199/208 (96%)	185 (93%)	14 (7%)	14	44
13	a	199/208 (96%)	185 (93%)	14 (7%)	14	44
14	N	162/162 (100%)	151 (93%)	11 (7%)	14	45
14	b	162/162 (100%)	151 (93%)	11 (7%)	14	45
All	All	5320/5540 (96%)	4788 (90%)	532 (10%)	7	29

All (532) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	THR
1	A	29	LYS
1	A	32	VAL
1	A	50	LYS
1	A	59	GLU
1	A	64	VAL
1	A	108	LYS
1	A	109	LEU
1	A	157	PHE
1	A	164	ILE
1	A	169	VAL
1	A	176	GLU
1	A	229	THR
1	A	231	LYS
1	A	248	GLU
2	B	2	SER
2	B	3	ARG
2	B	17	ARG
2	B	50	LYS
2	B	53	SER
2	B	55	LEU
2	B	58	GLN
2	B	62	THR
2	B	63	GLU
2	B	65	LEU
2	B	79	LEU
2	B	102	ASN
2	B	114	LEU
2	B	122	THR
2	B	155	ASN
2	B	173	THR
2	B	177	MET
2	B	180	LYS
2	B	191	LEU
2	B	197	SER
2	B	206	THR
2	B	217	LYS
2	B	237	ILE
2	B	239	VAL
2	B	244	THR
3	C	8	ILE
3	C	49	THR

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Mol	Chain	Res	Type
3	C	50	LEU
3	C	51	LYS
3	C	52	LEU
3	C	61	LYS
3	C	69	VAL
3	C	107	LEU
3	C	147	GLN
3	C	160	GLN
3	C	167	LYS
3	C	169	VAL
3	C	171	GLU
3	C	175	LYS
3	C	180	LYS
3	C	181	GLU
3	C	203	THR
3	C	213	VAL
3	C	214	LYS
3	C	224	SER
3	C	226	GLU
3	C	228	ASN
3	C	233	GLN
3	C	235	GLU
3	C	238	LYS
3	C	239	GLN
4	D	4	VAL
4	D	6	THR
4	D	12	ARG
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	60	VAL
4	D	64	ARG
4	D	99	ILE
4	D	102	GLU
4	D	111	LEU
4	D	117	GLU
4	D	169	GLU
4	D	176	LEU
4	D	183	LEU
4	D	190	LEU
4	D	193	LEU
4	D	202	GLU

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Mol	Chain	Res	Type
4	D	203	LYS
4	D	214	ILE
4	D	215	THR
4	D	224	ASP
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	8	ASP
5	E	9	THR
5	E	15	THR
5	E	25	LEU
5	E	29	LYS
5	E	44	VAL
5	E	46	VAL
5	E	55	LEU
5	E	71	LEU
5	E	76	LEU
5	E	87	LEU
5	E	95	SER
5	E	144	LEU
5	E	147	GLN
5	E	152	VAL
5	E	160	ILE
5	E	169	THR
5	E	174	THR
5	E	180	LYS
5	E	188	LEU
5	E	190	LYS
5	E	207	VAL
5	E	209	ASN
5	E	217	LYS
6	F	2	THR
6	F	14	ASP
6	F	53	LYS
6	F	94	SER
6	F	96	LYS
6	F	123	ASN
6	F	139	LYS
6	F	165	ARG
6	F	169	LYS
6	F	172	LEU
6	F	174	LYS

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Mol	Chain	Res	Type
6	F	181	GLU
6	F	186	ARG
6	F	206	LYS
6	F	221	ASN
7	G	24	LYS
7	G	26	THR
7	G	28	GLN
7	G	31	ILE
7	G	36	VAL
7	G	39	LYS
7	G	58	THR
7	G	70	ILE
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	148	THR
7	G	162	THR
7	G	166	GLN
7	G	171	THR
7	G	178	LYS
7	G	181	LYS
7	G	201	MET
7	G	221	LYS
7	G	223	LYS
7	G	235	ARG
7	G	236	LEU
7	G	237	VAL
7	G	239	ILE
7	G	241	GLU
7	G	242	GLN
8	H	3	ILE
8	H	9	ASN
8	H	13	VAL
8	H	22	GLN
8	H	30	ASN
8	H	34	LEU
8	H	53	GLU
8	H	56	THR
8	H	68	LEU
8	H	113	ILE
8	H	118	SER
8	H	121	VAL

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Mol	Chain	Res	Type
8	H	127	LEU
8	H	153	LYS
8	H	163	ILE
8	H	180	ILE
8	H	191	LEU
8	H	195	VAL
8	H	199	LYS
8	H	216	SER
8	H	218	VAL
8	H	224	GLN
9	I	17	LYS
9	I	30	SER
9	I	31	GLN
9	I	37	ASN
9	I	92	SER
9	I	96	GLU
9	I	97	ARG
9	I	117	LYS
9	I	126	ILE
9	I	133	LYS
9	I	151	SER
9	I	166	ILE
9	I	171	LEU
9	I	190	LYS
9	I	195	VAL
10	J	3	ILE
10	J	7	ILE
10	J	8	ARG
10	J	17	SER
10	J	23	ARG
10	J	25	ILE
10	J	35	THR
10	J	36	ARG
10	J	49	GLU
10	J	63	ASN
10	J	69	ILE
10	J	90	LYS
10	J	92	ILE
10	J	99	GLN
10	J	110	LYS
10	J	113	LYS
10	J	126	VAL

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Mol	Chain	Res	Type
10	J	161	LEU
10	J	162	LYS
10	J	166	GLN
10	J	189	ILE
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	45	MET
11	K	99	THR
11	K	147	ASP
11	K	148	LEU
11	K	186	ILE
11	K	211	ILE
12	L	18	GLU
12	L	23	LEU
12	L	43	VAL
12	L	49	ASN
12	L	65	VAL
12	L	85	SER
12	L	108	HIS
12	L	109	THR
12	L	150	LEU
12	L	169	LYS
12	L	172	LEU
12	L	173	LYS
12	L	177	VAL
12	L	189	THR
12	L	209	LYS
12	L	215	GLU
13	M	2	GLN
13	M	10	SER
13	M	29	SER
13	M	35	ARG
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	157	LYS
13	M	161	ARG
13	M	187	ARG
13	M	212	LEU
13	M	213	GLN

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Mol	Chain	Res	Type
13	M	214	VAL
14	N	9	LYS
14	N	68	SER
14	N	83	LYS
14	N	92	ASN
14	N	105	LYS
14	N	107	LYS
14	N	119	VAL
14	N	144	GLU
14	N	160	SER
14	N	176	VAL
14	N	178	LEU
1	O	1	MET
1	O	2	THR
1	O	29	LYS
1	O	32	VAL
1	O	50	LYS
1	O	59	GLU
1	O	64	VAL
1	O	108	LYS
1	O	109	LEU
1	O	157	PHE
1	O	164	ILE
1	O	169	VAL
1	O	176	GLU
1	O	229	THR
1	O	231	LYS
1	O	248	GLU
2	P	2	SER
2	P	3	ARG
2	P	17	ARG
2	P	50	LYS
2	P	53	SER
2	P	55	LEU
2	P	58	GLN
2	P	62	THR
2	P	63	GLU
2	P	65	LEU
2	P	79	LEU
2	P	102	ASN
2	P	114	LEU
2	P	122	THR

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Mol	Chain	Res	Type
2	P	155	ASN
2	P	173	THR
2	P	177	MET
2	P	180	LYS
2	P	191	LEU
2	P	197	SER
2	P	206	THR
2	P	217	LYS
2	P	237	ILE
2	P	239	VAL
2	P	244	THR
3	Q	8	ILE
3	Q	49	THR
3	Q	50	LEU
3	Q	51	LYS
3	Q	52	LEU
3	Q	61	LYS
3	Q	69	VAL
3	Q	107	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	167	LYS
3	Q	169	VAL
3	Q	171	GLU
3	Q	175	LYS
3	Q	180	LYS
3	Q	181	GLU
3	Q	203	THR
3	Q	213	VAL
3	Q	214	LYS
3	Q	224	SER
3	Q	226	GLU
3	Q	228	ASN
3	Q	233	GLN
3	Q	235	GLU
3	Q	238	LYS
3	Q	239	GLN
4	R	4	VAL
4	R	6	THR
4	R	12	ARG
4	R	20	LEU
4	R	40	LEU

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Mol	Chain	Res	Type
4	R	51	LEU
4	R	60	VAL
4	R	64	ARG
4	R	99	ILE
4	R	102	GLU
4	R	111	LEU
4	R	117	GLU
4	R	169	GLU
4	R	176	LEU
4	R	183	LEU
4	R	190	LEU
4	R	193	LEU
4	R	202	GLU
4	R	203	LYS
4	R	214	ILE
4	R	215	THR
4	R	224	ASP
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	8	ASP
5	S	9	THR
5	S	15	THR
5	S	25	LEU
5	S	29	LYS
5	S	44	VAL
5	S	46	VAL
5	S	55	LEU
5	S	71	LEU
5	S	76	LEU
5	S	87	LEU
5	S	95	SER
5	S	144	LEU
5	S	147	GLN
5	S	152	VAL
5	S	160	ILE
5	S	169	THR
5	S	174	THR
5	S	180	LYS
5	S	188	LEU
5	S	190	LYS
5	S	207	VAL

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Mol	Chain	Res	Type
5	S	209	ASN
5	S	217	LYS
5	S	227	GLU
6	T	2	THR
6	T	14	ASP
6	T	53	LYS
6	T	94	SER
6	T	96	LYS
6	T	123	ASN
6	T	139	LYS
6	T	165	ARG
6	T	169	LYS
6	T	172	LEU
6	T	174	LYS
6	T	181	GLU
6	T	186	ARG
6	T	206	LYS
6	T	221	ASN
7	U	24	LYS
7	U	26	THR
7	U	28	GLN
7	U	31	ILE
7	U	36	VAL
7	U	39	LYS
7	U	58	THR
7	U	70	ILE
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	148	THR
7	U	162	THR
7	U	166	GLN
7	U	171	THR
7	U	178	LYS
7	U	181	LYS
7	U	201	MET
7	U	221	LYS
7	U	223	LYS
7	U	235	ARG
7	U	236	LEU
7	U	237	VAL
7	U	239	ILE

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Mol	Chain	Res	Type
7	U	241	GLU
7	U	242	GLN
8	V	3	ILE
8	V	9	ASN
8	V	13	VAL
8	V	22	GLN
8	V	30	ASN
8	V	34	LEU
8	V	53	GLU
8	V	56	THR
8	V	68	LEU
8	V	113	ILE
8	V	118	SER
8	V	121	VAL
8	V	127	LEU
8	V	153	LYS
8	V	163	ILE
8	V	180	ILE
8	V	191	LEU
8	V	195	VAL
8	V	199	LYS
8	V	216	SER
8	V	218	VAL
8	V	224	GLN
9	W	17	LYS
9	W	30	SER
9	W	31	GLN
9	W	37	ASN
9	W	92	SER
9	W	96	GLU
9	W	97	ARG
9	W	117	LYS
9	W	126	ILE
9	W	133	LYS
9	W	151	SER
9	W	166	ILE
9	W	171	LEU
9	W	190	LYS
9	W	195	VAL
10	X	3	ILE
10	X	7	ILE
10	X	8	ARG

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Mol	Chain	Res	Type
10	X	17	SER
10	X	23	ARG
10	X	25	ILE
10	X	35	THR
10	X	36	ARG
10	X	49	GLU
10	X	63	ASN
10	X	69	ILE
10	X	90	LYS
10	X	92	ILE
10	X	99	GLN
10	X	110	LYS
10	X	113	LYS
10	X	126	VAL
10	X	161	LEU
10	X	162	LYS
10	X	166	GLN
10	X	189	ILE
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	45	MET
11	Y	99	THR
11	Y	147	ASP
11	Y	148	LEU
11	Y	186	ILE
11	Y	210	VAL
11	Y	211	ILE
12	Z	18	GLU
12	Z	23	LEU
12	Z	43	VAL
12	Z	49	ASN
12	Z	65	VAL
12	Z	85	SER
12	Z	108	HIS
12	Z	109	THR
12	Z	150	LEU
12	Z	169	LYS
12	Z	172	LEU
12	Z	173	LYS
12	Z	177	VAL
12	Z	189	THR

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Mol	Chain	Res	Type
12	Z	209	LYS
12	Z	215	GLU
13	a	2	GLN
13	a	10	SER
13	a	29	SER
13	a	35	ARG
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	157	LYS
13	a	161	ARG
13	a	187	ARG
13	a	212	LEU
13	a	213	GLN
13	a	214	VAL
14	b	9	LYS
14	b	68	SER
14	b	83	LYS
14	b	92	ASN
14	b	105	LYS
14	b	107	LYS
14	b	119	VAL
14	b	144	GLU
14	b	160	SER
14	b	176	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (155) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	102	ASN
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	155	ASN
2	B	172	GLN
3	C	17	GLN
3	C	38	ASN

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Mol	Chain	Res	Type
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	239	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	106	GLN
4	D	160	ASN
4	D	207	ASN
4	D	217	GLN
4	D	225	ASN
5	E	4	ASN
5	E	68	HIS
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
6	F	58	GLN
6	F	86	ASN
6	F	117	GLN
6	F	140	ASN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	184	HIS
7	G	186	ASN
7	G	212	ASN
7	G	242	GLN
8	H	35	HIS
8	H	66	HIS
8	H	114	HIS
8	H	116	HIS
8	H	165	ASN
8	H	172	ASN
9	I	63	ASN
9	I	71	ASN
9	I	88	GLN

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Mol	Chain	Res	Type
10	J	10	GLN
10	J	55	GLN
10	J	63	ASN
10	J	147	HIS
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	143	ASN
11	K	176	ASN
12	L	3	ASN
12	L	29	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	94	GLN
12	L	195	HIS
12	L	197	GLN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	203	ASN
13	M	213	GLN
14	N	38	HIS
14	N	141	ASN
14	N	161	GLN
1	O	190	HIS
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	155	ASN
2	P	172	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN

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Mol	Chain	Res	Type
3	Q	160	GLN
3	Q	239	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	160	ASN
4	R	207	ASN
4	R	225	ASN
5	S	4	ASN
5	S	68	HIS
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
6	T	58	GLN
6	T	86	ASN
6	T	117	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	186	ASN
7	U	212	ASN
7	U	242	GLN
8	V	35	HIS
8	V	66	HIS
8	V	114	HIS
8	V	116	HIS
9	W	63	ASN
9	W	71	ASN
9	W	203	GLN
10	X	10	GLN
10	X	55	GLN
10	X	63	ASN
10	X	86	GLN
10	X	147	HIS
11	Y	9	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	143	ASN
11	Y	176	ASN

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Mol	Chain	Res	Type
12	Z	3	ASN
12	Z	29	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	94	GLN
12	Z	153	GLN
12	Z	195	HIS
13	a	48	ASN
13	a	102	GLN
13	a	171	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	141	ASN
14	b	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.73	0 100 100	45, 63, 95, 132	0
1	O	250/250 (100%)	-0.69	0 100 100	46, 67, 106, 132	0
2	B	244/258 (94%)	-0.66	0 100 100	46, 68, 112, 159	0
2	P	244/258 (94%)	-0.63	0 100 100	45, 69, 119, 158	0
3	C	240/254 (94%)	-0.60	0 100 100	44, 69, 120, 139	0
3	Q	240/254 (94%)	-0.52	1 (0%) 88 76	52, 79, 138, 156	0
4	D	235/260 (90%)	-0.65	0 100 100	44, 69, 97, 118	0
4	R	235/260 (90%)	-0.67	0 100 100	50, 73, 102, 129	0
5	E	231/234 (98%)	-0.66	0 100 100	49, 74, 103, 134	0
5	S	231/234 (98%)	-0.59	0 100 100	53, 79, 111, 139	0
6	F	243/288 (84%)	-0.67	0 100 100	47, 68, 109, 142	0
6	T	243/288 (84%)	-0.62	0 100 100	44, 71, 112, 135	0
7	G	241/252 (95%)	-0.71	0 100 100	44, 62, 100, 142	0
7	U	241/252 (95%)	-0.69	0 100 100	46, 63, 95, 121	0
8	H	226/232 (97%)	-0.74	0 100 100	43, 60, 91, 150	0
8	V	226/232 (97%)	-0.77	0 100 100	46, 62, 90, 156	0
9	I	204/205 (99%)	-0.85	0 100 100	42, 61, 88, 112	0
9	W	204/205 (99%)	-0.84	0 100 100	41, 60, 88, 132	0
10	J	195/198 (98%)	-0.77	1 (0%) 87 72	41, 61, 90, 129	0
10	X	195/198 (98%)	-0.73	1 (0%) 87 72	43, 63, 89, 144	0
11	K	212/212 (100%)	-0.75	0 100 100	44, 61, 94, 113	0
11	Y	212/212 (100%)	-0.74	0 100 100	47, 63, 98, 127	0
12	L	222/222 (100%)	-0.79	0 100 100	43, 61, 85, 103	0
12	Z	222/222 (100%)	-0.79	0 100 100	43, 62, 91, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
13	M	233/246 (94%)	-0.80	0	100	100	42, 62, 86, 107	0
13	a	233/246 (94%)	-0.79	0	100	100	42, 60, 82, 105	0
14	N	196/196 (100%)	-0.81	0	100	100	41, 57, 84, 121	0
14	b	196/196 (100%)	-0.79	0	100	100	42, 58, 83, 112	0
15	1	2/4 (50%)	0.09	0	100	100	68, 68, 68, 71	0
15	2	2/4 (50%)	-0.63	0	100	100	57, 57, 57, 58	0
15	3	2/4 (50%)	-0.23	0	100	100	77, 77, 77, 81	0
15	4	2/4 (50%)	-0.84	0	100	100	65, 65, 65, 69	0
All	All	6352/6630 (95%)	-0.71	3 (0%)	100	100	41, 65, 103, 159	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	4.4
3	Q	50	LEU	3.3
10	J	1	MET	2.4

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

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

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(Å ²)	Q<0.9
16	MG	H	301	1/1	0.91	0.12	60,60,60,60	0
16	MG	Z	301	1/1	0.95	0.09	71,71,71,71	0
16	MG	I	302	1/1	0.96	0.12	67,67,67,67	0
16	MG	K	302	1/1	0.97	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	MG	N	201	1/1	0.97	0.03	48,48,48,48	0
16	MG	I	301	1/1	0.97	0.05	42,42,42,42	0
16	MG	V	301	1/1	0.98	0.04	68,68,68,68	0
16	MG	Y	301	1/1	0.98	0.06	50,50,50,50	0
16	MG	K	301	1/1	0.98	0.05	45,45,45,45	0
16	MG	G	301	1/1	0.99	0.03	53,53,53,53	0
16	MG	J	201	1/1	1.00	0.08	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.