



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:01 PM UTC

PDB ID : 4JSU / pdb_00004jsu
Title : Yeast 20S proteasome in complex with the dimerized linear mimetic of TMC-95A - yCP:3a
Authors : Desvergne, A.; Genin, E.; Marechal, X.; Gallastegui, N.; Dufau, L.; Richy, N.; Groll, M.; Vidal, J.; Reboud-Ravaux, M.
Deposited on : 2013-03-22
Resolution : 2.90 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

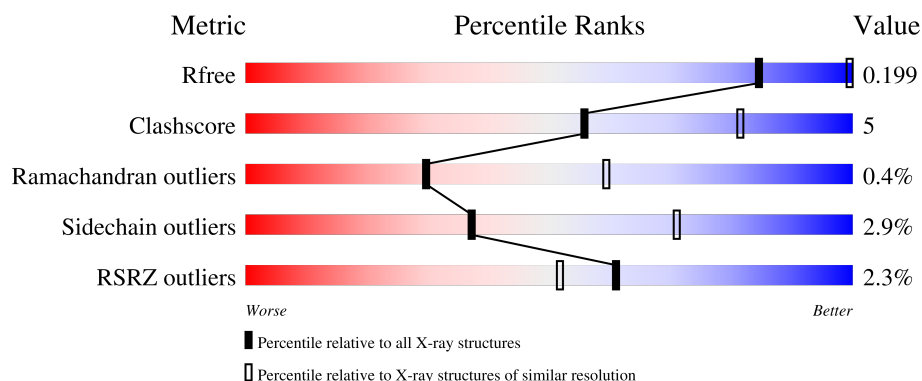
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	250	0.1% 91% 8%
1	O	250	0.1% 88% 11%
2	B	258	3% 79% 16% 5%
2	P	258	5% 80% 14% 5%
3	C	254	4% 79% 15% • 5%

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Mol	Chain	Length	Quality of chain
3	Q	254	 4% 80% 14% 5%
4	D	260	 4% 78% 14% 7%
4	R	260	 3% 78% 14% 7%
5	E	234	 % 82% 16%
5	S	234	 3% 82% 16%
6	F	288	 % 75% 9% 15%
6	T	288	 % 74% 10% 15%
7	G	252	 2% 85% 11%
7	U	252	 2% 84% 12%
8	H	232	 % 85% 10%
8	V	232	 % 85% 10%
9	I	205	 % 84% 15%
9	W	205	 % 84% 15%
10	J	198	 4% 84% 15%
10	X	198	 4% 85% 15%
11	K	212	 4% 86% 12%
11	Y	212	 5% 86% 13%
12	L	222	 % 92% 8%
12	Z	222	 3% 92% 8%
13	M	233	 % 85% 14%
13	a	233	 % 84% 15%
14	N	196	 % 86% 14%
14	b	196	 % 85% 15%
15	c	8	 25% 25% 12% 38%
15	d	8	 25% 25% 12% 38%

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Mol	Chain	Length	Quality of chain
15	e	8	12% 38% 25% 38%
15	f	8	12% 38% 25% 38%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 51118 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	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			
4	R	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
6	T	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	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	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	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 TMC-95A mimic ligand yCP:3a.

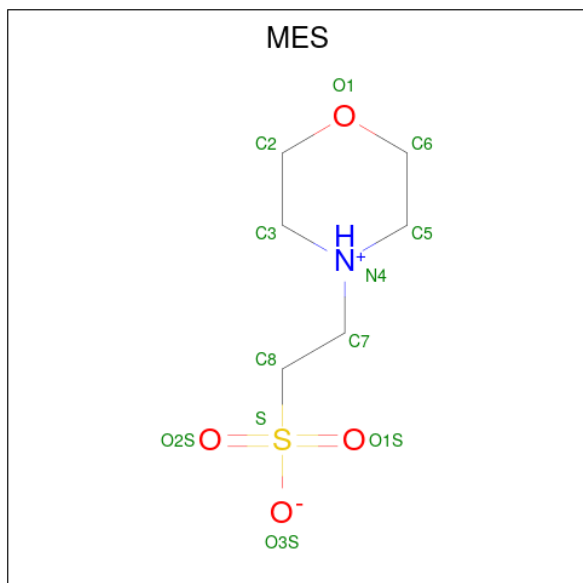
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	5	Total	C	N	O	0	0	0
			56	43	6	7			
15	d	5	Total	C	N	O	0	0	0
			56	43	6	7			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	5	Total	C	N	O	0	0	0
			56	43	6	7			
15	f	5	Total	C	N	O	0	0	0
			56	43	6	7			

- Molecule 16 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
16	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	58	Total	O	0	0
			58	58		
17	B	40	Total	O	0	0
			40	40		
17	C	40	Total	O	0	0
			40	40		
17	D	37	Total	O	0	0
			37	37		
17	E	22	Total	O	0	0
			22	22		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	F	47	Total O 47 47	0	0
17	G	58	Total O 58 58	0	0
17	H	53	Total O 53 53	0	0
17	I	62	Total O 62 62	0	0
17	J	53	Total O 53 53	0	0
17	K	49	Total O 49 49	0	0
17	L	58	Total O 58 58	0	0
17	M	75	Total O 75 75	0	0
17	N	57	Total O 57 57	0	0
17	O	33	Total O 33 33	0	0
17	P	29	Total O 29 29	0	0
17	Q	29	Total O 29 29	0	0
17	R	28	Total O 28 28	0	0
17	S	18	Total O 18 18	0	0
17	T	44	Total O 44 44	0	0
17	U	58	Total O 58 58	0	0
17	V	47	Total O 47 47	0	0
17	W	58	Total O 58 58	0	0
17	X	44	Total O 44 44	0	0
17	Y	46	Total O 46 46	0	0
17	Z	51	Total O 51 51	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	a	79	Total 79	O 79	0	0
17	b	57	Total 57	O 57	0	0
17	e	1	Total 1	O 1	0	0
17	f	1	Total 1	O 1	0	0

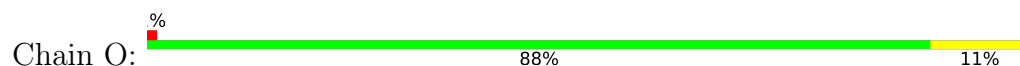
3 Residue-property plots [i](#)

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.

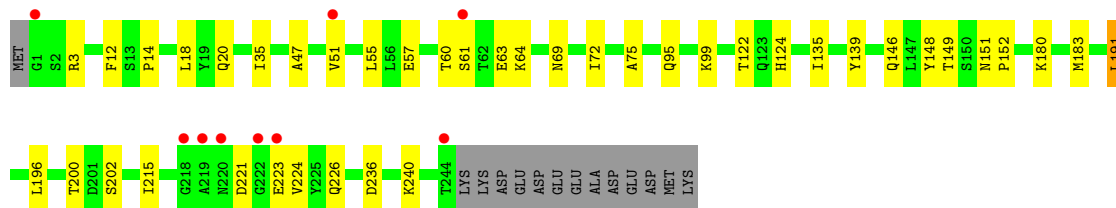
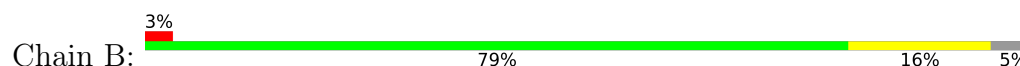
- Molecule 1: Proteasome subunit alpha type-2



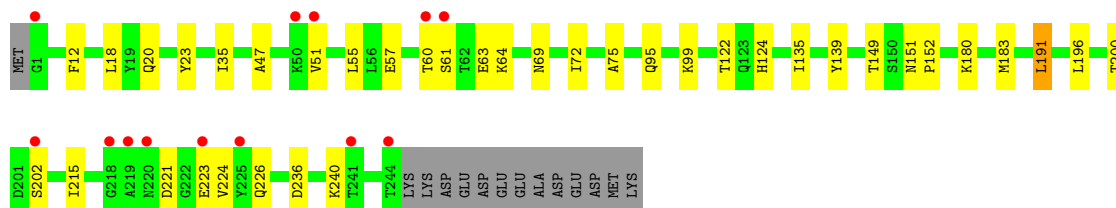
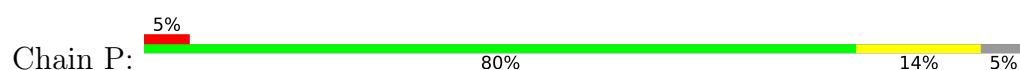
- Molecule 1: Proteasome subunit alpha type-2



- Molecule 2: Proteasome subunit alpha type-3

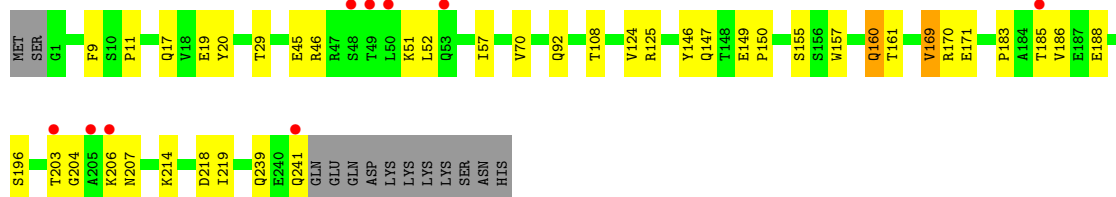


- Molecule 2: Proteasome subunit alpha type-3



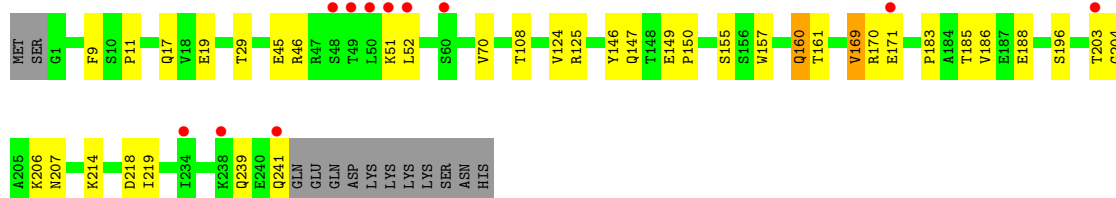
- Molecule 3: Proteasome subunit alpha type-4

Chain C: 



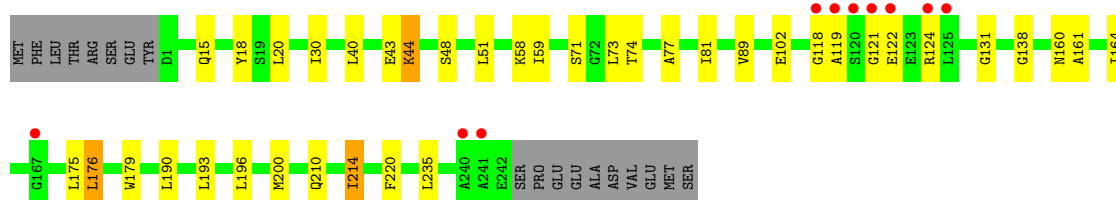
• Molecule 3: Proteasome subunit alpha type-4

Chain Q: 



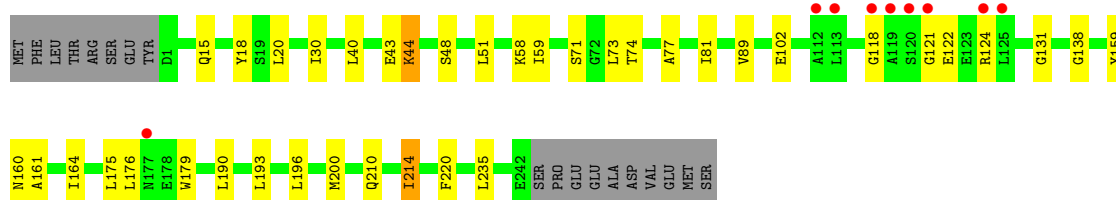
• Molecule 4: Proteasome subunit alpha type-5

Chain D: 



• Molecule 4: Proteasome subunit alpha type-5

Chain R: 



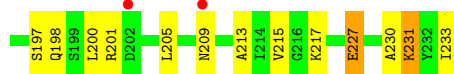
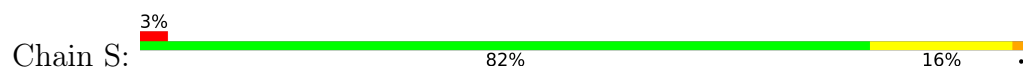
• Molecule 5: Proteasome subunit alpha type-6

Chain E: 

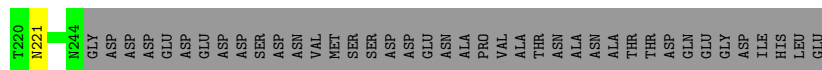
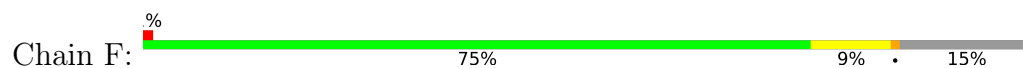




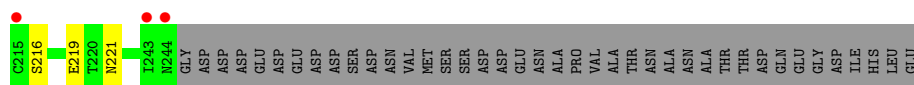
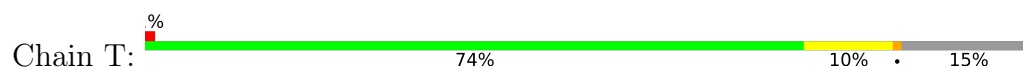
- Molecule 5: Proteasome subunit alpha type-6



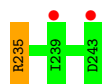
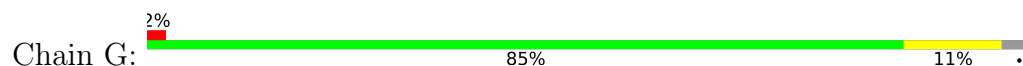
- Molecule 6: Probable proteasome subunit alpha type-7



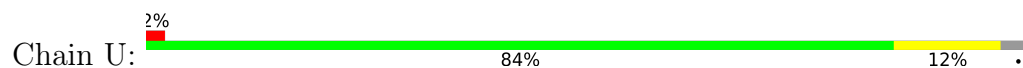
- Molecule 6: Probable proteasome subunit alpha type-7

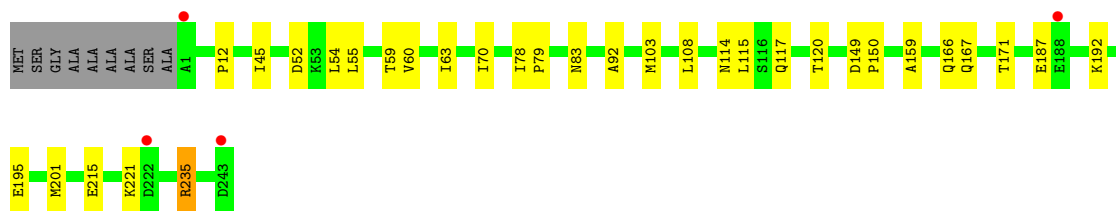


- Molecule 7: Proteasome subunit alpha type-1

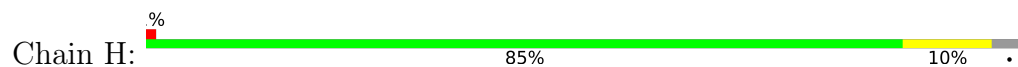


- Molecule 7: Proteasome subunit alpha type-1

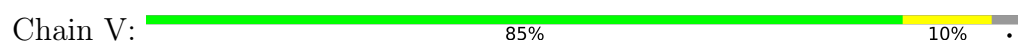




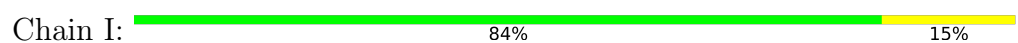
• Molecule 8: Proteasome subunit beta type-2



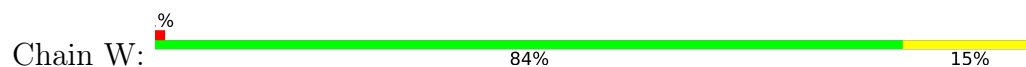
• Molecule 8: Proteasome subunit beta type-2



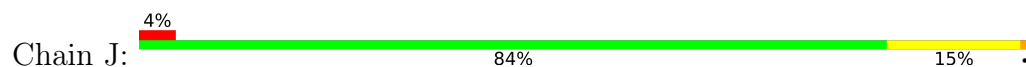
• Molecule 9: Proteasome subunit beta type-3



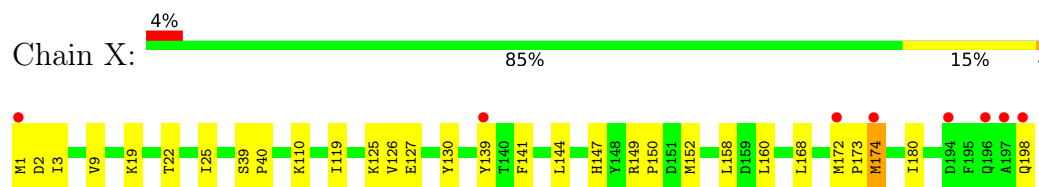
• Molecule 9: Proteasome subunit beta type-3



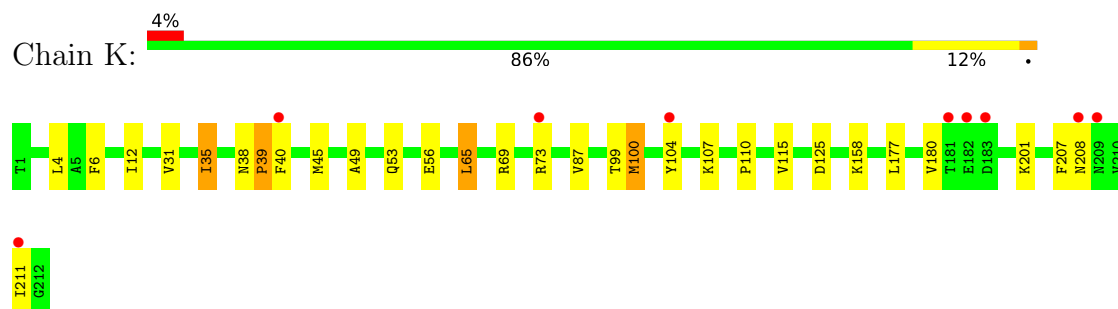
• Molecule 10: Proteasome subunit beta type-4



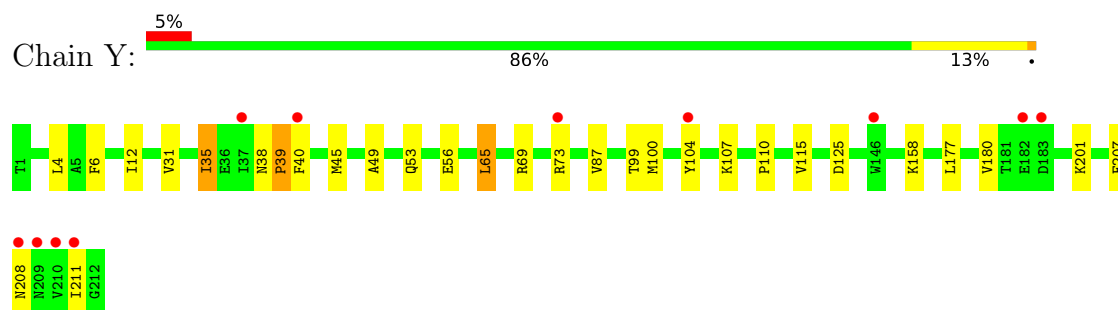
- Molecule 10: Proteasome subunit beta type-4



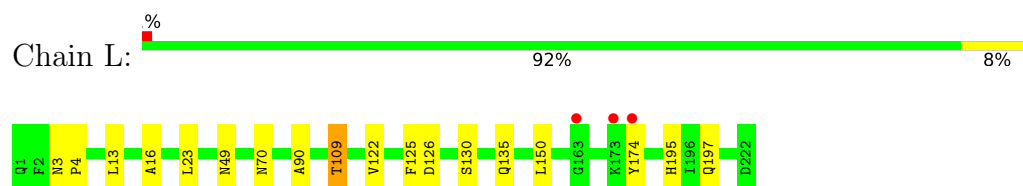
- Molecule 11: Proteasome subunit beta type-5



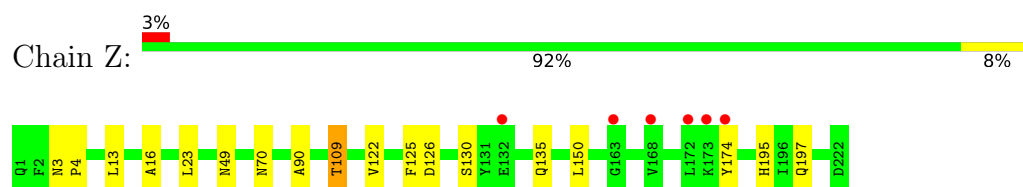
- Molecule 11: Proteasome subunit beta type-5



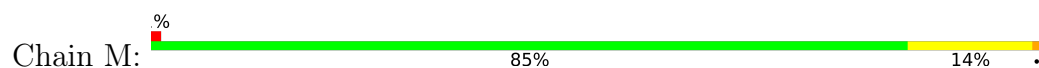
- Molecule 12: Proteasome subunit beta type-6

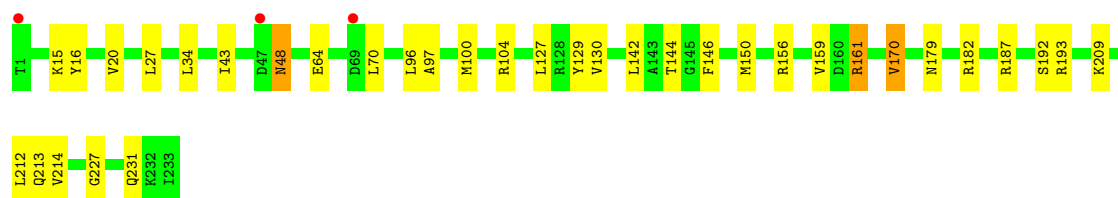


- Molecule 12: Proteasome subunit beta type-6



- Molecule 13: Proteasome subunit beta type-7





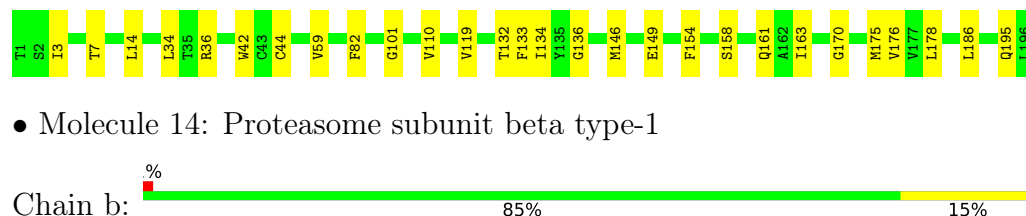
• Molecule 13: Proteasome subunit beta type-7

Chain a: 84% 15%



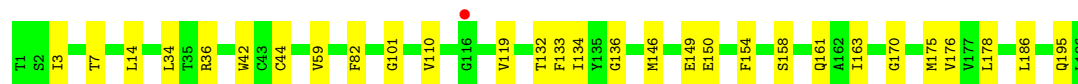
• Molecule 14: Proteasome subunit beta type-1

Chain N: 86% 14%



• Molecule 14: Proteasome subunit beta type-1

Chain b: 85% 15%



• Molecule 15: TMC-95A mimic ligand yCP:3a

Chain c: 25% 25% 12% 38%



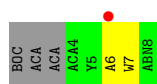
• Molecule 15: TMC-95A mimic ligand yCP:3a

Chain d: 25% 25% 12% 38%

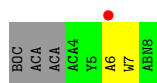


• Molecule 15: TMC-95A mimic ligand yCP:3a

Chain e: 12% 38% 25% 38%



- Molecule 15: TMC-95A mimic ligand yCP:3a



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.35Å 299.22Å 144.65Å 90.00° 112.97° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (15.00-2.90) 98.4 (15.00-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.221 , 0.227 (Not available) , 0.199	Depositor DCC
R_{free} test set	11475 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.2	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	0.92	EDS
Total number of atoms	51118	wwPDB-VP
Average B, all atoms (Å ²)	67.0	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: ABN, MES, TY5, ACA, RE0

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	0.48	0/1952	0.78	0/2642
1	O	0.48	0/1952	0.78	0/2642
2	B	0.46	0/1934	0.76	0/2618
2	P	0.46	0/1934	0.76	0/2618
3	C	0.47	0/1919	0.79	0/2598
3	Q	0.47	0/1919	0.79	0/2598
4	D	0.52	0/1886	0.77	0/2541
4	R	0.52	0/1886	0.76	0/2541
5	E	0.47	0/1823	0.76	2/2463 (0.1%)
5	S	0.47	0/1823	0.76	2/2463 (0.1%)
6	F	0.59	0/1936	0.83	0/2614
6	T	0.58	0/1936	0.82	0/2614
7	G	0.48	0/1959	0.76	0/2652
7	U	0.48	0/1959	0.76	0/2652
8	H	0.61	0/1715	0.75	0/2326
8	V	0.61	0/1715	0.75	0/2326
9	I	0.45	0/1611	0.76	0/2174
9	W	0.45	0/1611	0.76	0/2174
10	J	0.48	0/1613	0.76	0/2173
10	X	0.48	0/1613	0.76	0/2173
11	K	0.58	0/1681	0.77	0/2274
11	Y	0.58	0/1681	0.77	0/2274
12	L	0.50	0/1795	0.75	0/2420
12	Z	0.50	0/1795	0.75	0/2420
13	M	0.46	0/1855	0.75	0/2514
13	a	0.46	0/1855	0.75	0/2514
14	N	0.51	0/1541	0.75	0/2087
14	b	0.51	0/1541	0.76	0/2087
15	c	0.61	0/4	0.70	0/4
15	d	0.61	0/4	0.69	0/4
15	e	0.59	0/4	0.65	0/4
15	f	0.60	0/4	0.64	0/4

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.51	0/50456	0.77	4/68208 (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
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	147	GLN	CA-C-N	5.45	125.79	119.47
5	E	147	GLN	C-N-CA	5.45	125.79	119.47
5	S	147	GLN	CA-C-N	5.42	125.75	119.47
5	S	147	GLN	C-N-CA	5.42	125.75	119.47

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	e	6	ALA	Peptide
15	f	6	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	14	0
1	O	1915	0	1929	19	0
2	B	1904	0	1904	28	0
2	P	1904	0	1904	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1890	0	1903	29	0
3	Q	1890	0	1903	23	0
4	D	1861	0	1839	20	0
4	R	1861	0	1839	19	0
5	E	1795	0	1800	27	0
5	S	1795	0	1800	26	0
6	F	1896	0	1889	17	0
6	T	1896	0	1889	18	0
7	G	1921	0	1913	17	0
7	U	1921	0	1913	21	0
8	H	1684	0	1688	14	0
8	V	1684	0	1688	14	0
9	I	1581	0	1574	21	0
9	W	1581	0	1574	20	0
10	J	1585	0	1590	24	0
10	X	1585	0	1590	21	0
11	K	1644	0	1595	19	0
11	Y	1644	0	1595	18	0
12	L	1757	0	1711	11	0
12	Z	1757	0	1711	11	0
13	M	1824	0	1832	21	0
13	a	1824	0	1832	22	0
14	N	1512	0	1481	16	0
14	b	1512	0	1481	17	0
15	c	56	0	42	4	0
15	d	56	0	42	4	0
15	e	56	0	42	0	0
15	f	56	0	42	0	0
16	K	12	0	13	0	0
16	Y	12	0	13	0	0
17	A	58	0	0	0	0
17	B	40	0	0	0	0
17	C	40	0	0	0	0
17	D	37	0	0	0	0
17	E	22	0	0	0	0
17	F	47	0	0	0	0
17	G	58	0	0	0	0
17	H	53	0	0	0	0
17	I	62	0	0	0	0
17	J	53	0	0	2	0
17	K	49	0	0	0	0
17	L	58	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	M	75	0	0	0	0
17	N	57	0	0	0	0
17	O	33	0	0	0	0
17	P	29	0	0	0	0
17	Q	29	0	0	0	0
17	R	28	0	0	0	0
17	S	18	0	0	0	0
17	T	44	0	0	0	0
17	U	58	0	0	0	0
17	V	47	0	0	0	0
17	W	58	0	0	0	0
17	X	44	0	0	0	0
17	Y	46	0	0	0	0
17	Z	51	0	0	0	0
17	a	79	0	0	0	0
17	b	57	0	0	0	0
17	e	1	0	0	0	0
17	f	1	0	0	0	0
All	All	51118	0	49490	471	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 (471) 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)
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.55	0.88
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.57	0.86
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.57	0.86
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.55	0.86
10:J:174:MET:HE3	10:X:174:MET:HE3	1.58	0.85
1:O:12:PHE:H	2:P:20:GLN:HE22	1.29	0.80
2:B:12:PHE:H	3:C:17:GLN:HE22	1.28	0.79
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.50	0.76
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.51	0.75
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.50	0.75
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.51	0.75
2:B:122:THR:HG22	3:C:125:ARG:HH21	1.54	0.73
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.36	0.72
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.55	0.72
1:A:12:PHE:H	2:B:20:GLN:HE22	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.72	0.71
7:G:92:ALA:HA	7:G:103:MET:HE2	1.72	0.71
3:C:9:PHE:H	4:D:15:GLN:HE22	1.38	0.71
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.72	0.70
5:S:12:PHE:H	6:T:19:GLN:HE22	1.38	0.70
7:U:92:ALA:HA	7:U:103:MET:HE2	1.72	0.70
2:P:200:THR:HG22	2:P:202:SER:H	1.57	0.69
2:B:200:THR:HG22	2:B:202:SER:H	1.57	0.69
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.75	0.69
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.60	0.67
5:E:12:PHE:H	6:F:19:GLN:HE22	1.42	0.66
13:a:161:ARG:HG3	13:a:161:ARG:HH11	1.60	0.66
2:P:122:THR:HG22	3:Q:125:ARG:HH21	1.60	0.65
11:Y:45:MET:HB3	15:d:8:ABN:H3	1.79	0.64
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.28	0.64
11:K:31:VAL:HG11	15:c:8:ABN:C5	2.28	0.64
10:J:168:LEU:O	10:J:172:MET:HB2	1.99	0.63
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.47	0.63
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.45	0.63
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.64	0.62
10:J:139:TYR:OH	10:X:25:ILE:HG12	1.99	0.62
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.81	0.62
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.82	0.62
10:J:25:ILE:HG12	10:X:139:TYR:OH	1.99	0.62
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.82	0.62
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.48	0.62
3:Q:214:LYS:HB2	3:Q:218:ASP:HB3	1.82	0.62
4:R:73:LEU:HD12	4:R:131:GLY:HA3	1.82	0.62
10:X:168:LEU:O	10:X:172:MET:HB2	1.99	0.62
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.28	0.62
3:C:214:LYS:HB2	3:C:218:ASP:HB3	1.81	0.61
11:K:107:LYS:H	11:K:107:LYS:HD2	1.66	0.61
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.81	0.61
4:D:73:LEU:HD12	4:D:131:GLY:HA3	1.82	0.61
9:I:35:VAL:HG13	17:J:240:HOH:O	2.01	0.61
6:F:31:THR:HG21	6:F:47:GLU:O	2.01	0.61
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.82	0.61
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.83	0.61
4:D:119:ALA:HA	5:E:124:GLY:HA2	1.83	0.60
6:T:31:THR:HG21	6:T:47:GLU:O	2.01	0.60
11:Y:107:LYS:H	11:Y:107:LYS:HD2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:THR:HG21	3:C:169:VAL:HG13	1.84	0.60
12:Z:126:ASP:HB2	12:Z:130:SER:HB3	1.83	0.60
12:L:109:THR:HG23	12:L:125:PHE:HB2	1.82	0.60
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.83	0.60
13:a:127:LEU:HG	13:a:142:LEU:HD12	1.83	0.60
14:b:175:MET:HB2	14:b:186:LEU:HB2	1.83	0.59
7:G:195:GLU:HG3	7:G:235:ARG:HG3	1.83	0.59
12:L:195:HIS:HD2	12:L:197:GLN:H	1.51	0.59
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.84	0.59
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.84	0.59
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.84	0.59
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.83	0.59
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.84	0.59
11:Y:31:VAL:HG11	15:d:8:ABN:C5	2.32	0.58
15:c:5:TY5:H47	15:c:7:RE0:H18	1.83	0.58
2:B:63:GLU:HG3	2:B:64:LYS:HG3	1.86	0.58
10:J:3:ILE:HD13	10:J:168:LEU:HD13	1.85	0.58
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.50	0.58
3:C:155:SER:HB2	4:D:51:LEU:HD21	1.84	0.58
12:L:126:ASP:HB2	12:L:130:SER:HB3	1.84	0.58
8:H:35:HIS:CB	8:H:56:THR:HG21	2.34	0.58
10:X:3:ILE:HD13	10:X:168:LEU:HD13	1.86	0.58
12:Z:109:THR:HG23	12:Z:125:PHE:HB2	1.85	0.57
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.86	0.57
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.84	0.57
2:P:63:GLU:HG3	2:P:64:LYS:HG3	1.86	0.57
8:V:35:HIS:CB	8:V:56:THR:HG21	2.34	0.57
2:P:215:ILE:HG12	2:P:226:GLN:HG2	1.87	0.57
13:a:179:ASN:HD22	13:a:182:ARG:HH11	1.52	0.57
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.52	0.57
2:B:215:ILE:HG12	2:B:226:GLN:HG2	1.87	0.56
5:E:68:HIS:HE1	5:E:102:LEU:O	1.88	0.56
4:R:161:ALA:HB3	5:S:55:LEU:HD23	1.88	0.56
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.86	0.56
15:d:5:TY5:H47	15:d:7:RE0:H18	1.87	0.56
4:D:77:ALA:O	4:D:81:ILE:HG12	2.06	0.56
4:R:77:ALA:O	4:R:81:ILE:HG12	2.06	0.56
1:O:83:ARG:HE	7:U:114:ASN:HD21	1.53	0.55
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.89	0.55
10:J:119:ILE:HG12	10:J:125:LYS:HG3	1.88	0.55
5:E:205:LEU:HA	5:E:209:ASN:HD22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.89	0.54
5:S:68:HIS:HE1	5:S:102:LEU:O	1.88	0.54
10:X:119:ILE:HG12	10:X:125:LYS:HG3	1.88	0.54
11:Y:158:LYS:HB2	11:Y:177:LEU:HD11	1.90	0.54
2:B:35:ILE:HD12	2:B:196:LEU:HG	1.88	0.54
11:K:208:ASN:HD21	10:X:150:PRO:HG3	1.73	0.54
9:W:94:LEU:HD11	9:W:106:PRO:HG2	1.90	0.54
2:P:35:ILE:HD12	2:P:196:LEU:HG	1.88	0.54
5:S:205:LEU:HA	5:S:209:ASN:HD22	1.72	0.54
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.90	0.54
2:P:183:MET:HE1	2:P:191:LEU:HD12	1.89	0.54
11:K:73:ARG:NH2	11:K:104:TYR:O	2.41	0.53
2:P:75:ALA:HB3	2:P:135:ILE:HB	1.90	0.53
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.41	0.53
12:Z:135:GLN:HG3	12:Z:174:TYR:OH	2.08	0.53
3:Q:157:TRP:CE2	4:R:51:LEU:HD23	2.43	0.53
1:A:83:ARG:HE	7:G:114:ASN:HD21	1.56	0.53
7:U:63:ILE:HD12	7:U:215:GLU:HG2	1.90	0.53
13:a:27:LEU:HB2	13:a:192:SER:HB2	1.90	0.53
2:B:75:ALA:HB3	2:B:135:ILE:HB	1.90	0.53
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.39	0.53
8:H:35:HIS:HB2	8:H:56:THR:HG21	1.89	0.53
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.39	0.53
2:B:183:MET:HE1	2:B:191:LEU:HD12	1.89	0.53
12:L:135:GLN:HG3	12:L:174:TYR:OH	2.08	0.53
1:O:83:ARG:HE	7:U:114:ASN:ND2	2.06	0.53
6:T:91:GLU:HG3	6:T:111:ARG:HH11	1.74	0.53
8:V:35:HIS:HB2	8:V:56:THR:HG21	1.89	0.53
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.91	0.52
1:A:55:LEU:HD12	7:G:170:THR:HG23	1.90	0.52
13:M:27:LEU:HB2	13:M:192:SER:HB2	1.90	0.52
10:J:39:SER:HB2	10:J:40:PRO:HD2	1.92	0.52
6:T:32:THR:HG22	6:T:47:GLU:OE2	2.10	0.52
7:G:63:ILE:HD12	7:G:215:GLU:HG2	1.90	0.52
11:K:158:LYS:HB2	11:K:177:LEU:HD11	1.91	0.52
13:a:48:ASN:H	13:a:48:ASN:HD22	1.57	0.52
6:F:32:THR:HG22	6:F:47:GLU:OE2	2.09	0.52
10:J:150:PRO:HG3	11:Y:208:ASN:HD21	1.74	0.52
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.75	0.52
2:B:3:ARG:HB2	5:E:122:TYR:OH	2.10	0.52
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.91	0.52
13:M:48:ASN:H	13:M:48:ASN:HD22	1.57	0.52
4:R:44:LYS:HE3	4:R:210:GLN:HB2	1.92	0.52
13:a:15:LYS:HB3	13:a:20:VAL:HG12	1.92	0.52
3:C:204:GLY:HA3	3:C:207:ASN:HB2	1.92	0.51
4:D:44:LYS:HE3	4:D:210:GLN:HB2	1.92	0.51
9:I:28:LEU:HB3	9:I:36:SER:HB3	1.92	0.51
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.45	0.51
11:K:45:MET:HB3	15:c:8:ABN:H3	1.91	0.51
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.45	0.51
10:J:139:TYR:HD1	17:J:226:HOH:O	1.94	0.51
6:F:91:GLU:HG3	6:F:111:ARG:HH11	1.75	0.51
5:S:127:TYR:O	5:S:148:PRO:HB3	2.09	0.51
10:X:39:SER:HB2	10:X:40:PRO:HD2	1.92	0.51
5:E:127:TYR:O	5:E:148:PRO:HB3	2.10	0.51
11:K:38:ASN:HB2	11:K:39:PRO:HD2	1.93	0.51
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.93	0.51
1:A:30:GLN:HE21	1:A:30:GLN:HA	1.75	0.51
4:D:59:ILE:HG22	4:D:220:PHE:HZ	1.76	0.51
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.75	0.51
7:G:78:ILE:N	7:G:79:PRO:HD2	2.26	0.51
10:X:149:ARG:HB2	10:X:152:MET:HG3	1.93	0.51
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	1.93	0.51
3:Q:155:SER:HB2	4:R:51:LEU:HD21	1.93	0.50
8:H:165:ASN:HD22	13:a:156:ARG:HH11	1.59	0.50
1:O:30:GLN:HA	1:O:30:GLN:HE21	1.76	0.50
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.93	0.50
5:S:9:THR:HG21	5:S:119:THR:HA	1.94	0.50
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.93	0.50
2:P:57:GLU:O	2:P:61:SER:HB2	2.11	0.50
2:B:57:GLU:O	2:B:61:SER:HB2	2.11	0.50
13:M:15:LYS:HB3	13:M:20:VAL:HG12	1.92	0.50
9:W:28:LEU:HB3	9:W:36:SER:HB3	1.93	0.50
4:R:59:ILE:HG22	4:R:220:PHE:HZ	1.76	0.50
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.94	0.50
5:E:9:THR:HG21	5:E:119:THR:HA	1.93	0.50
7:U:78:ILE:N	7:U:79:PRO:HD2	2.26	0.50
5:E:205:LEU:H	5:E:205:LEU:HD23	1.77	0.50
5:S:205:LEU:HD23	5:S:205:LEU:H	1.77	0.50
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.47	0.49
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:204:GLY:HA3	3:Q:207:ASN:HB2	1.92	0.49
9:I:52:ILE:HB	9:I:59:VAL:HG13	1.94	0.49
10:J:149:ARG:HB2	10:J:152:MET:HG3	1.93	0.49
4:D:89:VAL:HG21	11:K:65:LEU:HD13	1.94	0.49
3:Q:239:GLN:C	3:Q:241:GLN:H	2.21	0.49
5:S:231:LYS:H	5:S:231:LYS:HD2	1.78	0.49
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.95	0.49
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.24	0.49
3:C:185:THR:HB	3:C:188:GLU:HG2	1.94	0.49
5:S:197:SER:HA	5:S:200:LEU:HG	1.95	0.49
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.95	0.49
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.61	0.49
5:E:231:LYS:H	5:E:231:LYS:HD2	1.78	0.49
13:a:227:GLY:HA3	13:a:231:GLN:HB3	1.95	0.49
4:D:176:LEU:HD22	5:E:55:LEU:HD13	1.95	0.48
6:T:201:GLU:O	6:T:204:LYS:HD2	2.13	0.48
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.61	0.48
3:Q:186:VAL:HG21	3:Q:214:LYS:HE2	1.95	0.48
5:S:80:ALA:HB2	5:S:129:VAL:HG21	1.95	0.48
5:S:155:LEU:HD23	6:T:55:LEU:HA	1.95	0.48
5:S:200:LEU:HD11	5:S:205:LEU:HD22	1.95	0.48
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.94	0.48
8:V:210:THR:HG21	9:W:167:SER:HB3	1.94	0.48
1:A:83:ARG:HE	7:G:114:ASN:ND2	2.11	0.48
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.94	0.48
10:X:147:HIS:HB2	10:X:160:LEU:HD11	1.95	0.48
5:E:193:VAL:HG13	5:E:205:LEU:HD11	1.95	0.48
11:K:35:ILE:HG21	11:K:56:GLU:HB3	1.96	0.48
6:F:31:THR:HG23	6:F:47:GLU:HB3	1.95	0.48
13:M:129:TYR:HE1	13:M:144:THR:HG22	1.78	0.48
3:C:186:VAL:HG21	3:C:214:LYS:HE2	1.95	0.48
5:E:197:SER:HA	5:E:200:LEU:HG	1.94	0.48
5:E:200:LEU:HD11	5:E:205:LEU:HD22	1.95	0.48
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.96	0.48
13:M:227:GLY:HA3	13:M:231:GLN:HB3	1.95	0.48
14:N:146:MET:HE1	14:N:154:PHE:HB2	1.96	0.48
2:P:180:LYS:HG3	2:P:183:MET:HG3	1.95	0.48
14:b:146:MET:HE1	14:b:154:PHE:HB2	1.96	0.48
3:Q:46:ARG:HD2	3:Q:206:LYS:O	2.14	0.48
4:R:89:VAL:HG21	11:Y:65:LEU:HD13	1.95	0.48
13:a:193:ARG:HG3	13:a:214:VAL:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:LYS:HG3	2:B:183:MET:HG3	1.96	0.48
11:K:99:THR:HG22	11:K:115:VAL:O	2.14	0.48
5:S:193:VAL:HG13	5:S:205:LEU:HD11	1.96	0.48
9:I:36:SER:HB2	10:J:126:VAL:HG21	1.96	0.47
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.61	0.47
5:E:80:ALA:HB2	5:E:129:VAL:HG21	1.95	0.47
3:Q:46:ARG:HB2	3:Q:207:ASN:HA	1.96	0.47
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.96	0.47
3:C:239:GLN:C	3:C:241:GLN:H	2.20	0.47
6:T:31:THR:HG23	6:T:47:GLU:HB3	1.95	0.47
9:W:10:ILE:HD11	9:W:174:ALA:HB2	1.96	0.47
13:a:129:TYR:HE1	13:a:144:THR:HG22	1.78	0.47
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.49	0.47
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.96	0.47
11:Y:201:LYS:HG3	11:Y:207:PHE:HB2	1.97	0.47
10:J:147:HIS:HB2	10:J:160:LEU:HD11	1.95	0.47
3:C:46:ARG:HD2	3:C:206:LYS:O	2.14	0.47
9:I:10:ILE:HD11	9:I:174:ALA:HB2	1.95	0.47
9:I:14:MET:HB3	9:I:162:LEU:HD11	1.97	0.47
11:K:201:LYS:HG3	11:K:207:PHE:HB2	1.97	0.47
13:M:193:ARG:HG3	13:M:214:VAL:HB	1.96	0.47
2:P:236:ASP:O	2:P:240:LYS:HG2	2.15	0.47
9:W:14:MET:HB3	9:W:162:LEU:HD11	1.97	0.47
11:Y:35:ILE:HG21	11:Y:56:GLU:HB3	1.96	0.47
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.49	0.47
3:Q:70:VAL:HG13	3:Q:219:ILE:HD13	1.97	0.47
8:V:4:VAL:HG22	8:V:159:ILE:HD11	1.97	0.47
7:G:103:MET:HE3	7:G:108:LEU:HB2	1.97	0.47
13:M:16:TYR:CE2	13:M:170:VAL:HG22	2.50	0.47
1:O:55:LEU:HB3	7:U:159:ALA:O	2.15	0.47
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.97	0.47
2:B:236:ASP:O	2:B:240:LYS:HG2	2.15	0.46
5:E:155:LEU:HD23	6:F:55:LEU:HA	1.96	0.46
8:H:210:THR:HG21	9:I:167:SER:HB3	1.96	0.46
7:U:103:MET:HE3	7:U:108:LEU:HB2	1.97	0.46
1:A:68:THR:HB	1:A:69:PRO:HD2	1.97	0.46
14:N:34:LEU:HD13	14:N:176:VAL:HG23	1.98	0.46
1:O:68:THR:HB	1:O:69:PRO:HD2	1.97	0.46
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.13	0.46
5:S:230:ALA:HA	5:S:233:ILE:HD12	1.98	0.46
9:W:36:SER:HB2	10:X:126:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.97	0.46
9:W:62:LEU:HD11	9:W:104:VAL:HG21	1.98	0.46
3:C:46:ARG:HB2	3:C:207:ASN:HA	1.96	0.46
10:J:152:MET:HE1	10:J:160:LEU:HD22	1.98	0.46
10:J:173:PRO:HB3	10:X:22:THR:HG21	1.98	0.46
1:O:158:PRO:HB2	2:P:57:GLU:HB3	1.97	0.46
1:A:110:LEU:O	1:A:114:VAL:HG23	2.16	0.46
13:M:96:LEU:O	13:M:100:MET:HG2	2.16	0.46
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.97	0.46
1:O:110:LEU:O	1:O:114:VAL:HG23	2.16	0.46
5:S:131:LEU:HB2	5:S:146:PHE:HB3	1.97	0.46
8:V:50:ALA:HB2	9:W:128:CYS:HB2	1.97	0.46
5:E:49:LYS:HB3	5:E:58:TYR:HB3	1.98	0.46
5:E:131:LEU:HB2	5:E:146:PHE:HB3	1.97	0.46
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.81	0.46
11:Y:99:THR:HG22	11:Y:115:VAL:O	2.14	0.46
5:E:230:ALA:HA	5:E:233:ILE:HD12	1.98	0.45
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.81	0.45
10:X:19:LYS:HD3	10:X:180:ILE:HG13	1.99	0.45
13:a:16:TYR:CE2	13:a:170:VAL:HG22	2.51	0.45
7:G:103:MET:HE3	7:G:108:LEU:HD13	1.98	0.45
3:C:108:THR:HG21	3:C:146:TYR:HB3	1.98	0.45
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.96	0.45
13:M:179:ASN:HD22	13:M:182:ARG:NH1	2.15	0.45
5:S:227:GLU:CD	5:S:227:GLU:H	2.25	0.45
6:T:52:SER:H	6:T:55:LEU:HD13	1.80	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.45
1:A:119:GLN:O	1:A:122:THR:HB	2.16	0.45
4:D:43:GLU:HG3	4:D:200:MET:HE3	1.99	0.45
6:F:52:SER:H	6:F:55:LEU:HD13	1.80	0.45
10:X:152:MET:HE1	10:X:160:LEU:HD22	1.98	0.45
11:Y:38:ASN:C	11:Y:40:PHE:H	2.25	0.45
13:a:96:LEU:O	13:a:100:MET:HG2	2.16	0.45
6:F:201:GLU:O	6:F:204:LYS:HD2	2.16	0.45
14:b:101:GLY:HA2	14:b:178:LEU:HD23	1.98	0.45
3:C:70:VAL:HG13	3:C:219:ILE:HD13	1.97	0.45
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.99	0.45
11:K:38:ASN:O	11:K:40:PHE:N	2.49	0.45
4:R:43:GLU:HG3	4:R:200:MET:HE3	1.99	0.45
7:U:103:MET:HE3	7:U:108:LEU:HD13	1.98	0.45
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.45
10:J:22:THR:HG21	10:X:173:PRO:HB3	1.97	0.45
14:b:14:LEU:O	14:b:175:MET:HA	2.17	0.45
14:b:34:LEU:HD13	14:b:176:VAL:HG23	1.99	0.45
10:J:19:LYS:HD3	10:J:180:ILE:HG13	1.99	0.45
11:K:38:ASN:C	11:K:40:PHE:H	2.25	0.45
2:P:69:ASN:HB3	2:P:72:ILE:H	1.82	0.45
5:S:49:LYS:HB3	5:S:58:TYR:HB3	1.99	0.45
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.13	0.45
3:C:157:TRP:CZ3	4:D:48:SER:HB3	2.51	0.44
14:N:14:LEU:O	14:N:175:MET:HA	2.17	0.44
13:M:150:MET:HE1	13:M:187:ARG:HG3	1.99	0.44
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.52	0.44
2:P:18:LEU:HD13	2:P:122:THR:HG23	1.99	0.44
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.99	0.44
6:T:49:LEU:HD22	6:T:206:LYS:HB2	1.99	0.44
3:C:149:GLU:HB2	3:C:150:PRO:HD2	1.98	0.44
11:K:31:VAL:HG11	15:c:8:ABN:H5	1.99	0.44
1:O:21:ILE:HD11	1:O:122:THR:HG21	2.00	0.44
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.99	0.44
9:W:33:LEU:HD11	10:X:141:PHE:HD2	1.81	0.44
11:Y:38:ASN:O	11:Y:40:PHE:N	2.50	0.44
2:B:99:LYS:HG3	9:I:64:GLU:HB3	1.98	0.44
9:I:62:LEU:HD11	9:I:104:VAL:HG21	1.98	0.44
14:N:101:GLY:HA2	14:N:178:LEU:HD23	1.98	0.44
13:a:209:LYS:HB3	13:a:212:LEU:HD11	1.99	0.44
2:B:18:LEU:HD13	2:B:122:THR:HG23	1.99	0.44
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.66	0.44
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	1.98	0.44
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.99	0.44
1:A:26:THR:O	1:A:30:GLN:HG2	2.18	0.44
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.99	0.44
9:I:33:LEU:HD11	10:J:141:PHE:HD2	1.82	0.44
13:M:209:LYS:HB3	13:M:212:LEU:HD11	1.99	0.44
1:O:119:GLN:O	1:O:122:THR:HB	2.16	0.44
6:T:118:ALA:HA	6:T:121:LEU:HD12	1.99	0.44
5:E:227:GLU:CD	5:E:227:GLU:H	2.25	0.44
13:a:150:MET:HE1	13:a:187:ARG:HG3	2.00	0.44
3:C:29:THR:HB	3:C:45:GLU:HG3	2.00	0.44
11:K:6:PHE:HA	11:K:125:ASP:O	2.18	0.44
6:F:118:ALA:HA	6:F:121:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ILE:HD11	1:A:122:THR:HG21	2.00	0.43
5:E:134:ILE:HD12	5:E:215:VAL:HG12	2.00	0.43
6:F:49:LEU:HD22	6:F:206:LYS:HB2	1.99	0.43
6:T:158:GLY:O	7:U:54:LEU:HB3	2.18	0.43
8:V:148:LYS:HE3	8:V:177:VAL:HG11	1.99	0.43
10:J:1:MET:HG2	10:J:2:ASP:N	2.33	0.43
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.66	0.43
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.00	0.43
1:O:21:ILE:HD11	1:O:122:THR:CG2	2.49	0.43
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.54	0.43
5:S:134:ILE:HD12	5:S:215:VAL:HG12	2.00	0.43
12:L:90:ALA:HA	12:L:125:PHE:HZ	1.84	0.43
14:N:7:THR:HG23	14:N:110:VAL:HG23	2.00	0.43
8:V:84:LYS:HG3	8:V:85:GLN:N	2.32	0.43
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.18	0.43
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	1.99	0.43
5:S:205:LEU:HA	5:S:209:ASN:ND2	2.34	0.43
1:A:21:ILE:HD11	1:A:122:THR:CG2	2.48	0.43
2:B:69:ASN:HB3	2:B:72:ILE:H	1.82	0.43
2:B:196:LEU:O	2:B:200:THR:OG1	2.35	0.43
6:F:66:VAL:HG11	6:F:108:PHE:CE1	2.53	0.43
8:H:148:LYS:HE3	8:H:177:VAL:HG11	1.99	0.43
1:O:26:THR:O	1:O:30:GLN:HG2	2.18	0.43
8:H:84:LYS:HG3	8:H:85:GLN:N	2.32	0.43
10:X:1:MET:HG2	10:X:2:ASP:N	2.34	0.43
13:a:161:ARG:HG3	13:a:161:ARG:NH1	2.32	0.43
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.54	0.43
6:T:66:VAL:HG11	6:T:108:PHE:CE1	2.53	0.43
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.54	0.43
6:T:155:GLY:HA3	7:U:59:THR:HG21	2.01	0.43
10:J:158:LEU:HD13	10:J:198:GLN:HE22	1.84	0.43
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.99	0.43
5:E:205:LEU:HA	5:E:209:ASN:ND2	2.33	0.42
6:F:158:GLY:O	7:G:54:LEU:HB3	2.19	0.42
9:I:148:MET:HE2	9:I:172:ASN:HB2	2.00	0.42
11:K:100:MET:HE2	11:K:100:MET:HB2	1.88	0.42
3:Q:29:THR:HB	3:Q:45:GLU:HG3	2.00	0.42
7:U:149:ASP:HB2	7:U:150:PRO:HD2	2.00	0.42
12:Z:90:ALA:HA	12:Z:125:PHE:HZ	1.83	0.42
14:b:7:THR:HG23	14:b:110:VAL:HG23	2.01	0.42
14:b:59:VAL:HG11	14:b:82:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:98:PHE:O	13:a:91:TYR:HA	2.19	0.42
6:F:34:ILE:HG12	6:F:196:ILE:HD11	2.01	0.42
2:P:99:LYS:HG3	9:W:64:GLU:HB3	2.00	0.42
11:Y:45:MET:CB	15:d:8:ABN:H3	2.48	0.42
3:C:92:GLN:HG3	10:J:66:LEU:HB2	2.01	0.42
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.02	0.42
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.54	0.42
13:a:1:THR:N	13:a:107:MET:O	2.50	0.42
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.54	0.42
8:H:50:ALA:HB2	9:I:128:CYS:HB2	2.01	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.42
14:b:163:ILE:HG23	14:b:170:GLY:HA2	2.02	0.42
2:B:47:ALA:HB1	2:B:64:LYS:HD3	2.02	0.42
7:G:149:ASP:HB2	7:G:150:PRO:HD2	2.00	0.42
14:N:59:VAL:HG11	14:N:82:PHE:CE2	2.55	0.42
4:R:161:ALA:HB1	4:R:175:LEU:HD22	2.02	0.42
3:C:155:SER:CB	4:D:51:LEU:HD21	2.49	0.42
6:F:8:ASN:HB3	6:F:123:ASN:HA	2.01	0.42
11:K:12:ILE:HB	11:K:180:VAL:HB	2.02	0.42
2:P:47:ALA:HB1	2:P:64:LYS:HD3	2.02	0.42
2:P:223:GLU:HG2	2:P:224:VAL:H	1.85	0.42
2:P:223:GLU:HG2	2:P:224:VAL:N	2.35	0.42
5:S:62:ILE:HG21	5:S:213:ALA:HB2	2.02	0.42
10:X:158:LEU:HD13	10:X:198:GLN:HE22	1.84	0.42
13:a:179:ASN:HD22	13:a:182:ARG:NH1	2.15	0.42
2:B:223:GLU:HG2	2:B:224:VAL:N	2.35	0.42
5:E:62:ILE:HG21	5:E:213:ALA:HB2	2.02	0.42
7:G:52:ASP:HB3	7:G:55:LEU:HG	2.02	0.42
9:W:148:MET:HE2	9:W:172:ASN:HB2	2.00	0.42
11:Y:104:TYR:CE2	11:Y:110:PRO:HG3	2.55	0.42
6:T:34:ILE:HG12	6:T:196:ILE:HD11	2.01	0.42
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.00	0.41
4:D:161:ALA:HB1	4:D:175:LEU:HD22	2.01	0.41
5:E:12:PHE:HB2	6:F:19:GLN:HE22	1.84	0.41
1:O:64:VAL:HG11	1:O:212:ALA:HB3	2.02	0.41
9:I:36:SER:CB	10:J:126:VAL:HG21	2.50	0.41
14:N:133:PHE:HA	14:b:132:THR:O	2.20	0.41
14:N:163:ILE:HG23	14:N:170:GLY:HA2	2.02	0.41
3:Q:157:TRP:CZ3	4:R:48:SER:HB3	2.56	0.41
10:X:130:TYR:HB2	10:X:144:LEU:HD13	2.02	0.41
13:M:129:TYR:CE1	13:M:144:THR:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:3:ILE:HB	14:N:44:CYS:HB3	2.02	0.41
7:U:70:ILE:HG21	7:U:108:LEU:HD23	2.02	0.41
13:a:43:ILE:HG12	13:a:64:GLU:HG2	2.02	0.41
5:E:92:ASN:HD22	5:E:92:ASN:HA	1.73	0.41
4:R:71:SER:HB3	4:R:164:ILE:HD12	2.03	0.41
2:B:223:GLU:HG2	2:B:224:VAL:H	1.85	0.41
11:K:104:TYR:CE2	11:K:110:PRO:HG3	2.55	0.41
13:M:161:ARG:HG3	13:M:161:ARG:NH1	2.32	0.41
13:M:213:GLN:HE21	13:M:213:GLN:HB3	1.69	0.41
3:C:11:PRO:HA	4:D:18:TYR:CD1	2.55	0.41
4:D:58:LYS:HE2	4:D:74:THR:HG21	2.03	0.41
10:J:130:TYR:HB2	10:J:144:LEU:HD13	2.02	0.41
14:N:134:ILE:HG21	14:N:158:SER:O	2.21	0.41
2:P:95:GLN:HE21	9:W:68:TYR:HA	1.86	0.41
7:U:52:ASP:HB3	7:U:55:LEU:HG	2.03	0.41
8:V:3:ILE:HG22	8:V:16:ALA:HB2	2.02	0.41
11:Y:49:ALA:O	11:Y:53:GLN:HB2	2.21	0.41
14:b:3:ILE:HB	14:b:44:CYS:HB3	2.02	0.41
11:K:49:ALA:O	11:K:53:GLN:HB2	2.21	0.41
4:R:58:LYS:HE2	4:R:74:THR:HG21	2.03	0.41
8:H:3:ILE:HG22	8:H:16:ALA:HB2	2.03	0.40
9:I:7:ASN:HA	9:I:29:GLY:O	2.22	0.40
13:M:43:ILE:HG12	13:M:64:GLU:HG2	2.03	0.40
9:W:141:ALA:HB2	9:W:177:ASP:HB2	2.03	0.40
13:a:129:TYR:CE1	13:a:144:THR:HG22	2.54	0.40
1:A:64:VAL:HG11	1:A:212:ALA:HB3	2.02	0.40
4:D:71:SER:HB3	4:D:164:ILE:HD12	2.03	0.40
7:G:70:ILE:HG21	7:G:108:LEU:HD23	2.02	0.40
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.40
9:I:62:LEU:CD1	9:I:104:VAL:HG21	2.51	0.40
10:J:173:PRO:HB2	10:X:174:MET:HE1	2.02	0.40
14:N:132:THR:O	14:b:133:PHE:HA	2.21	0.40
5:S:42:HIS:HB2	5:S:188:LEU:HD12	2.04	0.40
6:T:8:ASN:HB3	6:T:123:ASN:HA	2.01	0.40
9:W:62:LEU:CD1	9:W:104:VAL:HG21	2.51	0.40
14:b:134:ILE:HG21	14:b:158:SER:O	2.21	0.40
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.57	0.40
2:B:148:TYR:OH	3:C:57:ILE:HB	2.22	0.40
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.03	0.40
10:J:174:MET:HE1	10:X:173:PRO:HB2	2.02	0.40
9:W:111:ILE:HG21	9:W:191:LYS:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:146:MET:HE2	14:b:150:GLU:HB3	2.04	0.40
1:O:49:LYS:HG3	1:O:210:GLU:HB2	2.03	0.40
1:O:66:LEU:HD12	1:O:235:PHE:CD2	2.57	0.40
7:U:117:GLN:O	7:U:120:THR:HB	2.22	0.40
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	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%)	242 (98%)	4 (2%)	2 (1%)	16	44
1	O	248/250 (99%)	242 (98%)	4 (2%)	2 (1%)	16	44
2	B	242/258 (94%)	230 (95%)	10 (4%)	2 (1%)	16	44
2	P	242/258 (94%)	230 (95%)	10 (4%)	2 (1%)	16	44
3	C	239/254 (94%)	229 (96%)	7 (3%)	3 (1%)	9	32
3	Q	239/254 (94%)	230 (96%)	6 (2%)	3 (1%)	9	32
4	D	240/260 (92%)	231 (96%)	6 (2%)	3 (1%)	9	32
4	R	240/260 (92%)	230 (96%)	7 (3%)	3 (1%)	9	32
5	E	231/234 (99%)	221 (96%)	8 (4%)	2 (1%)	14	41
5	S	231/234 (99%)	221 (96%)	8 (4%)	2 (1%)	14	41
6	F	242/288 (84%)	235 (97%)	7 (3%)	0	100	100
6	T	242/288 (84%)	235 (97%)	7 (3%)	0	100	100
7	G	241/252 (96%)	233 (97%)	8 (3%)	0	100	100
7	U	241/252 (96%)	233 (97%)	8 (3%)	0	100	100
8	H	220/232 (95%)	212 (96%)	8 (4%)	0	100	100
8	V	220/232 (95%)	212 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	196/198 (99%)	189 (96%)	6 (3%)	1 (0%)	24	54
10	X	196/198 (99%)	189 (96%)	6 (3%)	1 (0%)	24	54
11	K	210/212 (99%)	203 (97%)	6 (3%)	1 (0%)	24	54
11	Y	210/212 (99%)	203 (97%)	6 (3%)	1 (0%)	24	54
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	231/233 (99%)	222 (96%)	9 (4%)	0	100	100
13	a	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
15	c	1/8 (12%)	1 (100%)	0	0	100	100
15	d	1/8 (12%)	1 (100%)	0	0	100	100
15	e	1/8 (12%)	1 (100%)	0	0	100	100
15	f	1/8 (12%)	1 (100%)	0	0	100	100
All	All	6316/6620 (95%)	6084 (96%)	204 (3%)	28 (0%)	30	59

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	52	LEU
3	Q	52	LEU
1	A	166	LYS
5	E	201	ARG
11	K	39	PRO
1	O	166	LYS
5	S	201	ARG
11	Y	39	PRO
1	A	2	THR
2	B	221	ASP
4	D	121	GLY
4	D	122	GLU
1	O	2	THR
2	P	221	ASP
4	R	121	GLY

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Mol	Chain	Res	Type
4	R	122	GLU
2	B	51	VAL
3	C	183	PRO
3	C	203	THR
5	E	217	LYS
2	P	51	VAL
3	Q	183	PRO
3	Q	203	THR
5	S	217	LYS
4	D	118	GLY
4	R	118	GLY
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%)	205 (98%)	4 (2%)	50	79
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	79
2	B	203/216 (94%)	199 (98%)	4 (2%)	48	78
2	P	203/216 (94%)	199 (98%)	4 (2%)	48	78
3	C	213/226 (94%)	207 (97%)	6 (3%)	38	72
3	Q	213/226 (94%)	207 (97%)	6 (3%)	38	72
4	D	198/215 (92%)	188 (95%)	10 (5%)	21	53
4	R	198/215 (92%)	188 (95%)	10 (5%)	21	53
5	E	192/193 (100%)	184 (96%)	8 (4%)	26	60
5	S	192/193 (100%)	184 (96%)	8 (4%)	26	60
6	F	201/239 (84%)	192 (96%)	9 (4%)	24	58
6	T	201/239 (84%)	192 (96%)	9 (4%)	24	58
7	G	207/210 (99%)	200 (97%)	7 (3%)	32	66
7	U	207/210 (99%)	200 (97%)	7 (3%)	32	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	181/190 (95%)	178 (98%)	3 (2%)	53	82
8	V	181/190 (95%)	178 (98%)	3 (2%)	53	82
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	82
9	W	172/173 (99%)	169 (98%)	3 (2%)	53	82
10	J	175/175 (100%)	172 (98%)	3 (2%)	53	82
10	X	175/175 (100%)	172 (98%)	3 (2%)	53	82
11	K	169/169 (100%)	162 (96%)	7 (4%)	27	61
11	Y	169/169 (100%)	162 (96%)	7 (4%)	27	61
12	L	185/185 (100%)	182 (98%)	3 (2%)	55	83
12	Z	185/185 (100%)	182 (98%)	3 (2%)	55	83
13	M	199/199 (100%)	192 (96%)	7 (4%)	32	66
13	a	199/199 (100%)	192 (96%)	7 (4%)	32	66
14	N	162/162 (100%)	159 (98%)	3 (2%)	50	79
14	b	162/162 (100%)	159 (98%)	3 (2%)	50	79
All	All	5332/5522 (97%)	5178 (97%)	154 (3%)	37	71

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	59	GLU
1	A	61	LEU
1	A	157	PHE
2	B	55	LEU
2	B	60	THR
2	B	149	THR
2	B	191	LEU
3	C	19	GLU
3	C	51	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	171	GLU
4	D	20	LEU
4	D	40	LEU
4	D	44	LYS
4	D	102	GLU

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Mol	Chain	Res	Type
4	D	124	ARG
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
5	E	9	THR
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	188	LEU
5	E	198	GLN
5	E	227	GLU
5	E	231	LYS
6	F	7	SER
6	F	31	THR
6	F	39	ASN
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	186	ARG
6	F	201	GLU
6	F	221	ASN
7	G	45	ILE
7	G	83	ASN
7	G	115	LEU
7	G	166	GLN
7	G	201	MET
7	G	221	LYS
7	G	235	ARG
8	H	34	LEU
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	110	LYS
10	J	127	GLU
10	J	174	MET
11	K	4	LEU
11	K	35	ILE
11	K	65	LEU

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Mol	Chain	Res	Type
11	K	69	ARG
11	K	87	VAL
11	K	100	MET
11	K	211	ILE
12	L	23	LEU
12	L	49	ASN
12	L	109	THR
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	146	PHE
13	M	159	VAL
13	M	161	ARG
13	M	170	VAL
14	N	119	VAL
14	N	149	GLU
14	N	195	GLN
1	O	30	GLN
1	O	59	GLU
1	O	61	LEU
1	O	157	PHE
2	P	55	LEU
2	P	60	THR
2	P	149	THR
2	P	191	LEU
3	Q	19	GLU
3	Q	51	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	171	GLU
4	R	20	LEU
4	R	40	LEU
4	R	44	LYS
4	R	102	GLU
4	R	124	ARG
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
5	S	9	THR

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Mol	Chain	Res	Type
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	188	LEU
5	S	198	GLN
5	S	227	GLU
5	S	231	LYS
6	T	7	SER
6	T	31	THR
6	T	39	ASN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	186	ARG
6	T	201	GLU
6	T	221	ASN
7	U	45	ILE
7	U	83	ASN
7	U	115	LEU
7	U	166	GLN
7	U	201	MET
7	U	221	LYS
7	U	235	ARG
8	V	34	LEU
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	110	LYS
10	X	127	GLU
10	X	174	MET
11	Y	4	LEU
11	Y	35	ILE
11	Y	65	LEU
11	Y	69	ARG
11	Y	87	VAL
11	Y	100	MET
11	Y	211	ILE
12	Z	23	LEU
12	Z	49	ASN
12	Z	109	THR

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Mol	Chain	Res	Type
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	146	PHE
13	a	159	VAL
13	a	161	ARG
13	a	170	VAL
14	b	119	VAL
14	b	149	GLU
14	b	195	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (194) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
2	B	20	GLN
2	B	69	ASN
2	B	93	HIS
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
2	B	220	ASN
2	B	232	GLN
3	C	17	GLN
3	C	77	ASN
3	C	92	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	165	ASN
3	C	241	GLN
4	D	15	GLN
4	D	146	GLN
4	D	160	ASN
4	D	210	GLN
4	D	225	ASN
5	E	4	ASN
5	E	30	GLN
5	E	59	GLN

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Mol	Chain	Res	Type
5	E	68	HIS
5	E	85	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
5	E	165	GLN
5	E	184	ASN
5	E	198	GLN
5	E	209	ASN
6	F	19	GLN
6	F	39	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	224	HIS
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
7	G	186	ASN
8	H	22	GLN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	44	HIS
9	I	63	ASN
9	I	88	GLN
9	I	203	GLN
10	J	37	GLN
10	J	55	GLN
10	J	63	ASN
10	J	191	GLN
10	J	198	GLN
11	K	9	GLN

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Mol	Chain	Res	Type
11	K	24	ASN
11	K	85	ASN
11	K	176	ASN
11	K	190	ASN
11	K	208	ASN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	92	ASN
12	L	153	GLN
12	L	158	ASN
12	L	165	ASN
12	L	197	GLN
13	M	2	GLN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	171	GLN
13	M	179	ASN
13	M	211	ASN
13	M	213	GLN
14	N	62	HIS
14	N	69	GLN
14	N	141	ASN
14	N	161	GLN
1	O	30	GLN
1	O	143	ASN
2	P	20	GLN
2	P	69	ASN
2	P	93	HIS
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
2	P	220	ASN
2	P	232	GLN
3	Q	17	GLN
3	Q	77	ASN

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Mol	Chain	Res	Type
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	241	GLN
4	R	15	GLN
4	R	146	GLN
4	R	160	ASN
4	R	210	GLN
4	R	225	ASN
5	S	4	ASN
5	S	59	GLN
5	S	68	HIS
5	S	85	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
5	S	198	GLN
5	S	209	ASN
6	T	19	GLN
6	T	39	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	224	HIS
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
7	U	231	ASN
8	V	22	GLN
8	V	30	ASN
8	V	66	HIS
8	V	144	GLN

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Mol	Chain	Res	Type
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	37	ASN
9	W	44	HIS
9	W	63	ASN
9	W	88	GLN
9	W	203	GLN
10	X	37	GLN
10	X	55	GLN
10	X	63	ASN
10	X	86	GLN
10	X	191	GLN
10	X	198	GLN
11	Y	9	GLN
11	Y	24	ASN
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	92	ASN
12	Z	153	GLN
12	Z	158	ASN
12	Z	165	ASN
12	Z	197	GLN
13	a	2	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	171	GLN
13	a	179	ASN
13	a	213	GLN
14	b	69	GLN
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 ⓘ

12 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	ACA	f	4	15	6,7,8	0.74	0	5,6,8	0.48	0
15	TY5	c	5	15	19,20,21	1.12	0	20,25,27	0.74	0
15	RE0	d	7	15	15,17,18	1.30	2 (13%)	19,25,27	1.94	5 (26%)
15	ACA	e	4	15	6,7,8	0.74	0	5,6,8	0.47	0
15	RE0	e	7	15	15,17,18	1.33	2 (13%)	19,25,27	1.83	5 (26%)
15	ACA	d	4	15	6,7,8	0.75	0	5,6,8	0.47	0
15	TY5	e	5	15	19,20,21	1.12	0	20,25,27	0.60	0
15	TY5	f	5	15	19,20,21	1.11	0	20,25,27	0.62	0
15	RE0	c	7	15	15,17,18	1.28	2 (13%)	19,25,27	1.98	5 (26%)
15	TY5	d	5	15	19,20,21	1.12	0	20,25,27	0.72	0
15	ACA	c	4	15	6,7,8	0.75	0	5,6,8	0.47	0
15	RE0	f	7	15	15,17,18	1.33	2 (13%)	19,25,27	1.85	5 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ACA	f	4	15	-	1/5/5/6	-
15	TY5	c	5	15	-	5/10/11/13	0/2/2/2
15	RE0	d	7	15	-	0/6/23/25	0/2/2/2
15	ACA	e	4	15	-	1/5/5/6	-
15	RE0	e	7	15	-	2/6/23/25	0/2/2/2
15	ACA	d	4	15	-	1/5/5/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	TY5	e	5	15	-	2/10/11/13	0/2/2/2
15	TY5	f	5	15	-	2/10/11/13	0/2/2/2
15	RE0	c	7	15	-	0/6/23/25	0/2/2/2
15	TY5	d	5	15	-	5/10/11/13	0/2/2/2
15	ACA	c	4	15	-	2/5/5/6	-
15	RE0	f	7	15	-	2/6/23/25	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	e	7	RE0	CG-CD2	3.06	1.54	1.51
15	f	7	RE0	CG-CD2	3.00	1.54	1.51
15	d	7	RE0	CG-CD2	2.99	1.54	1.51
15	c	7	RE0	CG-CD2	2.94	1.54	1.51
15	f	7	RE0	CB-CA	2.47	1.57	1.54
15	e	7	RE0	CB-CA	2.39	1.57	1.54
15	d	7	RE0	CB-CA	2.35	1.57	1.54
15	c	7	RE0	CB-CA	2.31	1.57	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	c	7	RE0	CG-CD2-CE2	-5.42	106.64	108.86
15	d	7	RE0	CG-CD2-CE2	-5.32	106.69	108.86
15	f	7	RE0	CG-CD2-CE2	-4.87	106.87	108.86
15	e	7	RE0	CG-CD2-CE2	-4.77	106.91	108.86
15	c	7	RE0	CD2-CE2-NE1	3.64	112.04	109.60
15	d	7	RE0	CD2-CE2-NE1	3.61	112.01	109.60
15	f	7	RE0	CD2-CE2-NE1	3.45	111.91	109.60
15	e	7	RE0	CD2-CE2-NE1	3.39	111.87	109.60
15	c	7	RE0	CE2-NE1-CD1	-3.01	109.85	111.85
15	d	7	RE0	CE2-NE1-CD1	-2.98	109.88	111.85
15	f	7	RE0	CE2-NE1-CD1	-2.93	109.91	111.85
15	e	7	RE0	CE2-NE1-CD1	-2.87	109.95	111.85
15	c	7	RE0	CZ2-CE2-NE1	-2.65	125.47	130.83
15	d	7	RE0	CZ2-CE2-NE1	-2.63	125.52	130.83
15	e	7	RE0	CZ2-CE2-NE1	-2.58	125.61	130.83
15	f	7	RE0	CZ2-CE2-NE1	-2.58	125.62	130.83
15	e	7	RE0	CG-CD1-NE1	2.38	109.85	108.43
15	f	7	RE0	CG-CD1-NE1	2.31	109.81	108.43
15	c	7	RE0	CG-CD1-NE1	2.15	109.71	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	d	7	RE0	CG-CD1-NE1	2.12	109.70	108.43

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	e	7	RE0	N-CA-CB-CG
15	e	7	RE0	C-CA-CB-CG
15	f	7	RE0	N-CA-CB-CG
15	f	7	RE0	C-CA-CB-CG
15	e	4	ACA	C-C2-C3-C4
15	e	5	TY5	CE1-CZ-OH-C49
15	f	5	TY5	CE1-CZ-OH-C49
15	e	5	TY5	CE2-CZ-OH-C49
15	f	5	TY5	CE2-CZ-OH-C49
15	d	5	TY5	CE2-CZ-OH-C49
15	d	5	TY5	CE1-CZ-OH-C49
15	c	5	TY5	CE2-CZ-OH-C49
15	c	5	TY5	CE1-CZ-OH-C49
15	d	4	ACA	C2-C3-C4-C5
15	d	5	TY5	N-CA-CB-CG
15	c	4	ACA	C2-C3-C4-C5
15	c	4	ACA	C-C2-C3-C4
15	f	4	ACA	C-C2-C3-C4
15	c	5	TY5	N-CA-CB-CG
15	d	5	TY5	CA-CB-CG-CD2
15	d	5	TY5	CA-CB-CG-CD1
15	c	5	TY5	CA-CB-CG-CD2
15	c	5	TY5	CA-CB-CG-CD1

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	c	5	TY5	1	0
15	d	7	RE0	1	0
15	c	7	RE0	1	0
15	d	5	TY5	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
16	MES	K	301	-	12,12,12	1.35	2 (16%)	15,16,16	1.53	3 (20%)
16	MES	Y	301	-	12,12,12	1.34	2 (16%)	15,16,16	1.57	3 (20%)

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
16	MES	K	301	-	-	2/6/14/14	0/1/1/1
16	MES	Y	301	-	-	2/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	301	MES	C8-S	2.83	1.81	1.77
16	Y	301	MES	C8-S	2.82	1.81	1.77
16	K	301	MES	O2S-S	2.07	1.51	1.45
16	Y	301	MES	O2S-S	2.04	1.50	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	301	MES	O3S-S-O1S	3.12	119.21	111.40
16	K	301	MES	O2S-S-C8	-2.91	102.33	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	301	MES	O3S-S-O1S	2.82	118.45	111.40
16	Y	301	MES	O2S-S-C8	-2.81	102.48	106.73
16	K	301	MES	C7-N4-C5	2.36	117.52	111.24
16	Y	301	MES	C7-N4-C5	2.31	117.41	111.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	K	301	MES	C8-C7-N4-C5
16	Y	301	MES	C8-C7-N4-C5
16	K	301	MES	C8-C7-N4-C3
16	Y	301	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%)	-0.15	3 (1%) 76 69	50, 63, 82, 94	0
1	O	250/250 (100%)	-0.07	3 (1%) 76 69	55, 71, 92, 105	0
2	B	244/258 (94%)	0.16	9 (3%) 45 37	53, 68, 98, 108	0
2	P	244/258 (94%)	0.30	13 (5%) 32 25	59, 72, 101, 117	0
3	C	241/254 (94%)	0.11	9 (3%) 45 37	51, 69, 105, 142	0
3	Q	241/254 (94%)	0.27	11 (4%) 37 29	61, 85, 125, 158	0
4	D	242/260 (93%)	0.10	10 (4%) 41 33	55, 69, 97, 108	0
4	R	242/260 (93%)	0.17	9 (3%) 45 37	60, 76, 105, 118	0
5	E	233/234 (99%)	-0.00	3 (1%) 75 67	57, 73, 91, 101	0
5	S	233/234 (99%)	0.21	6 (2%) 57 48	62, 81, 103, 115	0
6	F	244/288 (84%)	-0.09	3 (1%) 76 69	54, 67, 92, 108	0
6	T	244/288 (84%)	0.06	4 (1%) 70 62	58, 74, 101, 123	0
7	G	243/252 (96%)	-0.05	4 (1%) 70 62	49, 64, 86, 120	0
7	U	243/252 (96%)	0.01	4 (1%) 70 62	57, 66, 83, 114	0
8	H	222/232 (95%)	-0.23	2 (0%) 81 75	50, 60, 74, 88	0
8	V	222/232 (95%)	-0.19	1 (0%) 87 83	52, 61, 74, 99	0
9	I	204/205 (99%)	-0.32	1 (0%) 87 83	48, 57, 71, 78	0
9	W	204/205 (99%)	-0.22	2 (0%) 79 73	51, 59, 73, 83	0
10	J	198/198 (100%)	-0.07	7 (3%) 47 38	49, 59, 74, 116	0
10	X	198/198 (100%)	-0.08	8 (4%) 42 34	55, 62, 75, 117	0
11	K	212/212 (100%)	0.10	9 (4%) 40 32	48, 60, 78, 84	0
11	Y	212/212 (100%)	0.10	11 (5%) 33 26	53, 63, 82, 88	0
12	L	222/222 (100%)	-0.09	3 (1%) 73 65	50, 60, 84, 89	0
12	Z	222/222 (100%)	-0.14	6 (2%) 56 47	53, 61, 83, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/233 (100%)	-0.28	3 (1%) 75 67	49, 60, 71, 74	0
13	a	233/233 (100%)	-0.28	1 (0%) 88 85	51, 60, 69, 72	0
14	N	196/196 (100%)	-0.30	0 100 100	50, 56, 71, 78	0
14	b	196/196 (100%)	-0.21	1 (0%) 87 83	51, 57, 72, 81	0
15	c	1/8 (12%)	0.78	0 100 100	55, 55, 55, 55	0
15	d	1/8 (12%)	0.28	0 100 100	54, 54, 54, 54	0
15	e	1/8 (12%)	3.00	1 (100%) 0 0	77, 77, 77, 77	0
15	f	1/8 (12%)	2.34	1 (100%) 0 0	81, 81, 81, 81	0
All	All	6372/6620 (96%)	-0.03	148 (2%) 61 52	48, 65, 96, 158	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	174	TYR	8.0
4	D	119	ALA	7.6
11	K	104	TYR	7.3
4	R	119	ALA	7.0
11	Y	104	TYR	6.8
3	Q	50	LEU	6.7
12	Z	174	TYR	6.6
2	P	219	ALA	5.9
11	K	208	ASN	5.8
4	D	118	GLY	5.7
7	U	243	ASP	5.7
4	R	118	GLY	5.5
4	D	120	SER	5.5
3	C	49	THR	5.3
4	R	120	SER	5.2
10	X	139	TYR	5.2
11	Y	182	GLU	5.1
11	Y	209	ASN	5.0
11	K	209	ASN	5.0
3	C	50	LEU	4.9
11	K	182	GLU	4.8
10	J	197	ALA	4.6
10	J	1	MET	4.4
2	B	219	ALA	4.3
4	R	121	GLY	4.3
7	U	1	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
11	K	40	PHE	4.1
10	J	139	TYR	4.0
2	P	61	SER	3.9
7	G	1	ALA	3.8
2	B	218	GLY	3.8
6	F	202	ASP	3.8
3	Q	52	LEU	3.8
5	S	1	PHE	3.8
10	X	1	MET	3.7
13	M	1	THR	3.7
10	X	198	GLN	3.6
13	a	1	THR	3.6
6	F	1	GLY	3.6
9	W	1	SER	3.5
4	R	124	ARG	3.5
4	R	125	LEU	3.5
11	Y	40	PHE	3.5
1	O	1	MET	3.4
3	Q	49	THR	3.3
10	X	174	MET	3.3
2	B	222	GLY	3.3
2	B	220	ASN	3.2
1	A	1	MET	3.2
10	J	174	MET	3.2
3	Q	203	THR	3.2
5	E	1	PHE	3.1
11	Y	208	ASN	3.1
10	J	198	GLN	3.1
2	P	1	GLY	3.1
7	U	188	GLU	3.1
10	X	197	ALA	3.1
3	C	48	SER	3.0
1	A	201	GLU	3.0
15	e	6	ALA	3.0
11	K	73	ARG	3.0
4	D	125	LEU	3.0
11	K	183	ASP	3.0
2	P	244	THR	3.0
4	R	113	LEU	3.0
2	B	1	GLY	2.9
14	b	116	GLY	2.9
1	O	53	SER	2.9

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Mol	Chain	Res	Type	RSRZ
11	Y	183	ASP	2.9
2	B	244	THR	2.9
4	D	124	ARG	2.9
3	C	206	LYS	2.9
11	Y	73	ARG	2.9
12	Z	173	LYS	2.8
3	Q	48	SER	2.8
5	S	52	ALA	2.8
6	F	203	ASN	2.8
8	H	222	ASP	2.8
8	V	222	ASP	2.8
2	P	241	THR	2.7
6	T	9	SER	2.7
2	B	223	GLU	2.7
11	Y	211	ILE	2.7
11	Y	146	TRP	2.7
2	P	218	GLY	2.7
10	J	196	GLN	2.7
2	P	51	VAL	2.7
12	Z	168	VAL	2.7
4	R	112	ALA	2.6
5	S	209	ASN	2.6
5	S	202	ASP	2.6
10	X	196	GLN	2.5
13	M	47	ASP	2.5
12	L	173	LYS	2.5
2	P	50	LYS	2.5
3	Q	234	ILE	2.5
3	Q	238	LYS	2.5
6	T	243	ILE	2.5
12	Z	132	GLU	2.5
4	D	240	ALA	2.5
2	P	220	ASN	2.5
4	D	121	GLY	2.4
7	G	239	ILE	2.4
7	U	222	ASP	2.4
3	Q	241	GLN	2.4
4	D	167	GLY	2.4
5	S	2	ARG	2.4
2	B	51	VAL	2.4
15	f	6	ALA	2.3
2	P	223	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
5	S	30	GLN	2.3
6	T	215	CYS	2.3
2	B	61	SER	2.3
8	H	198	GLU	2.3
12	Z	172	LEU	2.3
1	A	2	THR	2.3
7	G	2	GLY	2.3
9	I	192	ASP	2.2
3	Q	60	SER	2.2
5	E	202	ASP	2.2
10	X	194	ASP	2.2
11	K	181	THR	2.2
10	X	172	MET	2.2
3	Q	171	GLU	2.2
2	P	225	TYR	2.2
6	T	244	ASN	2.2
9	W	192	ASP	2.2
11	Y	210	VAL	2.2
2	P	202	SER	2.2
3	C	205	ALA	2.2
10	J	172	MET	2.1
2	P	60	THR	2.1
12	Z	163	GLY	2.1
11	Y	37	ILE	2.1
12	L	163	GLY	2.1
4	D	122	GLU	2.1
3	C	53	GLN	2.1
3	Q	51	LYS	2.0
1	O	2	THR	2.0
3	C	203	THR	2.0
11	K	211	ILE	2.0
3	C	241	GLN	2.0
4	R	177	ASN	2.0
3	C	185	THR	2.0
4	D	241	ALA	2.0
5	E	53	ASP	2.0
7	G	243	ASP	2.0
13	M	69	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	RE0	f	7	16/17	0.51	0.23	81,90,91,91	0
15	ACA	f	4	8/9	0.59	0.21	76,77,79,79	0
15	ACA	e	4	8/9	0.65	0.19	72,72,73,74	0
15	ACA	c	4	8/9	0.66	0.14	59,59,60,60	0
15	RE0	e	7	16/17	0.70	0.18	79,85,86,86	0
15	ACA	d	4	8/9	0.73	0.13	57,58,58,58	0
15	TY5	f	5	19/20	0.83	0.12	75,76,80,81	0
15	TY5	d	5	19/20	0.84	0.12	55,56,57,57	0
15	TY5	e	5	19/20	0.85	0.12	70,71,75,76	0
15	RE0	c	7	16/17	0.87	0.11	53,54,54,54	0
15	RE0	d	7	16/17	0.87	0.11	52,53,53,53	0
15	TY5	c	5	19/20	0.88	0.12	57,58,58,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	MES	Y	301	12/12	0.89	0.16	56,57,58,58	0
16	MES	K	301	12/12	0.95	0.11	54,55,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.