



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 09:05 PM UTC

PDB ID : 9QD2 / pdb_00009qd2
Title : Yeast 20S proteasome mutant: beta1_G128V (b1-propeptide deleted) in complex with MG132
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2025-03-05
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

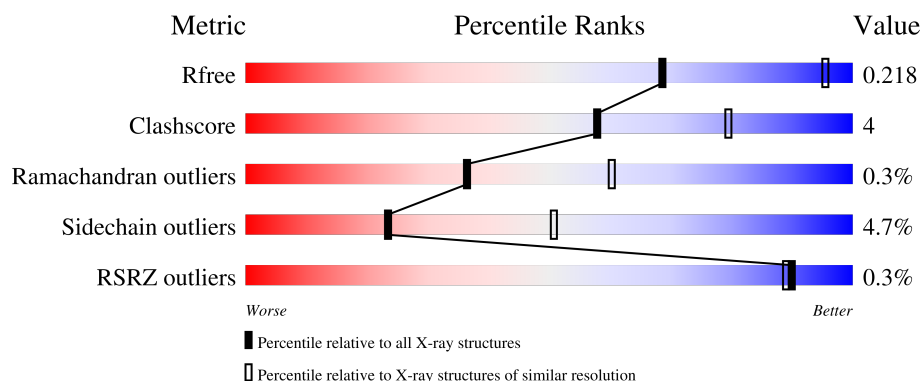
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	250	96% .
1	O	250	95% .
2	B	258	% 88% 5% • 5%
2	P	258	% 88% 5% • 5%
3	C	254	89% • • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	 2% 90% . . 6%
4	D	260	 84% 6% 10%
4	R	260	 85% 5% 10%
5	E	234	 92% 6% ..
5	S	234	 92% 6% ..
6	F	288	 80% . . 16%
6	T	288	 79% . . 16%
7	G	252	 88% 6% . .
7	U	252	 87% 8% . .
8	H	231	 80% 15% . .
8	V	231	 81% 14% . .
9	I	205	 94% 5%
9	W	205	 93% 6%
10	J	198	 82% 13% . .
10	X	198	 82% 14% . .
11	K	211	 70% 27% .
11	Y	211	 74% 22% .
12	L	222	 89% 9% .
12	Z	222	 86% 13% .
13	M	246	 74% 17% . 5%
13	a	246	 74% 19% . 5%
14	N	195	 74% 18% 7% %
14	b	195	 76% 19% 5%
15	d	4	 50% 25% 25%
15	e	4	 50% 50%

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Mol	Chain	Length	Quality of chain
15	f	4	 50% 25% 25%
15	g	4	 50% 25% 25%
15	h	4	 50% 50%
15	i	4	 50% 25% 25%

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49779 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	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	7			
8	V	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	7			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	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	195	Total	C	N	O	S	0	0	0
			1508	954	249	298	7			
14	b	195	Total	C	N	O	S	0	0	0
			1508	954	249	298	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	128	VAL	GLY	engineered mutation	UNP P38624
b	128	VAL	GLY	engineered mutation	UNP P38624

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

OLE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	d	4	Total 41	C 30	N 4	O 7	0	0	0
15	e	4	Total 41	C 30	N 4	O 7	0	0	0
15	f	4	Total 41	C 30	N 4	O 7	0	0	0
15	g	4	Total 41	C 30	N 4	O 7	0	0	0
15	h	4	Total 41	C 30	N 4	O 7	0	0	0
15	i	4	Total 41	C 30	N 4	O 7	0	0	0

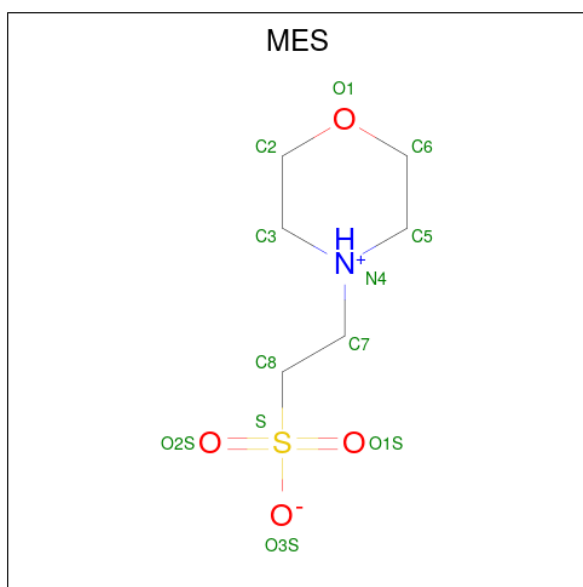
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total 1	Mg 1	0	0
16	I	1	Total 1	Mg 1	0	0
16	J	1	Total 1	Mg 1	0	0
16	Z	1	Total 1	Mg 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	2	Total 2	Cl 2	0	0
17	N	1	Total 1	Cl 1	0	0
17	U	1	Total 1	Cl 1	0	0
17	b	1	Total 1	Cl 1	0	0

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	a	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	6	Total	O	0	0
			6	6		
19	B	13	Total	O	0	0
			13	13		
19	C	12	Total	O	0	0
			12	12		
19	D	9	Total	O	0	0
			9	9		
19	E	4	Total	O	0	0
			4	4		
19	F	6	Total	O	0	0
			6	6		
19	G	7	Total	O	0	0
			7	7		
19	H	16	Total	O	0	0
			16	16		
19	I	8	Total	O	0	0
			8	8		
19	J	13	Total	O	0	0
			13	13		
19	K	9	Total	O	0	0
			9	9		

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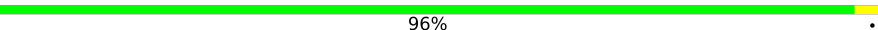
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	L	18	Total O 18 18	0	0
19	M	9	Total O 9 9	0	0
19	N	5	Total O 5 5	0	0
19	O	5	Total O 5 5	0	0
19	P	5	Total O 5 5	0	0
19	Q	8	Total O 8 8	0	0
19	R	3	Total O 3 3	0	0
19	S	4	Total O 4 4	0	0
19	T	8	Total O 8 8	0	0
19	U	11	Total O 11 11	0	0
19	V	9	Total O 9 9	0	0
19	W	9	Total O 9 9	0	0
19	X	14	Total O 14 14	0	0
19	Y	11	Total O 11 11	0	0
19	Z	7	Total O 7 7	0	0
19	a	9	Total O 9 9	0	0
19	b	9	Total O 9 9	0	0
19	d	1	Total O 1 1	0	0
19	e	1	Total O 1 1	0	0
19	g	1	Total O 1 1	0	0
19	h	2	Total O 2 2	0	0

3 Residue-property plots

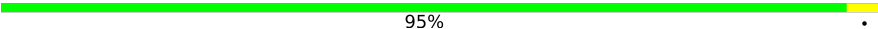
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

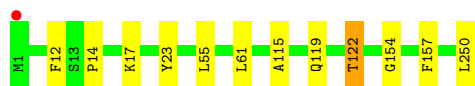
- Molecule 1: Proteasome subunit alpha type-2

Chain A:  96%



- Molecule 1: Proteasome subunit alpha type-2

Chain O:  95%



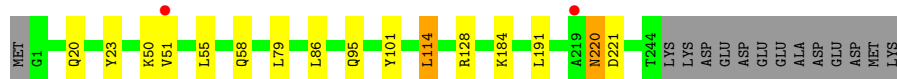
- Molecule 2: Proteasome subunit alpha type-3

Chain B:  88% 5% • 5%



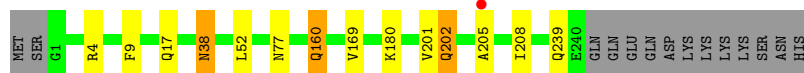
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  88% 5% • 5%

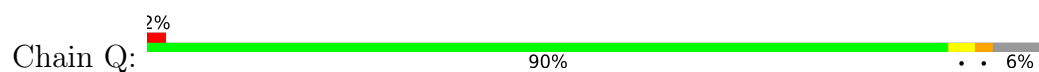


- Molecule 3: Proteasome subunit alpha type-4

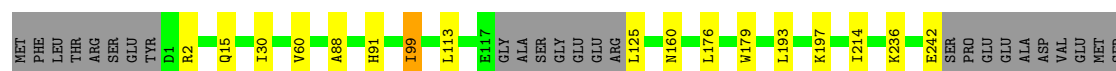
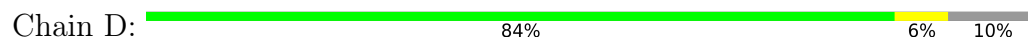
Chain C:  89% • • 6%



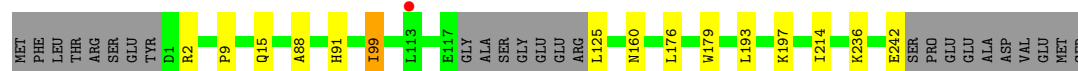
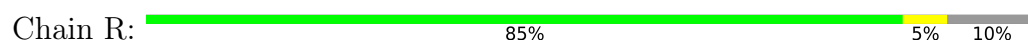
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-5



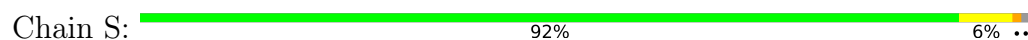
- Molecule 4: Proteasome subunit alpha type-5



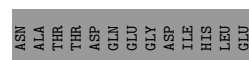
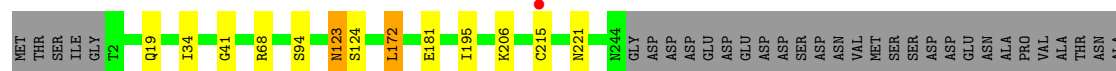
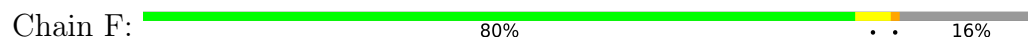
- Molecule 5: Proteasome subunit alpha type-6



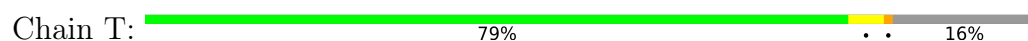
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 6: Probable proteasome subunit alpha type-7





- Molecule 7: Proteasome subunit alpha type-1

Chain G: 88% 6% . .



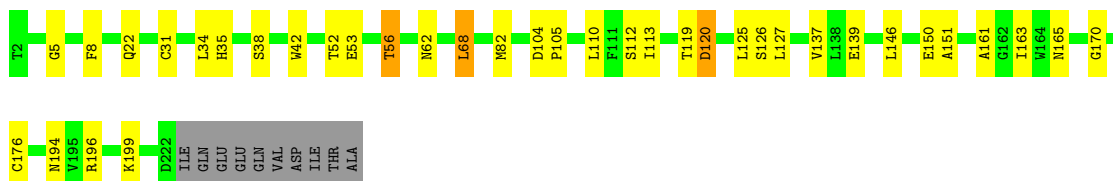
- Molecule 7: Proteasome subunit alpha type-1

Chain U: 87% 8% . .



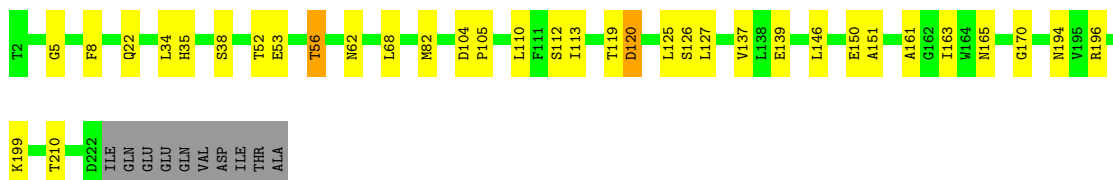
- Molecule 8: Proteasome subunit beta type-2

Chain H: 80% 15% . .



- Molecule 8: Proteasome subunit beta type-2

Chain V: 81% 14% . .



- Molecule 9: Proteasome subunit beta type-3

Chain I: 94% 5%

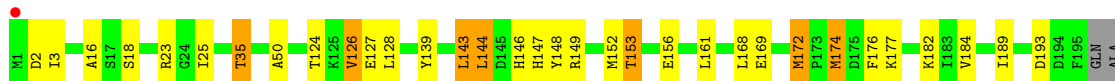
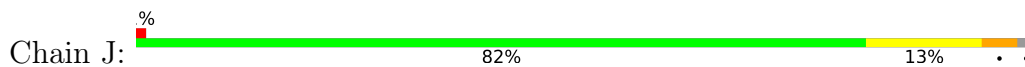


- Molecule 9: Proteasome subunit beta type-3

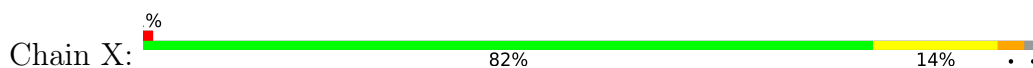
Chain W: 93% 6%



- Molecule 10: Proteasome subunit beta type-4



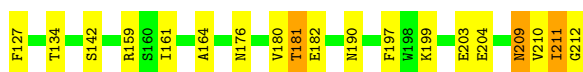
- Molecule 10: Proteasome subunit beta type-4



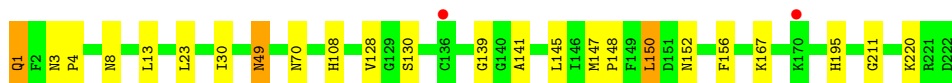
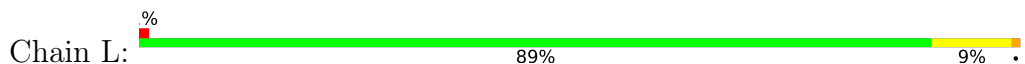
- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-6



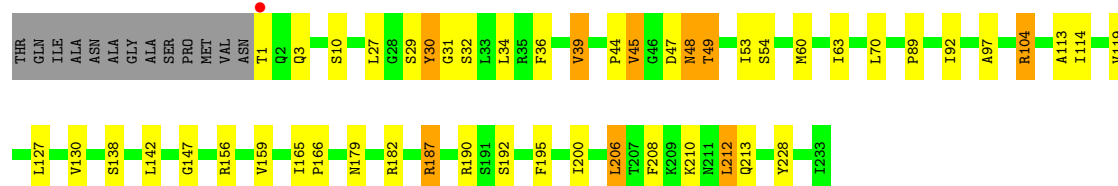
- Molecule 12: Proteasome subunit beta type-6

Chain Z:  86% 13% .



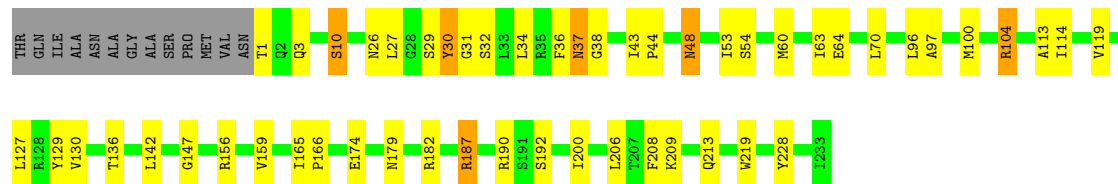
• Molecule 13: Proteasome subunit beta type-7

Chain M:  74% 17% . 5%



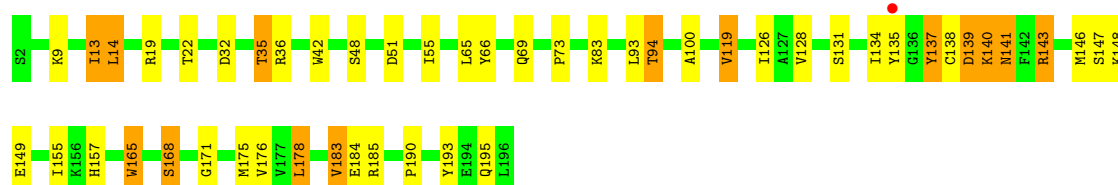
• Molecule 13: Proteasome subunit beta type-7

Chain a:  74% 19% . 5%



• Molecule 14: Proteasome subunit beta type-1

Chain N:  74% 18% 7%



• Molecule 14: Proteasome subunit beta type-1

Chain b:  76% 19% 5%



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

Chain d:  50% 25% 25%



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



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



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.23Å 300.11Å 145.77Å 90.00° 113.25° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (15.00-2.70) 97.2 (15.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.176 , 0.214 0.180 , 0.218	Depositor DCC
R_{free} test set	14253 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.6	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	0.97	EDS
Total number of atoms	49779	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: P6S, CL, MG, A1I48, MES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.03	0/1952	1.43	0/2642
1	O	1.03	0/1952	1.43	0/2642
2	B	1.03	0/1934	1.44	0/2618
2	P	1.03	0/1934	1.44	0/2618
3	C	1.03	0/1910	1.47	0/2586
3	Q	1.03	0/1910	1.47	0/2586
4	D	1.03	0/1837	1.47	4/2475 (0.2%)
4	R	1.03	0/1837	1.47	2/2475 (0.1%)
5	E	1.04	0/1800	1.45	4/2433 (0.2%)
5	S	1.04	0/1800	1.45	2/2433 (0.1%)
6	F	1.02	0/1932	1.46	2/2609 (0.1%)
6	T	1.02	0/1932	1.47	4/2609 (0.2%)
7	G	1.01	0/1945	1.42	0/2634
7	U	1.01	0/1945	1.43	0/2634
8	H	1.00	0/1708	1.41	1/2316 (0.0%)
8	V	1.00	0/1708	1.42	1/2316 (0.0%)
9	I	1.01	0/1611	1.42	1/2174 (0.0%)
9	W	1.01	0/1611	1.42	1/2174 (0.0%)
10	J	1.00	0/1589	1.40	0/2142
10	X	1.00	0/1589	1.38	0/2142
11	K	0.97	0/1674	1.38	1/2264 (0.0%)
11	Y	0.97	0/1674	1.39	1/2264 (0.0%)
12	L	1.00	0/1795	1.38	0/2420
12	Z	1.00	0/1795	1.38	1/2420 (0.0%)
13	M	0.98	0/1855	1.38	0/2514
13	a	0.99	0/1855	1.39	0/2514
14	N	0.97	0/1537	1.40	2/2082 (0.1%)
14	b	0.98	0/1537	1.39	1/2082 (0.0%)
15	d	0.70	0/15	0.76	0/19
15	e	0.79	0/15	0.78	0/19
15	f	0.61	0/15	0.83	0/19
15	g	0.63	0/15	0.75	0/19

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	h	0.76	0/15	0.78	0/19
15	i	0.64	0/15	0.85	0/19
All	All	1.01	0/50248	1.42	28/67932 (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	d	0	1
15	e	0	1
15	f	0	1
15	g	0	1
15	h	0	1
15	i	0	1
All	All	0	6

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	120	ASP	CA-CB-CG	9.68	122.28	112.60
8	H	120	ASP	CA-CB-CG	9.33	121.93	112.60
14	b	94	THR	CB-CA-C	8.53	124.66	111.70
14	N	94	THR	CB-CA-C	7.85	123.34	111.95
14	N	168	SER	N-CA-C	-6.12	104.53	111.14
9	I	183	GLY	CA-C-O	-6.12	118.25	122.22
9	W	183	GLY	CA-C-O	-6.08	118.27	122.22
6	T	34	ILE	CA-C-N	5.47	125.37	121.65
6	T	34	ILE	C-N-CA	5.47	125.37	121.65
6	F	34	ILE	CA-C-N	5.43	125.34	121.65
6	F	34	ILE	C-N-CA	5.43	125.34	121.65
5	S	35	VAL	CA-C-N	5.36	125.30	121.65
5	S	35	VAL	C-N-CA	5.36	125.30	121.65
6	T	77	LEU	CA-C-N	5.34	124.60	120.33
6	T	77	LEU	C-N-CA	5.34	124.60	120.33
12	Z	135	GLN	N-CA-C	-5.30	106.82	113.28
4	D	2	ARG	CA-C-N	5.14	124.99	120.10
4	D	2	ARG	C-N-CA	5.14	124.99	120.10
5	E	35	VAL	CA-C-N	5.14	125.15	121.65
5	E	35	VAL	C-N-CA	5.14	125.15	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	30	GLN	CA-C-N	5.12	124.96	120.10
5	E	30	GLN	C-N-CA	5.12	124.96	120.10
4	R	2	ARG	CA-C-N	5.05	124.89	120.10
4	R	2	ARG	C-N-CA	5.05	124.89	120.10
4	D	30	ILE	CA-C-N	5.02	125.06	121.65
4	D	30	ILE	C-N-CA	5.02	125.06	121.65
11	Y	57	THR	N-CA-C	-5.01	105.92	112.23
11	K	57	THR	N-CA-C	-5.01	105.92	112.23

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	d	3	LEU	Peptide
15	e	3	LEU	Peptide
15	f	3	LEU	Peptide
15	g	3	LEU	Peptide
15	h	3	LEU	Peptide
15	i	3	LEU	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	5	0
1	O	1915	0	1929	7	0
2	B	1904	0	1904	7	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	10	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	6	0
5	E	1773	0	1775	10	0
5	S	1773	0	1775	12	0
6	F	1892	0	1883	5	0
6	T	1892	0	1883	6	0
7	G	1907	0	1900	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	U	1907	0	1901	12	0
8	H	1677	0	1678	19	0
8	V	1677	0	1678	19	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	11	0
10	J	1561	0	1569	30	0
10	X	1561	0	1569	26	0
11	K	1637	0	1585	50	0
11	Y	1637	0	1585	45	0
12	L	1757	0	1711	20	0
12	Z	1757	0	1711	21	0
13	M	1824	0	1832	41	0
13	a	1824	0	1832	35	0
14	N	1508	0	1477	45	0
14	b	1508	0	1477	41	0
15	d	41	0	21	0	0
15	e	41	0	21	0	0
15	f	41	0	21	0	0
15	g	41	0	21	0	0
15	h	41	0	21	0	0
15	i	41	0	21	0	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	J	1	0	0	0	0
16	Z	1	0	0	0	0
17	G	2	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	b	1	0	0	0	0
18	a	12	0	13	0	0
19	A	6	0	0	0	0
19	B	13	0	0	0	0
19	C	12	0	0	1	0
19	D	9	0	0	0	0
19	E	4	0	0	0	0
19	F	6	0	0	0	0
19	G	7	0	0	0	0
19	H	16	0	0	0	0
19	I	8	0	0	0	0
19	J	13	0	0	1	0
19	K	9	0	0	0	0
19	L	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	M	9	0	0	0	0
19	N	5	0	0	0	0
19	O	5	0	0	0	0
19	P	5	0	0	0	0
19	Q	8	0	0	0	0
19	R	3	0	0	0	0
19	S	4	0	0	0	0
19	T	8	0	0	1	0
19	U	11	0	0	0	0
19	V	9	0	0	0	0
19	W	9	0	0	0	0
19	X	14	0	0	0	0
19	Y	11	0	0	0	0
19	Z	7	0	0	0	0
19	a	9	0	0	0	0
19	b	9	0	0	0	0
19	d	1	0	0	0	0
19	e	1	0	0	0	0
19	g	1	0	0	0	0
19	h	2	0	0	0	0
All	All	49779	0	49158	444	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 4.

All (444) 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)
14:N:14:LEU:HD11	14:N:100:ALA:HB3	1.21	1.17
14:b:143:ARG:H	14:b:146:MET:CE	1.67	1.08
13:M:45:VAL:HG11	13:M:92:ILE:HD13	1.30	1.08
14:b:143:ARG:H	14:b:146:MET:HE2	1.15	1.06
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.27	1.04
11:K:5:ALA:HB3	11:K:100:MET:CE	1.88	1.03
11:K:5:ALA:CB	11:K:100:MET:HE2	1.96	0.95
14:N:14:LEU:HD11	14:N:100:ALA:CB	2.00	0.90
11:Y:209:ASN:HD22	11:Y:209:ASN:H	1.18	0.88
13:M:45:VAL:CG1	13:M:92:ILE:HD13	2.03	0.87
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.39	0.87
13:M:45:VAL:HG11	13:M:92:ILE:CD1	2.03	0.87
11:Y:211:ILE:O	11:Y:212:GLY:OXT	1.94	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.41	0.86
13:a:36:PHE:HA	14:b:135:TYR:HB2	1.57	0.85
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.24	0.85
14:b:139:ASP:OD1	14:b:139:ASP:N	2.10	0.84
13:M:36:PHE:HA	14:N:135:TYR:HB2	1.60	0.84
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.26	0.81
14:b:143:ARG:O	14:b:146:MET:HE3	1.83	0.79
11:K:211:ILE:O	11:K:212:GLY:OXT	2.01	0.78
14:N:143:ARG:H	14:N:146:MET:HE2	1.49	0.77
11:K:51:ASP:HB3	11:K:97:MET:HE2	1.66	0.77
14:N:140:LYS:O	14:N:140:LYS:HD3	1.84	0.77
10:J:153:THR:HG23	10:J:156:GLU:OE2	1.85	0.77
14:N:14:LEU:CD1	14:N:100:ALA:HB3	2.11	0.77
10:X:143:LEU:HD23	10:X:143:LEU:O	1.87	0.75
13:M:45:VAL:CG1	13:M:92:ILE:CD1	2.62	0.75
14:b:143:ARG:N	14:b:146:MET:CE	2.48	0.75
14:N:165:TRP:CZ3	14:b:134:ILE:HG12	2.21	0.75
14:N:138:CYS:HB3	14:N:141:ASN:HB2	1.70	0.73
11:K:5:ALA:N	11:K:100:MET:HE1	2.03	0.73
11:K:5:ALA:CB	11:K:100:MET:CE	2.62	0.73
11:Y:33:LYS:HA	11:Y:45:MET:HG3	1.71	0.73
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	1.88	0.72
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	1.87	0.71
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.71	0.70
3:C:9:PHE:H	4:D:15:GLN:HE22	1.38	0.70
1:O:12:PHE:H	2:P:20:GLN:HE22	1.38	0.70
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.37	0.70
5:E:92:ASN:HD21	12:L:70:ASN:ND2	1.89	0.70
11:K:29:GLN:OE1	11:K:173:GLY:CA	2.41	0.69
14:N:165:TRP:HZ3	14:b:134:ILE:HG12	1.55	0.69
14:N:143:ARG:CG	14:N:143:ARG:HH11	2.06	0.68
1:A:12:PHE:H	2:B:20:GLN:HE22	1.42	0.68
5:E:92:ASN:ND2	12:L:70:ASN:HD21	1.90	0.68
10:J:139:TYR:CE1	11:Y:134:THR:HG22	2.30	0.67
14:b:143:ARG:N	14:b:146:MET:HE2	2.00	0.67
11:Y:209:ASN:HD22	11:Y:209:ASN:N	1.92	0.67
11:K:201:LYS:HE2	11:K:212:GLY:HA2	1.77	0.66
7:U:23:PHE:O	7:U:26:THR:HB	1.96	0.66
7:G:23:PHE:O	7:G:26:THR:HB	1.96	0.65
10:J:143:LEU:HD23	10:J:147:HIS:ND1	2.11	0.65
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:36:PHE:HA	14:b:135:TYR:CB	2.28	0.64
14:N:55:ILE:HD11	14:N:93:LEU:HD13	1.80	0.64
14:b:55:ILE:HD11	14:b:93:LEU:HD13	1.80	0.64
6:T:2:THR:N	19:T:301:HOH:O	2.32	0.63
10:J:174:MET:N	10:J:174:MET:HE3	2.13	0.63
13:M:48:ASN:H	13:M:48:ASN:HD22	1.44	0.63
10:X:153:THR:HG23	10:X:156:GLU:OE2	1.99	0.63
10:X:174:MET:N	10:X:174:MET:HE3	2.14	0.62
5:S:12:PHE:H	6:T:19:GLN:HE22	1.46	0.62
13:M:48:ASN:HD22	13:M:48:ASN:N	1.97	0.62
13:M:119:VAL:HG23	13:M:200:ILE:HG22	1.82	0.62
13:a:119:VAL:HG23	13:a:200:ILE:HG22	1.82	0.61
13:M:49:THR:OG1	13:M:89:PRO:HG3	2.00	0.61
10:J:146:HIS:ND1	11:Y:159:ARG:NH2	2.49	0.61
10:J:139:TYR:CZ	11:Y:134:THR:HG22	2.36	0.61
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.83	0.61
13:a:26:ASN:O	13:a:37:ASN:ND2	2.34	0.61
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.66	0.60
10:J:146:HIS:CE1	11:Y:204:GLU:OE2	2.53	0.60
13:M:44:PRO:HG3	13:M:208:PHE:CE2	2.35	0.60
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.01	0.60
14:b:143:ARG:HH11	14:b:143:ARG:CG	2.15	0.60
10:J:146:HIS:HE1	11:Y:204:GLU:CD	2.10	0.59
13:M:45:VAL:HG12	13:M:45:VAL:O	2.02	0.59
13:M:36:PHE:HA	14:N:135:TYR:CB	2.32	0.59
13:M:159:VAL:HG23	13:M:159:VAL:O	2.03	0.59
8:H:139:GLU:OE1	13:a:187:ARG:NH1	2.36	0.59
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.51	0.59
13:a:174:GLU:OE1	13:a:209:LYS:NZ	2.34	0.59
8:H:199:LYS:HE3	9:I:151:SER:O	2.02	0.59
11:K:45:MET:HB3	11:K:52:CYS:HB3	1.85	0.58
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.85	0.58
11:K:211:ILE:O	11:K:211:ILE:HG22	2.01	0.58
5:E:12:PHE:H	6:F:19:GLN:HE22	1.50	0.58
14:b:142:PHE:HA	14:b:146:MET:HE1	1.85	0.58
11:K:29:GLN:OE1	11:K:173:GLY:HA2	2.04	0.58
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.86	0.57
14:b:143:ARG:NH1	14:b:143:ARG:HG3	2.19	0.57
8:V:199:LYS:HE3	9:W:151:SER:O	2.03	0.57
13:a:27:LEU:HB2	13:a:192:SER:HB3	1.85	0.57
13:a:27:LEU:HD23	13:a:190:ARG:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:4:LEU:HD22	11:K:4:LEU:C	2.30	0.57
10:J:168:LEU:O	10:J:172:MET:HB2	2.04	0.57
14:N:185:ARG:HG2	14:N:185:ARG:HH11	1.70	0.56
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.88	0.56
11:K:56:GLU:OE2	11:K:99:THR:OG1	2.23	0.56
10:J:146:HIS:CE1	11:Y:204:GLU:CD	2.84	0.56
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.87	0.56
13:a:159:VAL:HG23	13:a:159:VAL:O	2.05	0.56
2:B:12:PHE:H	3:C:17:GLN:HE22	1.53	0.56
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.69	0.56
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.88	0.56
3:C:38:ASN:C	3:C:38:ASN:HD22	2.14	0.56
14:N:165:TRP:CD1	14:N:165:TRP:C	2.84	0.55
14:N:178:LEU:HD12	14:N:183:VAL:HG22	1.87	0.55
11:Y:211:ILE:C	11:Y:212:GLY:OXT	2.50	0.55
13:a:37:ASN:HD22	13:a:38:GLY:H	1.54	0.55
14:N:143:ARG:HH11	14:N:143:ARG:HG3	1.72	0.55
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.31	0.55
13:a:127:LEU:HG	13:a:142:LEU:HD12	1.89	0.55
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.88	0.55
14:b:124:TYR:OH	14:b:136:GLY:O	2.24	0.55
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.40	0.55
6:F:123:ASN:C	6:F:123:ASN:HD22	2.15	0.54
14:b:135:TYR:C	14:b:135:TYR:CD1	2.85	0.54
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.89	0.54
10:X:143:LEU:HD23	10:X:143:LEU:C	2.31	0.54
6:T:123:ASN:C	6:T:123:ASN:HD22	2.15	0.54
11:Y:199:LYS:O	11:Y:203:GLU:HG3	2.07	0.54
2:P:101:TYR:CE1	10:X:75:LEU:HD21	2.43	0.54
14:N:134:ILE:HD12	14:N:137:TYR:HD2	1.72	0.54
13:M:39:VAL:HG12	13:M:39:VAL:O	2.07	0.54
13:a:63:ILE:HD13	13:a:114:ILE:HD11	1.88	0.54
14:b:14:LEU:HD11	14:b:100:ALA:HB3	1.89	0.54
13:M:30:TYR:HB2	13:M:34:LEU:HB2	1.90	0.53
13:M:63:ILE:HD13	13:M:114:ILE:HD11	1.89	0.53
7:G:72:MET:HE3	7:G:74:VAL:CG2	2.38	0.53
10:J:152:MET:HE3	10:J:156:GLU:HB3	1.89	0.53
3:Q:38:ASN:C	3:Q:38:ASN:HD22	2.16	0.53
14:b:138:CYS:HB3	14:b:141:ASN:HB2	1.90	0.53
9:W:37:ASN:ND2	9:W:37:ASN:H	2.06	0.53
10:J:25:ILE:O	10:X:139:TYR:OH	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:211:ILE:C	11:K:212:GLY:OXT	2.50	0.53
10:J:143:LEU:HD23	10:J:147:HIS:CE1	2.44	0.53
14:N:178:LEU:CD1	14:N:183:VAL:HG22	2.39	0.53
11:K:199:LYS:O	11:K:203:GLU:HG3	2.09	0.52
11:K:155:TYR:OH	11:K:204:GLU:OE1	2.26	0.52
11:K:185:TRP:C	11:K:185:TRP:CE3	2.87	0.52
11:Y:35:ILE:HG23	11:Y:37:ILE:HG13	1.91	0.52
14:N:185:ARG:HG2	14:N:185:ARG:NH1	2.23	0.52
14:N:143:ARG:HG3	14:N:143:ARG:NH1	2.25	0.52
12:Z:1:GLN:HE21	13:a:1:THR:HG21	1.75	0.52
12:L:1:GLN:HE21	13:M:1:THR:HG21	1.75	0.51
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.58	0.51
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.92	0.51
8:V:52:THR:O	8:V:56:THR:HB	2.10	0.51
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.91	0.51
14:N:35:THR:HG21	13:a:228:TYR:HE2	1.75	0.51
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.46	0.51
13:a:48:ASN:H	13:a:48:ASN:HD22	1.57	0.51
14:b:143:ARG:NH2	14:b:150:GLU:OE2	2.32	0.51
13:M:45:VAL:CG1	13:M:92:ILE:HD11	2.41	0.51
13:a:179:ASN:HD22	13:a:182:ARG:HH11	1.59	0.51
14:b:143:ARG:CG	14:b:143:ARG:NH1	2.73	0.51
4:R:9:PRO:HA	5:S:23:TYR:CD1	2.45	0.51
14:b:165:TRP:CD1	14:b:165:TRP:C	2.88	0.51
8:H:52:THR:O	8:H:56:THR:HB	2.11	0.51
11:K:197:PHE:HZ	11:K:210:VAL:HG11	1.76	0.51
8:H:165:ASN:HD22	13:a:156:ARG:HH11	1.59	0.51
13:M:27:LEU:HB2	13:M:192:SER:HB3	1.92	0.51
14:N:135:TYR:C	14:N:135:TYR:CD2	2.88	0.51
11:Y:52:CYS:O	11:Y:56:GLU:HB2	2.10	0.51
14:b:14:LEU:O	14:b:175:MET:HA	2.10	0.51
10:J:139:TYR:OH	10:X:25:ILE:O	2.27	0.51
11:K:35:ILE:HG23	11:K:37:ILE:HG13	1.91	0.51
8:H:42:TRP:CG	8:H:176:CYS:HG	2.29	0.50
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.76	0.50
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.93	0.50
11:K:134:THR:HG22	10:X:139:TYR:CZ	2.47	0.50
13:M:45:VAL:HG12	13:M:92:ILE:CD1	2.40	0.50
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.77	0.50
12:L:8:ASN:HA	12:L:30:ILE:O	2.12	0.50
12:L:145:LEU:O	9:W:147:GLY:HA3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:55:LEU:HB3	7:U:159:ALA:O	2.11	0.50
7:U:78:ILE:N	7:U:79:PRO:CD	2.75	0.50
10:J:50:ALA:O	11:K:91:LYS:NZ	2.45	0.50
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.46	0.50
7:U:83:ASN:C	7:U:83:ASN:HD22	2.20	0.49
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.48	0.49
7:G:78:ILE:N	7:G:79:PRO:CD	2.75	0.49
11:K:99:THR:HG22	11:K:115:VAL:HB	1.94	0.49
13:M:30:TYR:CB	13:M:34:LEU:HB2	2.42	0.49
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.59	0.49
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.48	0.49
10:X:143:LEU:C	10:X:143:LEU:CD2	2.85	0.49
13:M:195:PHE:O	13:M:212:LEU:HB2	2.13	0.49
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.95	0.49
14:N:19:ARG:HD2	14:N:168:SER:O	2.13	0.48
9:W:37:ASN:ND2	9:W:37:ASN:N	2.61	0.48
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.13	0.48
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.78	0.48
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.95	0.48
14:N:143:ARG:CG	14:N:143:ARG:NH1	2.72	0.48
2:B:220:ASN:OD1	2:B:220:ASN:N	2.45	0.48
8:H:126:SER:O	8:H:127:LEU:HD12	2.14	0.48
7:G:68:ARG:O	7:G:223:LYS:HA	2.13	0.48
13:M:228:TYR:HE2	14:b:35:THR:HG21	1.78	0.48
14:N:134:ILE:HD12	14:N:137:TYR:CD2	2.48	0.48
2:P:220:ASN:OD1	2:P:220:ASN:N	2.46	0.48
11:K:4:LEU:HD22	11:K:4:LEU:O	2.14	0.48
1:O:119:GLN:O	1:O:122:THR:HB	2.13	0.48
14:N:66:TYR:CD1	14:N:73:PRO:HB3	2.49	0.48
11:Y:4:LEU:CD1	11:Y:161:ILE:HD11	2.44	0.48
13:M:27:LEU:CD2	13:M:190:ARG:O	2.62	0.47
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.12	0.47
11:Y:33:LYS:CA	11:Y:45:MET:HG3	2.43	0.47
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.29	0.47
12:L:147:MET:N	12:L:148:PRO:HD2	2.29	0.47
14:N:14:LEU:O	14:N:175:MET:HA	2.14	0.47
13:a:37:ASN:HB2	14:b:135:TYR:CZ	2.50	0.47
5:E:9:THR:HG21	5:E:119:THR:HA	1.96	0.47
14:b:65:LEU:HG	14:b:69:GLN:HE21	1.80	0.47
11:K:32:LYS:O	11:K:45:MET:HE2	2.14	0.47
11:K:134:THR:HG22	10:X:139:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:165:TRP:CE3	14:b:134:ILE:HG12	2.49	0.47
5:S:9:THR:HG21	5:S:119:THR:HA	1.97	0.47
7:U:68:ARG:O	7:U:223:LYS:HA	2.15	0.47
14:N:195:GLN:HG3	14:N:195:GLN:O	2.15	0.47
14:b:195:GLN:O	14:b:195:GLN:HG3	2.14	0.47
7:G:34:LEU:C	7:G:34:LEU:HD23	2.40	0.47
11:K:4:LEU:CD1	11:K:161:ILE:HD11	2.45	0.47
11:K:5:ALA:H	11:K:100:MET:HE1	1.75	0.47
12:L:108:HIS:HD2	12:L:139:GLY:HA3	1.79	0.47
14:N:65:LEU:HG	14:N:69:GLN:HE21	1.80	0.47
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.50	0.47
14:b:143:ARG:HH11	14:b:143:ARG:HG3	1.78	0.47
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.16	0.46
8:V:35:HIS:CE1	8:V:53:GLU:OE1	2.68	0.46
10:X:18:SER:HB2	10:X:176:PHE:HB2	1.97	0.46
10:X:136:SER:O	10:X:140:THR:HG23	2.15	0.46
12:Z:108:HIS:HD2	12:Z:139:GLY:HA3	1.80	0.46
13:a:44:PRO:HG3	13:a:208:PHE:CE2	2.50	0.46
3:C:201:VAL:HG13	3:C:202:GLN:N	2.29	0.46
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.44	0.46
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.79	0.46
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.30	0.46
14:b:66:TYR:CD1	14:b:73:PRO:HB3	2.50	0.46
8:H:35:HIS:CE1	8:H:53:GLU:OE1	2.68	0.46
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.45	0.46
8:V:126:SER:O	8:V:127:LEU:HD12	2.16	0.46
10:X:35:THR:HG21	10:X:182:LYS:HD2	1.98	0.46
13:a:27:LEU:CD2	13:a:190:ARG:O	2.63	0.46
7:U:34:LEU:C	7:U:34:LEU:HD23	2.41	0.46
1:A:119:GLN:O	1:A:122:THR:HB	2.15	0.46
10:J:35:THR:HG21	10:J:182:LYS:HD2	1.98	0.46
11:K:159:ARG:NH2	10:X:146:HIS:ND1	2.64	0.46
5:E:65:CYS:SG	5:E:71:LEU:CD1	3.04	0.45
10:J:18:SER:HB2	10:J:176:PHE:HB2	1.98	0.45
11:K:6:PHE:HA	11:K:125:ASP:O	2.16	0.45
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.98	0.45
10:X:3:ILE:HD12	10:X:176:PHE:CD2	2.51	0.45
12:Z:4:PRO:O	13:a:104:ARG:NH1	2.46	0.45
14:b:83:LYS:HB2	14:b:119:VAL:HG22	1.98	0.45
12:L:4:PRO:O	13:M:104:ARG:NH1	2.46	0.45
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:30:TYR:HB3	13:a:34:LEU:HB2	1.97	0.45
11:K:95:LEU:HD13	11:K:97:MET:HE1	1.97	0.45
13:a:43:ILE:HD12	13:a:64:GLU:HG3	1.98	0.45
14:b:165:TRP:CD1	14:b:165:TRP:O	2.70	0.45
6:F:123:ASN:HD22	6:F:124:SER:N	2.14	0.45
11:K:197:PHE:CE2	9:W:203:GLN:HG3	2.52	0.45
7:U:83:ASN:C	7:U:83:ASN:ND2	2.75	0.45
7:U:66:ILE:HB	7:U:70:ILE:HG22	1.98	0.45
9:I:56:ALA:HB3	10:J:124:THR:HG23	1.98	0.45
14:N:155:ILE:HG21	14:N:175:MET:HE3	1.99	0.45
11:K:185:TRP:CE3	11:K:185:TRP:O	2.70	0.45
14:N:135:TYR:CD2	14:N:135:TYR:O	2.70	0.45
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.45
7:U:78:ILE:HG22	7:U:79:PRO:HD3	1.99	0.45
12:L:108:HIS:HD2	12:L:139:GLY:CA	2.31	0.44
11:Y:12:ILE:HG23	11:Y:112:ILE:HD11	2.00	0.44
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	1.99	0.44
10:J:3:ILE:HD12	10:J:176:PHE:CD2	2.52	0.44
10:J:144:LEU:O	10:J:148:TYR:HB3	2.18	0.44
11:Y:4:LEU:CD1	11:Y:161:ILE:CD1	2.95	0.44
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.00	0.44
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.53	0.44
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.50	0.44
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.16	0.44
10:J:177:LYS:NZ	10:X:169:GLU:O	2.50	0.44
11:Y:197:PHE:HZ	11:Y:210:VAL:HG21	1.82	0.44
12:Z:141:ALA:HB1	12:Z:195:HIS:NE2	2.32	0.44
3:C:201:VAL:O	3:C:202:GLN:CB	2.66	0.44
11:K:16:VAL:HG21	11:K:34:VAL:HG23	2.00	0.44
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.48	0.44
14:b:141:ASN:HD22	14:b:141:ASN:HA	1.54	0.44
7:G:78:ILE:HG22	7:G:79:PRO:HD3	1.99	0.44
8:H:163:ILE:HG23	8:H:170:GLY:HA2	2.00	0.44
11:K:4:LEU:C	11:K:4:LEU:CD2	2.91	0.44
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.17	0.44
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.99	0.44
7:G:83:ASN:C	7:G:83:ASN:HD22	2.26	0.44
8:H:62:ASN:HB3	8:H:82:MET:HE1	2.00	0.44
1:O:115:ALA:HB1	1:O:154:GLY:O	2.18	0.44
13:M:54:SER:OG	13:M:113:ALA:HB3	2.17	0.43
5:E:77:ALA:N	5:E:78:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:92:ASN:CG	12:L:70:ASN:HD21	2.27	0.43
9:I:203:GLN:HG3	11:Y:197:PHE:CE2	2.52	0.43
8:V:146:LEU:HD22	8:V:150:GLU:HB3	2.00	0.43
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.99	0.43
14:b:155:ILE:HG21	14:b:175:MET:HE3	2.00	0.43
10:J:143:LEU:CD2	10:J:147:HIS:ND1	2.78	0.43
11:K:4:LEU:CD1	11:K:161:ILE:CD1	2.96	0.43
14:N:13:ILE:HG21	14:N:175:MET:HE2	2.01	0.43
14:N:32:ASP:OD2	14:N:185:ARG:NH2	2.51	0.43
5:S:77:ALA:N	5:S:78:PRO:CD	2.81	0.43
11:Y:2:THR:HG21	11:Y:164:ALA:CB	2.47	0.43
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.99	0.43
12:L:1:GLN:HE21	13:M:1:THR:CG2	2.31	0.43
13:M:27:LEU:HD23	13:M:190:ARG:O	2.18	0.43
14:N:83:LYS:HB2	14:N:119:VAL:HG22	1.99	0.43
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.99	0.43
8:H:146:LEU:HD22	8:H:150:GLU:HB3	2.00	0.43
11:K:2:THR:HG21	11:K:164:ALA:CB	2.49	0.43
12:L:220:LYS:HE3	8:V:194:ASN:HB3	2.00	0.43
8:V:137:VAL:HG21	8:V:161:ALA:HB2	1.99	0.43
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.01	0.43
9:I:147:GLY:HA3	12:Z:145:LEU:O	2.18	0.43
11:K:36:GLU:O	11:K:38:ASN:N	2.52	0.43
14:N:139:ASP:OD1	14:N:139:ASP:N	2.44	0.43
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.53	0.43
12:Z:108:HIS:HD2	12:Z:139:GLY:CA	2.32	0.43
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.99	0.43
8:H:137:VAL:HG21	8:H:161:ALA:HB2	2.00	0.43
11:K:176:ASN:HD21	11:K:190:ASN:HB2	1.82	0.43
14:N:35:THR:CG2	13:a:228:TYR:HE2	2.32	0.43
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.66	0.43
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.01	0.43
10:X:144:LEU:HD12	10:X:144:LEU:HA	1.81	0.43
4:D:113:LEU:HD12	5:E:78:PRO:HB2	2.00	0.43
5:S:92:ASN:CG	12:Z:70:ASN:HD21	2.25	0.43
7:U:73:VAL:HG12	7:U:133:THR:HB	2.00	0.43
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.49	0.43
11:Y:176:ASN:HD21	11:Y:190:ASN:HB2	1.84	0.43
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.48	0.43
12:Z:134:GLU:OE1	12:Z:137:ARG:NH2	2.52	0.43
2:B:86:LEU:HB3	2:B:114:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:68:ARG:HE	7:G:68:ARG:HB2	1.37	0.43
6:T:123:ASN:HD22	6:T:124:SER:N	2.17	0.43
8:V:62:ASN:HB3	8:V:82:MET:HE1	2.00	0.43
11:Y:104:TYR:CE2	11:Y:109:GLY:HA2	2.53	0.43
7:G:73:VAL:HG12	7:G:133:THR:HB	2.00	0.42
14:N:55:ILE:HD11	14:N:93:LEU:CD1	2.48	0.42
2:P:86:LEU:HB3	2:P:114:LEU:HD21	2.01	0.42
13:a:96:LEU:O	13:a:100:MET:HG2	2.19	0.42
6:F:41:GLY:HA3	6:F:215:CYS:O	2.19	0.42
10:J:2:ASP:OD1	19:J:301:HOH:O	2.22	0.42
14:b:48:SER:HB3	14:b:51:ASP:HB2	2.01	0.42
10:J:143:LEU:CD2	10:J:147:HIS:CE1	3.02	0.42
11:K:104:TYR:CE2	11:K:109:GLY:HA2	2.55	0.42
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.00	0.42
9:W:56:ALA:HB3	10:X:124:THR:HG23	2.01	0.42
14:b:55:ILE:HD11	14:b:93:LEU:CD1	2.48	0.42
2:B:161:ALA:HB3	3:C:52:LEU:HD23	2.01	0.42
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.01	0.42
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.55	0.42
11:K:104:TYR:CD1	11:K:104:TYR:C	2.98	0.42
14:N:35:THR:HG21	13:a:228:TYR:CE2	2.53	0.42
5:S:65:CYS:SG	5:S:71:LEU:CD1	3.07	0.42
11:K:12:ILE:HG23	11:K:112:ILE:HD11	2.02	0.42
12:L:141:ALA:HB1	12:L:195:HIS:NE2	2.34	0.42
13:a:54:SER:OG	13:a:113:ALA:HB3	2.19	0.42
10:J:169:GLU:O	10:X:177:LYS:NZ	2.52	0.42
13:M:10:SER:HB3	13:M:147:GLY:H	1.84	0.42
6:T:41:GLY:HA3	6:T:215:CYS:O	2.19	0.42
11:Y:100:MET:HE3	11:Y:127:PHE:CB	2.49	0.42
11:K:161:ILE:HD13	11:K:161:ILE:HA	1.91	0.42
8:V:163:ILE:HG23	8:V:170:GLY:HA2	2.01	0.42
11:Y:4:LEU:HD22	11:Y:4:LEU:O	2.20	0.42
11:Y:36:GLU:O	11:Y:38:ASN:N	2.52	0.42
13:a:10:SER:HB3	13:a:147:GLY:H	1.85	0.42
10:J:126:VAL:CG1	10:J:128:LEU:HG	2.50	0.42
13:M:206:LEU:O	13:M:206:LEU:HG	2.12	0.42
11:Y:86:LEU:HD13	11:Y:86:LEU:C	2.45	0.42
1:A:115:ALA:HB1	1:A:154:GLY:O	2.19	0.41
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.49	0.41
8:H:194:ASN:HB3	12:Z:220:LYS:HE3	2.02	0.41
13:M:127:LEU:O	13:M:138:SER:OG	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:1:GLN:HE21	13:a:1:THR:CG2	2.31	0.41
5:S:71:LEU:C	5:S:71:LEU:CD2	2.93	0.41
5:S:71:LEU:C	5:S:71:LEU:HD22	2.45	0.41
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.93	0.41
11:Y:50:ALA:CB	12:Z:128:VAL:HG23	2.50	0.41
3:C:208:ILE:N	19:C:302:HOH:O	2.50	0.41
11:Y:211:ILE:O	11:Y:211:ILE:HG22	2.19	0.41
11:K:12:ILE:HB	11:K:180:VAL:HB	2.03	0.41
11:K:86:LEU:C	11:K:86:LEU:HD13	2.44	0.41
10:X:147:HIS:HB3	10:X:160:LEU:HD13	2.02	0.41
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.56	0.41
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	2.02	0.41
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.02	0.41
8:H:5:GLY:HA3	8:H:110:LEU:HD11	2.02	0.41
14:N:48:SER:HB3	14:N:51:ASP:HB2	2.02	0.41
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.51	0.41
7:U:72:MET:HE3	7:U:74:VAL:CG2	2.50	0.41
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.02	0.41
11:Y:104:TYR:CD1	11:Y:104:TYR:C	2.98	0.41
10:J:184:VAL:HG22	10:J:189:ILE:HG12	2.03	0.41
13:M:45:VAL:HG12	13:M:92:ILE:HD11	2.01	0.41
10:X:1:MET:HA	10:X:34:LYS:CE	2.51	0.41
13:a:53:ILE:HB	13:a:60:MET:HG3	2.02	0.41
3:C:77:ASN:N	3:C:77:ASN:HD22	2.18	0.41
13:M:212:LEU:HA	13:M:212:LEU:HD12	1.89	0.41
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.51	0.41
4:D:91:HIS:HB3	4:D:99:ILE:HG21	2.03	0.41
7:G:83:ASN:C	7:G:83:ASN:ND2	2.78	0.41
10:J:146:HIS:HE1	11:Y:204:GLU:OE1	2.03	0.41
13:M:53:ILE:HB	13:M:60:MET:HG3	2.03	0.41
8:V:5:GLY:HA3	8:V:110:LEU:HD11	2.02	0.41
10:X:126:VAL:CG1	10:X:128:LEU:HG	2.50	0.41
14:b:13:ILE:CG2	14:b:175:MET:HE2	2.51	0.41
14:b:14:LEU:HD23	14:b:44:CYS:SG	2.61	0.41
8:H:68:LEU:HD12	8:H:68:LEU:HA	1.89	0.41
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.03	0.41
8:V:35:HIS:HB3	8:V:56:THR:HG21	2.03	0.41
10:X:174:MET:N	10:X:174:MET:SD	2.94	0.41
11:Y:41:LEU:HD23	11:Y:41:LEU:HA	1.86	0.41
11:Y:181:THR:HB	11:Y:182:GLU:H	1.67	0.41
11:K:50:ALA:CB	12:L:128:VAL:HG23	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.40
14:N:148:LYS:NZ	14:N:184:GLU:OE2	2.54	0.40
8:V:210:THR:HG21	9:W:167:SER:HB3	2.02	0.40
1:A:149:GLN:O	1:A:156:TYR:HA	2.22	0.40
7:G:61:SER:OG	7:G:215:GLU:OE2	2.29	0.40
7:G:68:ARG:O	7:G:68:ARG:HG3	2.20	0.40
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.54	0.40
10:J:144:LEU:HD12	10:J:144:LEU:HA	1.93	0.40
11:K:7:ARG:O	11:K:144:TYR:OH	2.35	0.40
13:a:129:TYR:O	13:a:136:THR:HA	2.21	0.40
13:a:187:ARG:HA	13:a:187:ARG:HD2	1.86	0.40
14:b:32:ASP:OD2	14:b:185:ARG:NH2	2.54	0.40
4:R:91:HIS:HB3	4:R:99:ILE:HG21	2.03	0.40
11:Y:4:LEU:HD12	11:Y:161:ILE:CD1	2.51	0.40
11:K:158:LYS:HB2	11:K:177:LEU:HD11	2.04	0.40
12:L:152:ASN:O	12:L:156:PHE:HA	2.21	0.40
13:M:47:ASP:N	13:M:47:ASP:OD1	2.54	0.40
14:N:190:PRO:HA	14:N:193:TYR:CE2	2.57	0.40
14:b:3:ILE:HG22	14:b:16:ALA:CB	2.52	0.40
3:Q:77:ASN:HD22	3:Q:77:ASN:N	2.19	0.40
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
1	O	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	16	37
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	16	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	9	25
3	Q	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	9	25
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
6	T	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
7	G	239/252 (95%)	233 (98%)	6 (2%)	0	100	100
7	U	239/252 (95%)	233 (98%)	6 (2%)	0	100	100
8	H	219/231 (95%)	215 (98%)	4 (2%)	0	100	100
8	V	219/231 (95%)	215 (98%)	4 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
11	K	209/211 (99%)	201 (96%)	6 (3%)	2 (1%)	12	32
11	Y	209/211 (99%)	203 (97%)	5 (2%)	1 (0%)	24	48
12	L	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
12	Z	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
13	M	231/246 (94%)	220 (95%)	10 (4%)	1 (0%)	30	54
13	a	231/246 (94%)	218 (94%)	12 (5%)	1 (0%)	30	54
14	N	193/195 (99%)	183 (95%)	9 (5%)	1 (0%)	24	48
14	b	193/195 (99%)	186 (96%)	6 (3%)	1 (0%)	24	48
15	d	1/4 (25%)	1 (100%)	0	0	100	100
15	e	1/4 (25%)	1 (100%)	0	0	100	100
15	f	1/4 (25%)	1 (100%)	0	0	100	100
15	g	1/4 (25%)	1 (100%)	0	0	100	100
15	h	1/4 (25%)	1 (100%)	0	0	100	100
15	i	1/4 (25%)	1 (100%)	0	0	100	100
All	All	6276/6632 (95%)	6095 (97%)	164 (3%)	17 (0%)	36	60

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
11	K	37	ILE
2	P	51	VAL
3	Q	202	GLN
11	Y	37	ILE
3	C	205	ALA
11	K	211	ILE
3	Q	205	ALA
2	B	221	ASP
14	N	137	TYR
2	P	221	ASP
14	b	137	TYR
3	C	239	GLN
3	Q	239	GLN
13	M	31	GLY
13	a	31	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	204 (98%)	5 (2%)	43	72
1	O	209/209 (100%)	204 (98%)	5 (2%)	43	72
2	B	203/216 (94%)	195 (96%)	8 (4%)	28	57
2	P	203/216 (94%)	195 (96%)	8 (4%)	28	57
3	C	212/226 (94%)	207 (98%)	5 (2%)	43	72
3	Q	212/226 (94%)	206 (97%)	6 (3%)	38	68
4	D	194/215 (90%)	185 (95%)	9 (5%)	24	51
4	R	194/215 (90%)	186 (96%)	8 (4%)	27	56
5	E	190/193 (98%)	185 (97%)	5 (3%)	40	70
5	S	190/193 (98%)	185 (97%)	5 (3%)	40	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	201/239 (84%)	194 (96%)	7 (4%)	32	61
6	T	201/239 (84%)	193 (96%)	8 (4%)	28	56
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	62
7	U	206/210 (98%)	198 (96%)	8 (4%)	28	57
8	H	180/189 (95%)	172 (96%)	8 (4%)	25	53
8	V	180/189 (95%)	173 (96%)	7 (4%)	28	57
9	I	172/173 (99%)	170 (99%)	2 (1%)	63	84
9	W	172/173 (99%)	170 (99%)	2 (1%)	63	84
10	J	173/175 (99%)	162 (94%)	11 (6%)	16	38
10	X	173/175 (99%)	164 (95%)	9 (5%)	21	47
11	K	168/168 (100%)	152 (90%)	16 (10%)	8	20
11	Y	168/168 (100%)	152 (90%)	16 (10%)	8	20
12	L	185/185 (100%)	179 (97%)	6 (3%)	34	64
12	Z	185/185 (100%)	177 (96%)	8 (4%)	26	54
13	M	199/208 (96%)	184 (92%)	15 (8%)	12	31
13	a	199/208 (96%)	187 (94%)	12 (6%)	17	41
14	N	162/162 (100%)	142 (88%)	20 (12%)	4	12
14	b	162/162 (100%)	143 (88%)	19 (12%)	5	13
15	d	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	e	2/2 (100%)	2 (100%)	0	100	100
15	f	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	g	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	h	2/2 (100%)	2 (100%)	0	100	100
15	i	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	5320/5548 (96%)	5071 (95%)	249 (5%)	23	51

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	250	LEU

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Mol	Chain	Res	Type
2	B	50	LYS
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	114	LEU
2	B	184	LYS
2	B	191	LEU
2	B	220	ASN
3	C	4	ARG
3	C	38	ASN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
4	D	60	VAL
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	197	LYS
4	D	214	ILE
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	188	LEU
6	F	68	ARG
6	F	94	SER
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	206	LYS
6	F	221	ASN
7	G	68	ARG
7	G	72	MET
7	G	83	ASN
7	G	115	LEU
7	G	125	MET
7	G	181	LYS
7	G	235	ARG
8	H	22	GLN

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Mol	Chain	Res	Type
8	H	31	CYS
8	H	34	LEU
8	H	38	SER
8	H	56	THR
8	H	68	LEU
8	H	120	ASP
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	23	ARG
10	J	35	THR
10	J	126	VAL
10	J	127	GLU
10	J	143	LEU
10	J	144	LEU
10	J	149	ARG
10	J	153	THR
10	J	172	MET
10	J	174	MET
10	J	193	ASP
11	K	4	LEU
11	K	9	GLN
11	K	31	VAL
11	K	35	ILE
11	K	38	ASN
11	K	71	LYS
11	K	73	ARG
11	K	99	THR
11	K	117	SER
11	K	118	ASP
11	K	142	SER
11	K	148	LEU
11	K	181	THR
11	K	183	ASP
11	K	210	VAL
11	K	211	ILE
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	130	SER
12	L	150	LEU
12	L	167	LYS

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Mol	Chain	Res	Type
13	M	3	GLN
13	M	29	SER
13	M	30	TYR
13	M	32	SER
13	M	39	VAL
13	M	45	VAL
13	M	48	ASN
13	M	49	THR
13	M	70	LEU
13	M	104	ARG
13	M	187	ARG
13	M	206	LEU
13	M	210	LYS
13	M	212	LEU
13	M	213	GLN
14	N	9	LYS
14	N	13	ILE
14	N	14	LEU
14	N	22	THR
14	N	35	THR
14	N	94	THR
14	N	119	VAL
14	N	126	ILE
14	N	128	VAL
14	N	131	SER
14	N	139	ASP
14	N	140	LYS
14	N	141	ASN
14	N	143	ARG
14	N	147	SER
14	N	149	GLU
14	N	157	HIS
14	N	165	TRP
14	N	178	LEU
14	N	183	VAL
1	O	17	LYS
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU

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Mol	Chain	Res	Type
2	P	58	GLN
2	P	79	LEU
2	P	114	LEU
2	P	184	LYS
2	P	191	LEU
2	P	220	ASN
3	Q	4	ARG
3	Q	38	ASN
3	Q	77	ASN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	197	LYS
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	188	LEU
6	T	2	THR
6	T	68	ARG
6	T	94	SER
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	206	LYS
6	T	221	ASN
7	U	13	GLU
7	U	26	THR
7	U	83	ASN
7	U	115	LEU
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
8	V	22	GLN

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Mol	Chain	Res	Type
8	V	34	LEU
8	V	38	SER
8	V	56	THR
8	V	68	LEU
8	V	120	ASP
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	23	ARG
10	X	35	THR
10	X	126	VAL
10	X	127	GLU
10	X	136	SER
10	X	144	LEU
10	X	172	MET
10	X	174	MET
10	X	193	ASP
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	38	ASN
11	Y	45	MET
11	Y	67	GLU
11	Y	71	LYS
11	Y	73	ARG
11	Y	99	THR
11	Y	100	MET
11	Y	117	SER
11	Y	118	ASP
11	Y	142	SER
11	Y	181	THR
11	Y	209	ASN
11	Y	211	ILE
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	130	SER
12	Z	132	GLU
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
13	a	3	GLN

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Mol	Chain	Res	Type
13	a	10	SER
13	a	29	SER
13	a	30	TYR
13	a	32	SER
13	a	37	ASN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	187	ARG
13	a	206	LEU
13	a	213	GLN
14	b	9	LYS
14	b	13	ILE
14	b	14	LEU
14	b	22	THR
14	b	35	THR
14	b	94	THR
14	b	119	VAL
14	b	135	TYR
14	b	139	ASP
14	b	140	LYS
14	b	141	ASN
14	b	143	ARG
14	b	147	SER
14	b	148	LYS
14	b	149	GLU
14	b	157	HIS
14	b	164	LYS
14	b	165	TRP
14	b	178	LEU
15	d	3	LEU
15	f	3	LEU
15	g	3	LEU
15	i	3	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (195) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
2	B	20	GLN
2	B	93	HIS
2	B	95	GLN

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Mol	Chain	Res	Type
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	155	ASN
2	B	176	GLN
2	B	232	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	165	ASN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	106	GLN
4	D	146	GLN
4	D	160	ASN
4	D	198	GLN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	147	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	143	HIS
6	F	178	HIS
6	F	191	GLN
6	F	203	ASN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	117	GLN

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Mol	Chain	Res	Type
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	22	GLN
8	H	30	ASN
8	H	35	HIS
8	H	57	GLN
8	H	66	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	31	GLN
9	I	44	HIS
9	I	63	ASN
9	I	88	GLN
9	I	168	GLN
9	I	203	GLN
10	J	37	GLN
10	J	55	GLN
10	J	63	ASN
10	J	191	GLN
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	143	ASN
11	K	176	ASN
11	K	188	HIS
11	K	209	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	80	ASN
12	L	152	ASN
12	L	153	GLN
12	L	158	ASN
12	L	165	ASN
12	L	197	GLN
13	M	18	ASN
13	M	26	ASN

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Mol	Chain	Res	Type
13	M	37	ASN
13	M	48	ASN
13	M	108	ASN
13	M	179	ASN
13	M	194	ASN
13	M	211	ASN
13	M	213	GLN
14	N	69	GLN
14	N	141	ASN
2	P	20	GLN
2	P	93	HIS
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	176	GLN
2	P	232	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	165	ASN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	146	GLN
4	R	160	ASN
4	R	198	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	147	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN

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Mol	Chain	Res	Type
6	T	117	GLN
6	T	123	ASN
6	T	143	HIS
6	T	191	GLN
6	T	203	ASN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
8	V	22	GLN
8	V	30	ASN
8	V	35	HIS
8	V	57	GLN
8	V	66	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	31	GLN
9	W	37	ASN
9	W	44	HIS
9	W	63	ASN
9	W	88	GLN
9	W	168	GLN
9	W	203	GLN
10	X	37	GLN
10	X	55	GLN
10	X	63	ASN
10	X	147	HIS
10	X	191	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	176	ASN
11	Y	188	HIS
11	Y	208	ASN
11	Y	209	ASN
12	Z	1	GLN
12	Z	3	ASN

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Mol	Chain	Res	Type
12	Z	29	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	80	ASN
12	Z	135	GLN
12	Z	152	ASN
12	Z	153	GLN
12	Z	158	ASN
12	Z	197	GLN
13	a	18	ASN
13	a	26	ASN
13	a	37	ASN
13	a	48	ASN
13	a	108	ASN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	69	GLN
14	b	141	ASN
14	b	145	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	A1I48	h	4	15,11	12,14,15	1.37	1 (8%)	10,18,20	1.48	3 (30%)
15	A1I48	i	4	15,14	12,14,15	1.55	1 (8%)	10,18,20	1.53	1 (10%)
15	A1I48	e	4	15,11	12,14,15	1.12	1 (8%)	10,18,20	1.24	1 (10%)
15	A1I48	f	4	15,14	12,14,15	1.18	1 (8%)	10,18,20	1.12	1 (10%)
15	A1I48	d	4	15,8	12,14,15	1.38	1 (8%)	10,18,20	1.58	2 (20%)
15	A1I48	g	4	15,8	12,14,15	1.38	1 (8%)	10,18,20	1.55	2 (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
15	A1I48	h	4	15,11	-	4/15/18/20	-
15	A1I48	i	4	15,14	-	3/15/18/20	-
15	A1I48	e	4	15,11	-	4/15/18/20	-
15	A1I48	f	4	15,14	-	3/15/18/20	-
15	A1I48	d	4	15,8	-	4/15/18/20	-
15	A1I48	g	4	15,8	-	4/15/18/20	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	i	4	A1I48	CA-N2	-4.93	1.33	1.47
15	g	4	A1I48	CA-N2	-4.25	1.35	1.47
15	h	4	A1I48	CA-N2	-4.23	1.35	1.47
15	d	4	A1I48	CA-N2	-4.22	1.35	1.47
15	f	4	A1I48	CA-N2	-3.44	1.37	1.47
15	e	4	A1I48	CA-N2	-3.14	1.38	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	i	4	A1I48	CB-CA-N2	-3.65	90.29	114.17
15	g	4	A1I48	CB-CA-N2	-3.33	92.44	114.17
15	d	4	A1I48	CB-CA-N2	-3.33	92.44	114.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	h	4	A1I48	CB-CA-N2	-2.61	97.13	114.17
15	f	4	A1I48	O-C-CA	-2.25	119.00	124.77
15	d	4	A1I48	CG2-CB-CA	2.21	117.58	113.26
15	g	4	A1I48	CG2-CB-CA	2.16	117.46	113.26
15	h	4	A1I48	CG2-CB-CA	2.15	117.45	113.26
15	h	4	A1I48	OG1-CB-CG2	-2.10	103.49	109.53
15	e	4	A1I48	CG2-CB-CA	2.02	117.19	113.26

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	d	4	A1I48	O23-C22-OG1-CB
15	d	4	A1I48	O-C-CA-CB
15	e	4	A1I48	O23-C22-OG1-CB
15	e	4	A1I48	O-C-CA-CB
15	f	4	A1I48	O23-C22-OG1-CB
15	g	4	A1I48	O23-C22-OG1-CB
15	g	4	A1I48	O-C-CA-CB
15	h	4	A1I48	O23-C22-OG1-CB
15	h	4	A1I48	O-C-CA-CB
15	i	4	A1I48	O23-C22-OG1-CB
15	e	4	A1I48	C-CA-CB-CG2
15	f	4	A1I48	C-CA-CB-CG2
15	h	4	A1I48	C-CA-CB-CG2
15	i	4	A1I48	C-CA-CB-CG2
15	e	4	A1I48	C-CA-CB-OG1
15	f	4	A1I48	C-CA-CB-OG1
15	h	4	A1I48	C-CA-CB-OG1
15	d	4	A1I48	C-CA-CB-CG2
15	g	4	A1I48	C-CA-CB-CG2
15	d	4	A1I48	C-CA-CB-OG1
15	g	4	A1I48	C-CA-CB-OG1
15	i	4	A1I48	C-CA-CB-OG1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	MES	a	301	-	12,12,12	0.67	0	15,16,16	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MES	a	301	-	-	3/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	a	301	MES	C7-C8-S-O2S
18	a	301	MES	C7-C8-S-O3S
18	a	301	MES	C7-C8-S-O1S

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 ⓘ

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%)	-0.64	1 (0%) 88 87	54, 70, 101, 177	0
1	O	250/250 (100%)	-0.59	1 (0%) 88 87	59, 77, 115, 172	0
2	B	244/258 (94%)	-0.48	3 (1%) 76 75	56, 74, 121, 169	0
2	P	244/258 (94%)	-0.44	2 (0%) 82 81	61, 79, 124, 173	0
3	C	240/254 (94%)	-0.53	1 (0%) 88 87	56, 77, 131, 156	0
3	Q	240/254 (94%)	-0.39	4 (1%) 69 67	60, 90, 152, 178	0
4	D	235/260 (90%)	-0.58	0 100 100	58, 79, 110, 151	0
4	R	235/260 (90%)	-0.50	1 (0%) 88 87	56, 80, 115, 151	0
5	E	231/234 (98%)	-0.57	0 100 100	59, 82, 114, 139	0
5	S	231/234 (98%)	-0.48	0 100 100	62, 86, 120, 157	0
6	F	243/288 (84%)	-0.55	1 (0%) 88 87	55, 77, 117, 140	0
6	T	243/288 (84%)	-0.50	0 100 100	58, 83, 128, 147	0
7	G	241/252 (95%)	-0.60	0 100 100	54, 70, 100, 134	0
7	U	241/252 (95%)	-0.60	0 100 100	58, 73, 104, 143	0
8	H	221/231 (95%)	-0.70	0 100 100	54, 66, 89, 120	0
8	V	221/231 (95%)	-0.66	0 100 100	56, 69, 91, 135	0
9	I	204/205 (99%)	-0.72	0 100 100	50, 65, 90, 117	0
9	W	204/205 (99%)	-0.73	0 100 100	51, 68, 96, 116	0
10	J	195/198 (98%)	-0.52	1 (0%) 87 86	52, 68, 95, 128	0
10	X	195/198 (98%)	-0.52	1 (0%) 87 86	55, 72, 94, 138	0
11	K	211/211 (100%)	-0.63	0 100 100	53, 66, 91, 177	0
11	Y	211/211 (100%)	-0.57	0 100 100	52, 67, 96, 181	0
12	L	222/222 (100%)	-0.52	2 (0%) 81 80	52, 70, 101, 121	0
12	Z	222/222 (100%)	-0.55	1 (0%) 87 86	53, 67, 99, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.66	1 (0%) 88 87	53, 71, 91, 111	0
13	a	233/246 (94%)	-0.69	0 100 100	51, 69, 91, 111	0
14	N	195/195 (100%)	-0.52	1 (0%) 87 86	53, 69, 117, 149	0
14	b	195/195 (100%)	-0.53	0 100 100	52, 69, 118, 151	0
15	d	2/4 (50%)	0.03	0 100 100	87, 87, 87, 96	0
15	e	2/4 (50%)	-0.69	0 100 100	71, 71, 71, 71	0
15	f	2/4 (50%)	-0.28	0 100 100	86, 86, 86, 89	0
15	g	2/4 (50%)	0.91	0 100 100	92, 92, 92, 101	0
15	h	2/4 (50%)	-1.14	0 100 100	77, 77, 77, 77	0
15	i	2/4 (50%)	-0.07	0 100 100	81, 81, 81, 84	0
All	All	6342/6632 (95%)	-0.57	21 (0%) 90 89	50, 73, 114, 181	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	205	ALA	4.2
10	X	1	MET	3.8
14	N	135	TYR	3.6
1	A	1	MET	3.4
2	B	219	ALA	3.4
1	O	1	MET	3.3
2	P	219	ALA	3.3
3	Q	50	LEU	2.8
3	Q	51	LYS	2.7
10	J	1	MET	2.7
13	M	1	THR	2.6
12	Z	160	TYR	2.6
2	B	218	GLY	2.5
2	B	51	VAL	2.5
2	P	51	VAL	2.5
4	R	113	LEU	2.5
3	C	205	ALA	2.4
3	Q	49	THR	2.3
12	L	136	CYS	2.2
6	F	215	CYS	2.1
12	L	170	LYS	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(Å ²)	Q<0.9
15	A1I48	f	4	15/16	0.94	0.11	69,75,88,93	0
15	A1I48	d	4	15/16	0.95	0.11	62,76,89,90	0
15	A1I48	h	4	15/16	0.95	0.09	67,71,73,74	0
15	A1I48	g	4	15/16	0.96	0.09	66,77,86,90	0
15	A1I48	i	4	15/16	0.97	0.09	71,80,84,84	0
15	A1I48	e	4	15/16	0.98	0.06	62,67,70,71	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(Å ²)	Q<0.9
16	MG	I	301	1/1	0.85	0.17	109,109,109,109	0
18	MES	a	301	12/12	0.87	0.14	122,130,143,149	0
16	MG	Z	301	1/1	0.93	0.13	99,99,99,99	0
16	MG	G	301	1/1	0.93	0.11	82,82,82,82	0
16	MG	J	201	1/1	0.94	0.10	30,30,30,30	0
17	CL	G	303	1/1	0.95	0.21	30,30,30,30	0
17	CL	U	301	1/1	0.97	0.04	70,70,70,70	0
17	CL	G	302	1/1	0.98	0.03	64,64,64,64	0
17	CL	b	201	1/1	0.98	0.06	81,81,81,81	0
17	CL	N	201	1/1	0.98	0.04	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.