



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2025 – 11:18 am BST

PDB ID : 9QDS / pdb_00009qds
Title : Yeast 20S proteasome mutant: beta1_G128V (b1-propeptide deleted) in complex with Carfilzomib
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2025-03-06
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

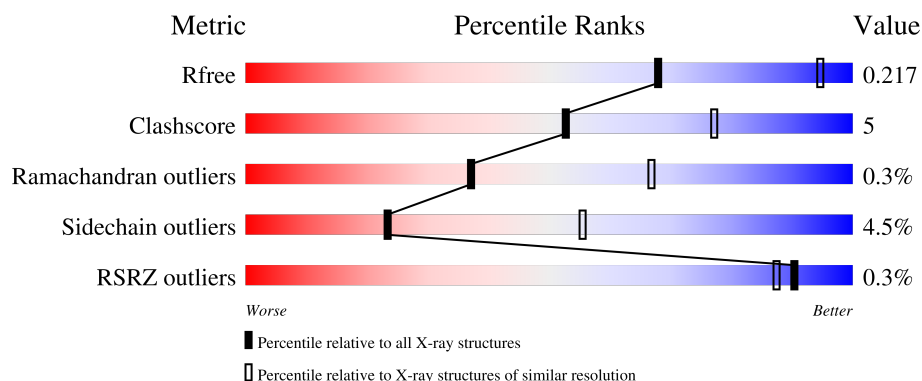
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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







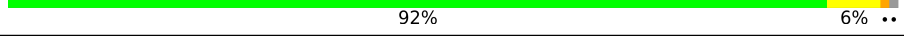



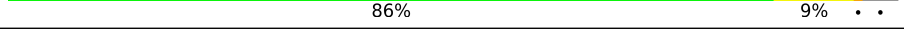

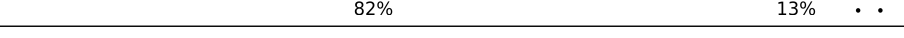
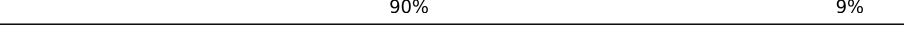




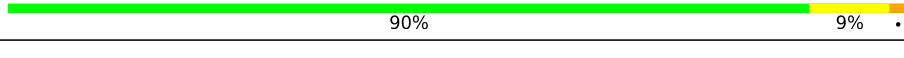

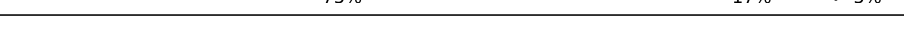


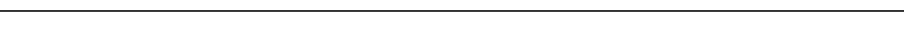
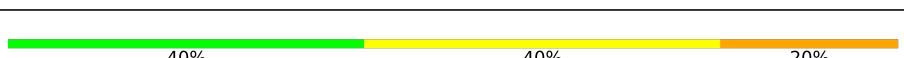


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	231	
8	V	231	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	211	
11	Y	211	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	195	
14	b	195	
15	d	5	
15	e	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	f	5	<div><div></div><div></div><div></div><div>20%</div><div>40%</div><div>40%</div></div>
15	g	5	<div><div></div><div></div><div></div><div>40%</div><div>60%</div><div></div></div>
15	h	5	<div><div></div><div></div><div></div><div>40%</div><div>40%</div><div>20%</div></div>
15	i	5	<div><div></div><div></div><div></div><div>20%</div><div>40%</div><div>40%</div></div>

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49954 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			

Continued on next page...

Continued from previous page...

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	1	0
			1767	1121	306	336	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	5	Total	C	N	O	0	0	0
			59	44	6	9			
15	e	5	Total	C	N	O	0	0	0
			59	44	6	9			
15	f	5	Total	C	N	O	0	0	0
			59	44	6	9			
15	g	5	Total	C	N	O	0	0	0
			59	44	6	9			
15	h	5	Total	C	N	O	0	0	0
			59	44	6	9			
15	i	5	Total	C	N	O	0	0	0
			59	44	6	9			

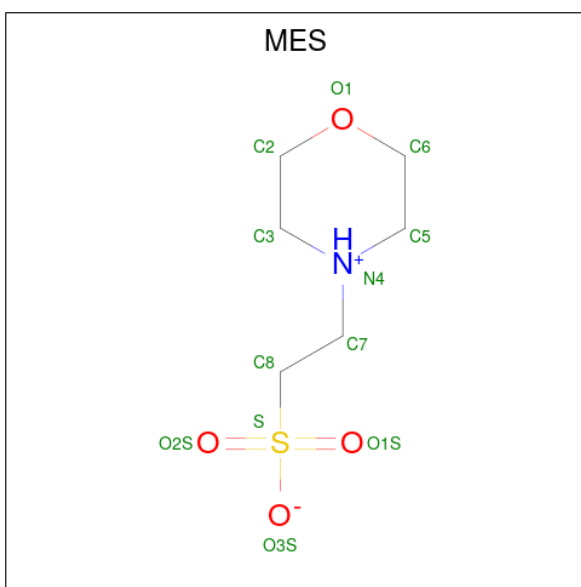
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	a	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	d	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	e	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	14	Total	O	0	0
			14	14		
19	C	7	Total	O	0	0
			7	7		
19	D	4	Total	O	0	0
			4	4		
19	E	7	Total	O	0	0
			7	7		
19	F	5	Total	O	0	0
			5	5		
19	G	13	Total	O	0	0
			13	13		
19	H	14	Total	O	0	0
			14	14		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	I	13	Total O 13 13	0	0
19	J	16	Total O 16 16	0	0
19	K	9	Total O 9 9	0	0
19	L	18	Total O 18 18	0	0
19	M	10	Total O 10 10	0	0
19	N	6	Total O 6 6	0	0
19	O	9	Total O 9 9	0	0
19	P	12	Total O 12 12	0	0
19	Q	9	Total O 9 9	0	0
19	R	6	Total O 6 6	0	0
19	S	2	Total O 2 2	0	0
19	T	7	Total O 7 7	0	0
19	U	8	Total O 8 8	0	0
19	V	14	Total O 14 14	0	0
19	W	7	Total O 7 7	0	0
19	X	12	Total O 12 12	0	0
19	Y	13	Total O 13 13	0	0
19	Z	7	Total O 7 7	0	0
19	a	10	Total O 10 10	0	0
19	b	9	Total O 9 9	0	0
19	e	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	f	2	Total 2	O 2	0	0
19	g	2	Total 2	O 2	0	0
19	i	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Proteasome subunit alpha type-2

Chain A:  95% .




- Molecule 1: Proteasome subunit alpha type-2

Chain O:  95% 5% .




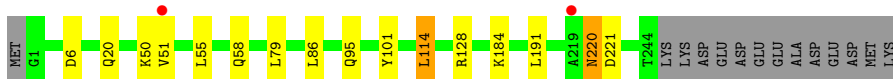
- Molecule 2: Proteasome subunit alpha type-3

Chain B:  88% 6% . 5% .




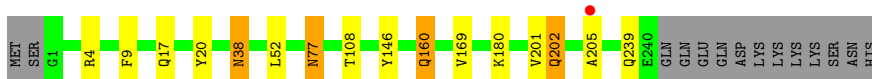
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  88% 5% . 5% .

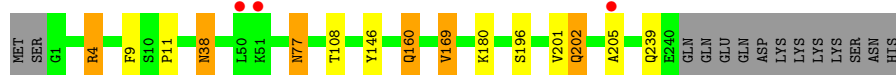
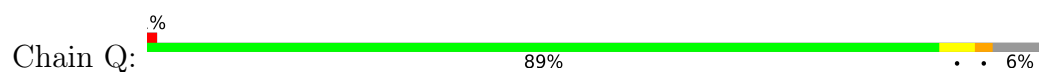


- Molecule 3: Proteasome subunit alpha type-4

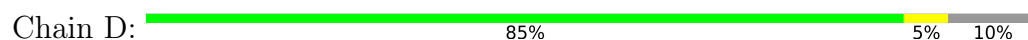
Chain C:  88% 5% . 6% .



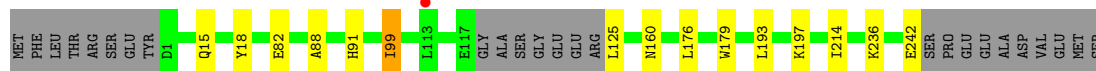
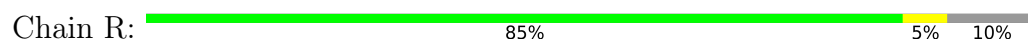
- Molecule 3: Proteasome subunit alpha type-4



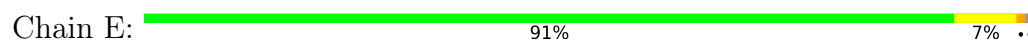
- Molecule 4: Proteasome subunit alpha type-5



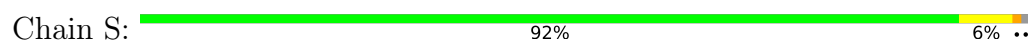
- Molecule 4: Proteasome subunit alpha type-5



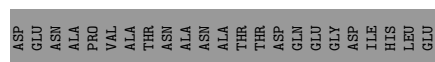
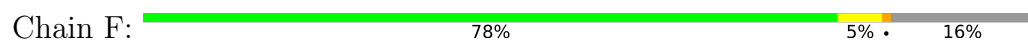
- Molecule 5: Proteasome subunit alpha type-6



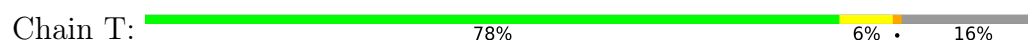
- Molecule 5: Proteasome subunit alpha type-6

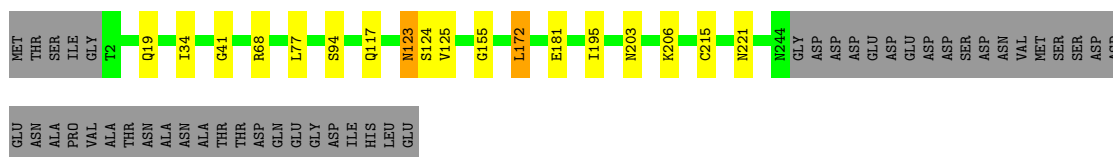


- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 6: Probable proteasome subunit alpha type-7





- Molecule 7: Proteasome subunit alpha type-1

Chain G: 88% 7% . .



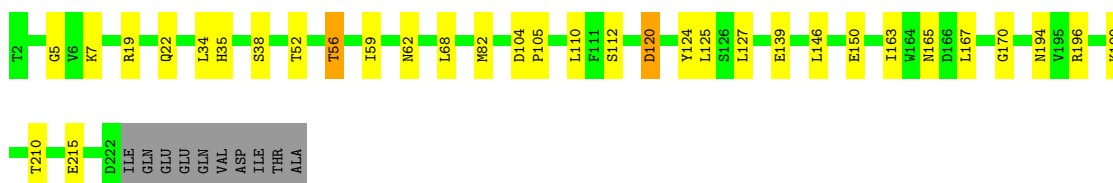
- Molecule 7: Proteasome subunit alpha type-1

Chain U: 86% 9% . .



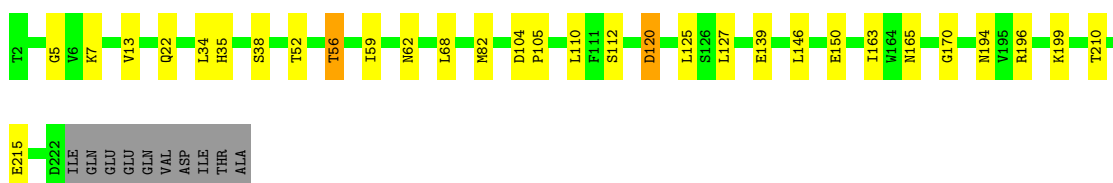
- Molecule 8: Proteasome subunit beta type-2

Chain H: 81% 13% . .



- Molecule 8: Proteasome subunit beta type-2

Chain V: 82% 13% . .



- Molecule 9: Proteasome subunit beta type-3

Chain I: 90% 9%

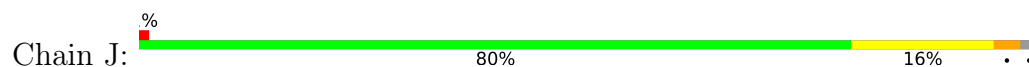


- Molecule 9: Proteasome subunit beta type-3

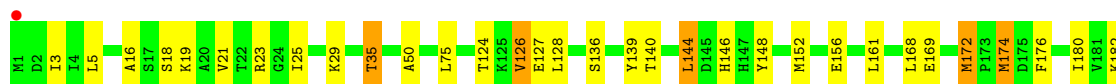
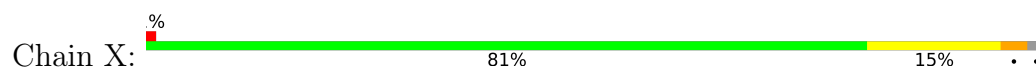
Chain W: 89% 9%



- Molecule 10: Proteasome subunit beta type-4



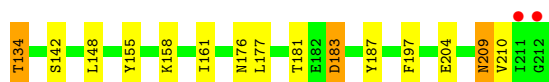
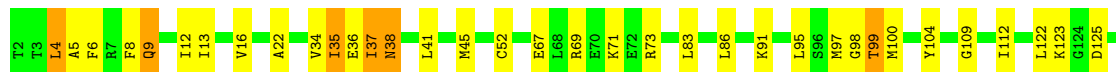
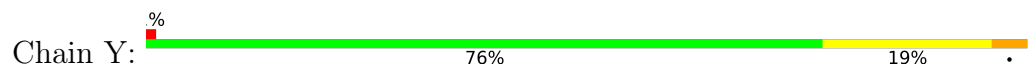
- Molecule 10: Proteasome subunit beta type-4



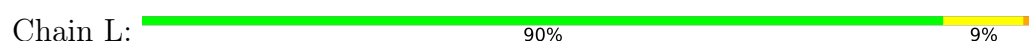
- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5

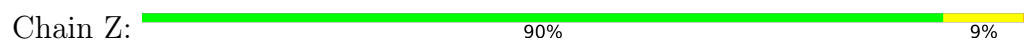


- Molecule 12: Proteasome subunit beta type-6

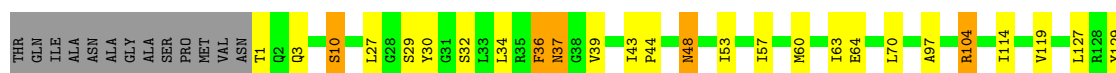
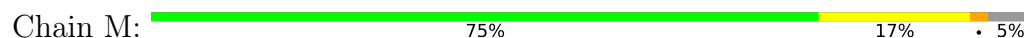




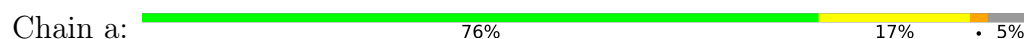
- Molecule 12: Proteasome subunit beta type-6



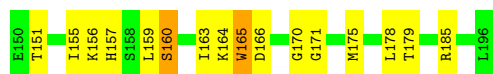
- Molecule 13: Proteasome subunit beta type-7



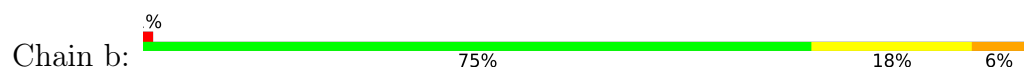
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1

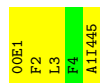


- Molecule 14: Proteasome subunit beta type-1

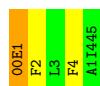




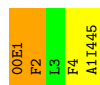
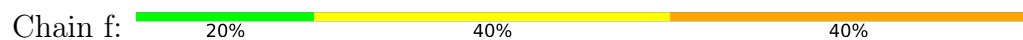
- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE



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



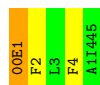
- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE



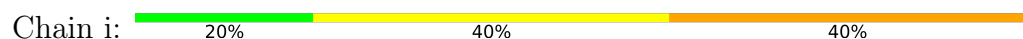
- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE



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



- 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	136.75Å 300.88Å 145.06Å 90.00° 113.56° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.7 (15.00-2.80) 95.7 (15.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.173 , 0.211 0.180 , 0.217	Depositor DCC
R_{free} test set	12570 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.3	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	0.96	EDS
Total number of atoms	49954	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: CL, A1I44, HPE, MES, MG, 00E

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	1.44	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	1.46	0/2586
3	Q	1.03	0/1910	1.47	0/2586
4	D	1.04	0/1837	1.48	2/2475 (0.1%)
4	R	1.04	0/1837	1.48	0/2475
5	E	1.03	0/1800	1.45	2/2433 (0.1%)
5	S	1.04	0/1800	1.45	4/2433 (0.2%)
6	F	1.02	0/1932	1.46	4/2609 (0.2%)
6	T	1.02	0/1932	1.47	4/2609 (0.2%)
7	G	1.01	0/1945	1.43	0/2634
7	U	1.01	0/1945	1.44	0/2634
8	H	0.99	0/1708	1.41	1/2316 (0.0%)
8	V	0.99	0/1708	1.42	1/2316 (0.0%)
9	I	1.01	0/1611	1.42	1/2174 (0.0%)
9	W	1.02	0/1611	1.41	2/2174 (0.1%)
10	J	1.00	0/1589	1.40	0/2142
10	X	0.99	0/1589	1.39	0/2142
11	K	0.97	0/1674	1.39	0/2264
11	Y	0.97	0/1674	1.42	0/2264
12	L	1.00	0/1795	1.39	0/2420
12	Z	1.01	0/1806	1.38	0/2435
13	M	0.99	0/1855	1.39	0/2514
13	a	1.00	0/1855	1.40	1/2514 (0.0%)
14	N	0.99	0/1537	1.42	1/2082 (0.0%)
14	b	0.99	0/1537	1.41	0/2082
15	d	1.12	0/19	1.24	0/24
15	e	1.16	0/19	1.51	1/24 (4.2%)
15	f	1.52	1/19 (5.3%)	1.44	0/24
15	g	1.09	0/19	1.25	0/24

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	h	1.17	0/19	1.51	1/24 (4.2%)
15	i	1.66	1/19 (5.3%)	1.74	0/24
All	All	1.01	2/50283 (0.0%)	1.43	25/67977 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	i	4	PHE	CB-CG	-6.12	1.36	1.50
15	f	4	PHE	CB-CG	-5.81	1.37	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	37	ASN	CA-CB-CG	8.45	121.05	112.60
14	N	94	THR	CB-CA-C	8.09	123.67	111.95
15	e	4	PHE	CA-CB-CG	-6.36	107.44	113.80
15	h	4	PHE	CA-CB-CG	-6.32	107.48	113.80
9	W	183	GLY	CA-C-O	-6.17	118.21	122.22
9	I	183	GLY	CA-C-O	-5.91	118.38	122.22
6	T	77	LEU	CA-C-N	5.62	124.83	120.33
6	T	77	LEU	C-N-CA	5.62	124.83	120.33
9	W	9	GLY	CA-C-O	-5.60	118.28	122.37
6	F	34	ILE	CA-C-N	5.49	125.38	121.65
6	F	34	ILE	C-N-CA	5.49	125.38	121.65
6	T	34	ILE	CA-C-N	5.48	125.38	121.65
6	T	34	ILE	C-N-CA	5.48	125.38	121.65
8	H	120	ASP	CA-CB-CG	5.29	117.89	112.60
8	V	120	ASP	CA-CB-CG	5.24	117.83	112.60
5	S	30	GLN	CA-C-N	5.14	124.99	120.10
5	S	30	GLN	C-N-CA	5.14	124.99	120.10
6	F	77	LEU	CA-C-N	5.09	124.41	120.33
6	F	77	LEU	C-N-CA	5.09	124.41	120.33
5	S	35	VAL	CA-C-N	5.05	125.09	121.65
5	S	35	VAL	C-N-CA	5.05	125.09	121.65
5	E	30	GLN	CA-C-N	5.02	124.87	120.10
5	E	30	GLN	C-N-CA	5.02	124.87	120.10
4	D	30	ILE	CA-C-N	5.00	125.05	121.65
4	D	30	ILE	C-N-CA	5.00	125.05	121.65

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	5	0
1	O	1915	0	1929	6	0
2	B	1904	0	1904	9	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	11	0
3	Q	1881	0	1895	11	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	7	0
5	E	1773	0	1775	14	0
5	S	1773	0	1775	12	0
6	F	1892	0	1883	8	0
6	T	1892	0	1883	7	0
7	G	1907	0	1901	13	0
7	U	1907	0	1901	13	0
8	H	1677	0	1678	19	0
8	V	1677	0	1678	17	0
9	I	1581	0	1574	14	0
9	W	1581	0	1574	15	0
10	J	1561	0	1569	32	0
10	X	1561	0	1569	35	0
11	K	1637	0	1585	55	0
11	Y	1637	0	1585	49	0
12	L	1757	0	1711	18	0
12	Z	1767	0	1717	17	0
13	M	1824	0	1832	37	0
13	a	1824	0	1832	31	0
14	N	1508	0	1477	60	0
14	b	1508	0	1477	52	0
15	d	59	0	40	3	0
15	e	59	0	40	2	0
15	f	59	0	40	3	0
15	g	59	0	40	2	0
15	h	59	0	40	4	0
15	i	59	0	40	5	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	V	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	Y	12	0	13	1	0
18	a	12	0	13	0	0
18	d	12	0	13	1	0
18	e	12	0	13	0	0
19	A	6	0	0	0	0
19	B	14	0	0	0	0
19	C	7	0	0	0	0
19	D	4	0	0	0	0
19	E	7	0	0	0	0
19	F	5	0	0	0	0
19	G	13	0	0	0	0
19	H	14	0	0	0	0
19	I	13	0	0	0	0
19	J	16	0	0	1	0
19	K	9	0	0	0	0
19	L	18	0	0	0	0
19	M	10	0	0	0	0
19	N	6	0	0	0	0
19	O	9	0	0	1	0
19	P	12	0	0	0	0
19	Q	9	0	0	0	0
19	R	6	0	0	0	0
19	S	2	0	0	0	0
19	T	7	0	0	0	0
19	U	8	0	0	0	0
19	V	14	0	0	0	0
19	W	7	0	0	0	0
19	X	12	0	0	1	0
19	Y	13	0	0	0	0
19	Z	7	0	0	0	0
19	a	10	0	0	0	0
19	b	9	0	0	0	0
19	e	1	0	0	0	0
19	f	2	0	0	0	0
19	g	2	0	0	0	0
19	i	1	0	0	1	0
All	All	49954	0	49318	486	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 (486) 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:b:135:TYR:HD1	14:b:136:GLY:N	1.37	1.20
13:M:37:ASN:CB	14:N:135:TYR:CE2	2.28	1.16
11:Y:5:ALA:HB3	11:Y:100:MET:HE3	1.17	1.16
14:b:135:TYR:CD1	14:b:136:GLY:N	2.13	1.14
13:M:37:ASN:HB3	14:N:135:TYR:HE2	1.09	1.08
13:M:37:ASN:HB3	14:N:135:TYR:CE2	1.86	1.06
14:N:135:TYR:CD1	14:N:136:GLY:N	2.25	1.03
14:b:165:TRP:CD1	14:b:165:TRP:C	2.38	1.01
14:b:165:TRP:C	14:b:165:TRP:HD1	1.68	1.01
14:N:165:TRP:HD1	14:N:165:TRP:C	1.69	1.00
14:N:165:TRP:C	14:N:165:TRP:CD1	2.40	0.98
11:Y:5:ALA:CB	11:Y:100:MET:CE	2.41	0.98
11:Y:5:ALA:CB	11:Y:100:MET:HE3	1.93	0.97
11:Y:5:ALA:HB3	11:Y:100:MET:CE	1.95	0.95
13:M:37:ASN:HB2	14:N:135:TYR:CE2	2.00	0.92
13:M:37:ASN:H	14:N:135:TYR:HD2	0.99	0.92
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.39	0.88
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.38	0.88
13:M:37:ASN:N	14:N:135:TYR:CD2	2.41	0.87
13:M:37:ASN:CB	14:N:135:TYR:HE2	1.75	0.86
10:J:152:MET:HE3	10:J:156:GLU:HB3	1.57	0.85
11:K:209:ASN:H	11:K:209:ASN:HD22	1.22	0.84
14:N:165:TRP:HD1	14:N:166:ASP:N	1.76	0.83
15:i:1:00E:HE2	19:i:101:HOH:O	1.78	0.82
14:N:135:TYR:HD1	14:N:136:GLY:N	1.75	0.82
11:K:159:ARG:HE	10:X:146:HIS:CE1	1.98	0.82
13:M:37:ASN:N	14:N:135:TYR:HD2	1.77	0.82
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.29	0.81
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.30	0.79
14:b:14:LEU:HD11	14:b:100:ALA:HB3	1.66	0.77
12:Z:108[B]:HIS:NE2	15:h:1:00E:HD1	1.99	0.77
14:b:165:TRP:HD1	14:b:166:ASP:N	1.82	0.77
11:Y:5:ALA:HB2	11:Y:100:MET:CE	2.14	0.76
15:f:1:00E:HD2A	15:f:2:HPE:N	1.99	0.76
11:Y:45:MET:HB3	11:Y:52:CYS:HB3	1.67	0.76
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.34	0.75
10:X:29:LYS:HE3	11:Y:123:LYS:O	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:i:1:00E:HD2A	15:i:2:HPE:N	2.00	0.75
10:J:23:ARG:HG3	10:J:23:ARG:HH11	1.50	0.75
11:Y:197:PHE:HZ	11:Y:210:VAL:HG21	1.51	0.74
14:N:134:ILE:HG22	14:N:135:TYR:O	1.88	0.73
11:K:209:ASN:H	11:K:209:ASN:ND2	1.87	0.72
1:O:12:PHE:H	2:P:20:GLN:HE22	1.38	0.72
14:N:165:TRP:CD1	14:N:166:ASP:N	2.57	0.71
5:E:92:ASN:HD21	12:L:70:ASN:ND2	1.88	0.70
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	1.89	0.70
3:C:9:PHE:H	4:D:15:GLN:HE22	1.39	0.70
11:K:159:ARG:NH2	10:X:146:HIS:ND1	2.40	0.70
11:K:45:MET:HB3	11:K:52:CYS:HB3	1.74	0.70
7:U:45:ILE:HG22	7:U:216:VAL:HG13	1.72	0.69
14:b:165:TRP:CD1	14:b:166:ASP:N	2.59	0.69
5:E:92:ASN:ND2	12:L:70:ASN:HD21	1.89	0.69
7:U:23:PHE:O	7:U:26:THR:HB	1.93	0.68
7:G:23:PHE:O	7:G:26:THR:HB	1.94	0.68
11:Y:5:ALA:N	11:Y:100:MET:HE1	2.09	0.68
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	1.91	0.68
10:J:23:ARG:HH11	10:J:23:ARG:CG	2.07	0.67
13:M:30:TYR:HB2	13:M:34:LEU:HB2	1.74	0.67
5:S:12:PHE:H	6:T:19:GLN:HE22	1.41	0.67
10:J:139:TYR:CZ	11:Y:134:THR:HG22	2.29	0.66
13:M:36:PHE:HA	14:N:135:TYR:HB2	1.75	0.66
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.78	0.66
14:N:139:ASP:CG	14:b:164:LYS:NZ	2.54	0.65
8:V:22:GLN:HG3	15:g:3:LEU:HD23	1.78	0.65
5:E:12:PHE:H	6:F:19:GLN:HE22	1.45	0.65
8:H:22:GLN:HG3	15:d:3:LEU:HD23	1.79	0.64
11:K:134:THR:HG22	10:X:139:TYR:CZ	2.32	0.64
11:K:211:ILE:HD11	9:W:38:LYS:HG2	1.79	0.64
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.78	0.64
1:A:12:PHE:H	2:B:20:GLN:HE22	1.45	0.64
11:K:159:ARG:NH1	11:K:207:PHE:CZ	2.66	0.64
14:N:139:ASP:OD2	14:b:164:LYS:NZ	2.31	0.64
10:J:18:SER:HB2	10:J:176:PHE:HB2	1.81	0.63
13:a:27:LEU:HD12	13:a:37:ASN:HB2	1.80	0.63
14:b:55:ILE:HD11	14:b:93:LEU:HD13	1.79	0.62
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.47	0.62
10:X:18:SER:HB2	10:X:176:PHE:HB2	1.82	0.62
14:b:135:TYR:HD1	14:b:135:TYR:C	2.03	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:68:ARG:O	7:G:223:LYS:HA	2.00	0.62
11:Y:9:GLN:NE2	11:Y:148:LEU:O	2.33	0.62
6:T:123:ASN:C	6:T:123:ASN:HD22	2.08	0.61
6:F:123:ASN:C	6:F:123:ASN:HD22	2.09	0.61
14:N:164:LYS:NZ	14:b:139:ASP:CG	2.58	0.61
14:N:164:LYS:NZ	14:b:139:ASP:OD2	2.33	0.61
13:a:119:VAL:HG23	13:a:200:ILE:HG22	1.82	0.61
13:M:119:VAL:HG23	13:M:200:ILE:HG22	1.83	0.61
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.83	0.60
11:K:159:ARG:NE	10:X:146:HIS:ND1	2.50	0.60
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.83	0.60
11:K:9:GLN:NE2	11:K:148:LEU:O	2.36	0.59
14:N:14:LEU:HD11	14:N:100:ALA:HB3	1.84	0.59
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.84	0.59
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.49	0.59
11:K:56:GLU:OE2	11:K:99:THR:OG1	2.21	0.59
14:N:139:ASP:OD1	14:b:164:LYS:NZ	2.34	0.59
14:N:149:GLU:CD	14:N:149:GLU:H	2.11	0.59
14:b:14:LEU:HD11	14:b:100:ALA:CB	2.32	0.59
13:a:220:ASP:O	13:a:223:LYS:HG2	2.04	0.58
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.85	0.58
13:a:48:ASN:H	13:a:48:ASN:HD22	1.51	0.58
13:M:48:ASN:H	13:M:48:ASN:HD22	1.49	0.57
13:M:159:VAL:HG23	13:M:159:VAL:O	2.04	0.57
10:J:50:ALA:O	11:K:91:LYS:NZ	2.37	0.57
10:J:174:MET:HA	10:X:174:MET:HA	1.86	0.57
13:M:36:PHE:CD1	13:M:36:PHE:C	2.83	0.57
13:M:220:ASP:O	13:M:223:LYS:HG2	2.05	0.57
14:N:13:ILE:HG13	14:N:151:THR:HG21	1.85	0.57
10:X:25:ILE:HG13	10:X:25:ILE:O	2.03	0.57
11:K:4:LEU:HD22	11:K:4:LEU:C	2.30	0.57
13:M:174:GLU:OE1	13:M:209:LYS:NZ	2.37	0.57
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.86	0.57
13:a:159:VAL:HG23	13:a:159:VAL:O	2.04	0.57
12:L:4:PRO:O	13:M:104:ARG:NH1	2.37	0.56
14:N:164:LYS:HZ3	14:b:139:ASP:CG	2.13	0.56
2:B:12:PHE:H	3:C:17:GLN:HE22	1.52	0.56
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.30	0.56
14:N:138:CYS:HB3	14:N:141:ASN:HB2	1.88	0.56
8:V:210:THR:HG21	9:W:167:SER:HB3	1.85	0.56
13:a:174:GLU:OE1	13:a:209:LYS:NZ	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.87	0.55
3:C:38:ASN:C	3:C:38:ASN:HD22	2.14	0.55
10:X:152:MET:HE3	10:X:156:GLU:HB3	1.88	0.55
14:N:164:LYS:NZ	14:b:139:ASP:OD1	2.38	0.55
11:K:159:ARG:HH12	11:K:207:PHE:HZ	1.54	0.55
10:J:153:THR:HG23	10:J:156:GLU:OE2	2.07	0.55
13:a:30:TYR:HB2	13:a:34:LEU:HB2	1.88	0.55
11:K:159:ARG:NH1	11:K:207:PHE:CE2	2.75	0.54
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.72	0.54
14:b:138:CYS:HB3	14:b:141:ASN:HB2	1.88	0.54
14:N:128:VAL:HG12	14:N:129:SER:N	2.22	0.54
11:K:158:LYS:HB2	11:K:177:LEU:HD11	1.89	0.54
14:N:139:ASP:CG	14:b:164:LYS:HZ3	2.12	0.54
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.89	0.54
12:Z:4:PRO:O	13:a:104:ARG:NH1	2.36	0.54
13:a:127:LEU:HG	13:a:142:LEU:HD12	1.90	0.54
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.90	0.54
13:M:36:PHE:C	13:M:36:PHE:HD1	2.16	0.54
3:Q:38:ASN:C	3:Q:38:ASN:HD22	2.16	0.53
13:a:27:LEU:HB2	13:a:192:SER:HB3	1.91	0.53
15:i:1:00E:CD2	15:i:2:HPE:N	2.72	0.53
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.06	0.53
13:a:27:LEU:HD12	13:a:37:ASN:CB	2.38	0.53
14:N:135:TYR:O	14:N:137:TYR:N	2.42	0.53
11:Y:4:LEU:CD1	11:Y:161:ILE:HD11	2.39	0.53
10:X:5:LEU:HD21	10:X:140:THR:HG21	1.91	0.53
11:K:204:GLU:OE2	10:X:146:HIS:CE1	2.62	0.52
8:V:35:HIS:CG	8:V:56:THR:HG21	2.44	0.52
14:b:13:ILE:CG2	14:b:175:MET:HE2	2.40	0.52
8:H:139:GLU:OE1	13:a:187:ARG:NH1	2.41	0.52
11:Y:5:ALA:CB	11:Y:100:MET:HE1	2.37	0.52
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.92	0.52
8:H:210:THR:HG21	9:I:167:SER:HB3	1.92	0.52
11:K:4:LEU:CD1	11:K:161:ILE:HD11	2.40	0.52
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	1.92	0.52
14:b:135:TYR:O	14:b:137:TYR:N	2.42	0.52
1:O:55:LEU:HB3	7:U:159:ALA:O	2.10	0.51
11:Y:4:LEU:C	11:Y:100:MET:HE1	2.35	0.51
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.92	0.51
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.75	0.51
10:J:5:LEU:HD21	10:J:140:THR:HG21	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:16:VAL:HG21	11:K:34:VAL:HG23	1.92	0.51
13:a:179:ASN:HD22	13:a:182:ARG:HH11	1.58	0.51
13:M:63:ILE:HD13	13:M:114:ILE:HD11	1.92	0.51
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.58	0.51
11:Y:22:ALA:HB1	15:h:1:00E:HD2	1.92	0.51
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.75	0.51
11:K:22:ALA:HB1	15:e:1:00E:HD2	1.92	0.51
6:F:123:ASN:HD22	6:F:124:SER:N	2.09	0.51
8:H:35:HIS:CG	8:H:56:THR:HG21	2.44	0.51
13:a:63:ILE:HD13	13:a:114:ILE:HD11	1.92	0.51
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.92	0.51
10:J:152:MET:CE	10:J:156:GLU:HB3	2.36	0.51
13:M:27:LEU:HB2	13:M:192:SER:HB3	1.92	0.51
6:T:123:ASN:HD22	6:T:124:SER:N	2.08	0.51
11:K:154:LEU:HD23	11:K:177:LEU:HD22	1.93	0.50
8:V:52:THR:O	8:V:56:THR:HB	2.12	0.50
10:X:174:MET:HE3	19:X:210:HOH:O	2.11	0.50
12:Z:1:GLN:HE21	13:a:1:THR:HG21	1.76	0.50
11:Y:35:ILE:HG23	11:Y:37:ILE:HG13	1.93	0.50
11:K:22:ALA:HB1	15:e:1:00E:CD2	2.41	0.50
11:Y:22:ALA:HB1	15:h:1:00E:CD2	2.41	0.50
5:E:92:ASN:CG	12:L:70:ASN:HD21	2.20	0.49
8:H:52:THR:O	8:H:56:THR:HB	2.11	0.49
11:K:35:ILE:HG23	11:K:37:ILE:HG13	1.93	0.49
13:a:39:VAL:HG11	13:a:57:ILE:HD12	1.94	0.49
7:G:78:ILE:N	7:G:79:PRO:CD	2.75	0.49
10:J:149:ARG:HB2	10:J:152:MET:HG3	1.94	0.49
14:N:165:TRP:HD1	14:N:166:ASP:CA	2.25	0.49
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.48	0.49
7:U:78:ILE:N	7:U:79:PRO:CD	2.75	0.49
8:V:215:GLU:HG2	9:W:197:ARG:HG2	1.95	0.49
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.76	0.49
11:K:99:THR:HG22	11:K:115:VAL:HB	1.95	0.49
11:K:4:LEU:HD22	11:K:4:LEU:O	2.13	0.49
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.78	0.49
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.77	0.49
11:K:185:TRP:C	11:K:185:TRP:CE3	2.91	0.49
2:P:101:TYR:CE1	10:X:75:LEU:HD21	2.48	0.49
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.48	0.49
10:J:35:THR:HG21	10:J:182:LYS:HD2	1.95	0.49
12:L:145:LEU:O	9:W:147:GLY:HA3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:55:ILE:HD11	14:N:93:LEU:HD13	1.95	0.49
11:Y:197:PHE:CZ	11:Y:210:VAL:HG21	2.40	0.49
5:E:9:THR:HG21	5:E:119:THR:HA	1.95	0.49
14:N:134:ILE:C	14:N:135:TYR:O	2.53	0.49
13:M:39:VAL:HG11	13:M:57:ILE:HD12	1.94	0.48
10:X:35:THR:HG21	10:X:182:LYS:HD2	1.95	0.48
10:X:174:MET:SD	10:X:174:MET:N	2.85	0.48
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.95	0.48
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.95	0.48
10:J:145:ASP:OD1	11:Y:209:ASN:ND2	2.46	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.95	0.48
14:N:83:LYS:HB2	14:N:119:VAL:HG22	1.95	0.48
12:L:1:GLN:HE21	13:M:1:THR:HG21	1.78	0.48
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.46	0.48
11:Y:45:MET:HB3	11:Y:52:CYS:CB	2.40	0.48
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.29	0.48
14:b:83:LYS:HB2	14:b:119:VAL:HG22	1.95	0.48
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.49	0.47
5:S:9:THR:HG21	5:S:119:THR:HA	1.96	0.47
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.79	0.47
14:b:134:ILE:C	14:b:135:TYR:O	2.57	0.47
12:L:147:MET:N	12:L:148:PRO:HD2	2.29	0.47
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.95	0.47
14:N:149:GLU:CD	14:N:149:GLU:N	2.72	0.47
7:G:34:LEU:C	7:G:34:LEU:HD23	2.40	0.47
13:M:44:PRO:HG3	13:M:208:PHE:CE2	2.49	0.47
13:a:44:PRO:HG3	13:a:208:PHE:CE2	2.49	0.47
8:H:199:LYS:HE3	9:I:151:SER:O	2.14	0.47
7:U:78:ILE:HG22	7:U:79:PRO:HD3	1.97	0.47
2:B:220:ASN:OD1	2:B:220:ASN:N	2.47	0.47
9:I:147:GLY:HA3	12:Z:145:LEU:O	2.15	0.47
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.50	0.47
14:N:155:ILE:HG21	14:N:175:MET:HE3	1.97	0.47
10:X:152:MET:CE	10:X:156:GLU:HB3	2.45	0.47
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.95	0.47
14:N:66:TYR:CD1	14:N:73:PRO:HB3	2.50	0.47
2:P:220:ASN:OD1	2:P:220:ASN:N	2.47	0.47
5:S:92:ASN:CG	12:Z:70:ASN:HD21	2.22	0.47
11:K:4:LEU:CD1	11:K:161:ILE:CD1	2.93	0.47
7:G:83:ASN:C	7:G:83:ASN:HD22	2.23	0.46
8:V:22:GLN:HG3	15:g:3:LEU:CD2	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:4:LEU:HD22	11:Y:4:LEU:O	2.15	0.46
14:b:143:ARG:O	14:b:146:MET:HG3	2.15	0.46
14:b:155:ILE:HG21	14:b:175:MET:HE3	1.97	0.46
10:J:130:TYR:CE1	10:J:144:LEU:HB3	2.51	0.46
10:J:174:MET:SD	10:J:174:MET:N	2.84	0.46
11:K:209:ASN:ND2	11:K:209:ASN:N	2.60	0.46
8:H:194:ASN:HB3	12:Z:220:LYS:HE3	1.97	0.46
13:M:37:ASN:CA	14:N:135:TYR:CE2	2.97	0.46
13:a:37:ASN:C	13:a:37:ASN:HD22	2.23	0.46
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.13	0.46
10:J:139:TYR:OH	10:X:25:ILE:O	2.20	0.46
13:a:43:ILE:HD12	13:a:64:GLU:HG3	1.98	0.46
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.96	0.46
10:X:19:LYS:HD3	10:X:180:ILE:HG13	1.97	0.46
11:Y:4:LEU:CD1	11:Y:161:ILE:CD1	2.93	0.46
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.50	0.46
3:C:201:VAL:HG13	3:C:202:GLN:N	2.30	0.46
10:J:3:ILE:HD12	10:J:176:PHE:CD2	2.51	0.46
7:U:34:LEU:C	7:U:34:LEU:HD23	2.41	0.46
14:b:135:TYR:O	14:b:136:GLY:C	2.59	0.46
14:b:33:LYS:HE2	15:i:5:A1I44:C65	2.46	0.46
14:b:139:ASP:OD1	14:b:139:ASP:N	2.44	0.46
7:G:78:ILE:HG22	7:G:79:PRO:HD3	1.97	0.46
10:J:25:ILE:O	10:J:25:ILE:HG13	2.15	0.46
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.30	0.46
14:b:165:TRP:HD1	14:b:166:ASP:CA	2.29	0.46
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.16	0.45
14:b:149:GLU:CD	14:b:149:GLU:H	2.22	0.45
2:B:86:LEU:HB3	2:B:114:LEU:HD21	1.98	0.45
12:L:110:ILE:CD1	12:L:137:ARG:HG3	2.47	0.45
12:L:220:LYS:HE3	8:V:194:ASN:HB3	1.99	0.45
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.46	0.45
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.46	0.45
2:P:86:LEU:HB3	2:P:114:LEU:HD21	1.98	0.45
14:b:66:TYR:CD1	14:b:73:PRO:HB3	2.51	0.45
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.99	0.45
11:K:159:ARG:CZ	10:X:146:HIS:ND1	2.78	0.45
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.46	0.45
14:b:94:THR:HG22	14:b:94:THR:O	2.16	0.45
10:J:177:LYS:NZ	10:X:169:GLU:O	2.49	0.45
13:M:48:ASN:HD22	13:M:48:ASN:N	2.12	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:3:ILE:HD12	10:X:176:PHE:CD2	2.51	0.45
10:J:19:LYS:HD3	10:J:180:ILE:HG13	1.97	0.45
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.65	0.45
13:M:43:ILE:HD12	13:M:64:GLU:HG3	1.99	0.45
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.99	0.45
7:U:83:ASN:C	7:U:83:ASN:HD22	2.25	0.45
13:a:36:PHE:O	13:a:36:PHE:CD1	2.69	0.45
8:H:146:LEU:HD22	8:H:150:GLU:HB3	1.99	0.45
10:J:25:ILE:O	10:X:139:TYR:OH	2.26	0.45
11:K:197:PHE:CE2	9:W:203:GLN:HG3	2.52	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.45
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.15	0.45
9:I:56:ALA:HB3	10:J:124:THR:HG23	1.99	0.45
12:L:8:ASN:HA	12:L:30:ILE:O	2.17	0.45
7:G:73:VAL:HG12	7:G:133:THR:HB	1.97	0.44
8:H:62:ASN:HB3	8:H:82:MET:HE1	1.99	0.44
14:N:139:ASP:OD1	14:N:139:ASP:N	2.45	0.44
11:K:6:PHE:HA	11:K:125:ASP:O	2.17	0.44
8:V:146:LEU:HD22	8:V:150:GLU:HB3	1.99	0.44
14:b:138:CYS:CB	14:b:141:ASN:HB2	2.47	0.44
2:B:161:ALA:HB3	3:C:52:LEU:HD23	1.99	0.44
11:K:185:TRP:CE3	11:K:185:TRP:O	2.70	0.44
14:N:13:ILE:CG2	14:N:175:MET:HE2	2.47	0.44
7:U:73:VAL:HG12	7:U:133:THR:HB	1.98	0.44
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.48	0.44
8:H:215:GLU:HG2	9:I:197:ARG:HG2	2.00	0.44
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.58	0.44
8:V:62:ASN:HB3	8:V:82:MET:HE1	1.99	0.44
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.48	0.44
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.99	0.44
14:b:13:ILE:HD13	14:b:177:VAL:HG22	1.99	0.44
7:G:61:SER:OG	7:G:215:GLU:OE2	2.23	0.44
6:F:158:GLY:O	7:G:54:LEU:HB3	2.18	0.44
8:V:199:LYS:HE3	9:W:151:SER:O	2.18	0.44
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.48	0.44
11:K:100:MET:HE3	11:K:127:PHE:CB	2.48	0.44
5:S:77:ALA:N	5:S:78:PRO:CD	2.81	0.44
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.00	0.43
13:M:10:SER:HB3	13:M:147:GLY:H	1.83	0.43
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.52	0.43
12:Z:108[B]:HIS:NE2	15:h:1:00E:CD1	2.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:104:TYR:CE2	11:Y:109:GLY:HA2	2.53	0.43
8:H:22:GLN:HG3	15:d:3:LEU:CD2	2.45	0.43
10:J:3:ILE:HB	10:J:18:SER:HB3	1.99	0.43
11:Y:4:LEU:HD12	11:Y:161:ILE:CD1	2.48	0.43
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.17	0.43
13:a:10:SER:HB3	13:a:147:GLY:H	1.83	0.43
14:b:149:GLU:CD	14:b:149:GLU:N	2.76	0.43
5:E:68:HIS:HE1	5:E:102:LEU:O	2.01	0.43
5:E:77:ALA:N	5:E:78:PRO:CD	2.82	0.43
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.99	0.43
10:J:2:ASP:OD1	19:J:201:HOH:O	2.21	0.43
11:K:159:ARG:NE	10:X:146:HIS:CE1	2.76	0.43
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.81	0.43
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.48	0.43
1:O:119:GLN:O	1:O:122:THR:HB	2.18	0.43
10:J:23:ARG:CG	10:J:23:ARG:NH1	2.73	0.43
14:N:138:CYS:CB	14:N:141:ASN:HB2	2.47	0.43
14:N:164:LYS:HZ1	14:b:139:ASP:CG	2.26	0.43
19:O:308:HOH:O	7:U:122:ARG:HD2	2.18	0.43
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.16	0.43
10:X:139:TYR:CD2	10:X:172:MET:HE3	2.53	0.43
13:a:36:PHE:HA	14:b:135:TYR:HB2	2.01	0.43
14:b:159:LEU:O	14:b:163:ILE:HG13	2.19	0.43
10:J:184:VAL:HG22	10:J:189:ILE:HG12	2.01	0.43
14:N:40:LYS:HE2	14:N:179:THR:O	2.19	0.43
14:N:128:VAL:HG12	14:N:129:SER:H	1.83	0.43
3:C:201:VAL:O	3:C:202:GLN:CB	2.67	0.43
11:K:4:LEU:HD12	11:K:161:ILE:CD1	2.49	0.43
1:O:115:ALA:HB1	1:O:154:GLY:O	2.19	0.43
14:b:134:ILE:HG22	14:b:135:TYR:O	2.18	0.43
11:K:4:LEU:C	11:K:4:LEU:CD2	2.92	0.43
11:K:8:PHE:CE1	11:K:13:ILE:HG12	2.54	0.43
1:A:149:GLN:O	1:A:156:TYR:HA	2.19	0.42
5:E:18:LEU:HD21	6:F:126:ARG:HD2	2.01	0.42
5:E:65:CYS:SG	5:E:71:LEU:CD1	3.07	0.42
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	2.01	0.42
7:U:68:ARG:O	7:U:223:LYS:HA	2.19	0.42
10:X:3:ILE:HB	10:X:18:SER:HB3	2.00	0.42
10:X:75:LEU:HD12	10:X:75:LEU:HA	1.90	0.42
14:b:128:VAL:O	14:b:132:THR:HB	2.19	0.42
6:F:41:GLY:HA3	6:F:215:CYS:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:176:ASN:HD21	11:K:190:ASN:HB2	1.84	0.42
12:L:12:ILE:CD1	12:L:110:ILE:HG13	2.49	0.42
14:N:65:LEU:HG	14:N:69:GLN:HE21	1.84	0.42
1:O:149:GLN:O	1:O:156:TYR:HA	2.19	0.42
14:b:132:THR:O	14:b:132:THR:HG22	2.19	0.42
9:W:56:ALA:HB3	10:X:124:THR:HG23	2.01	0.42
11:Y:36:GLU:O	11:Y:38:ASN:N	2.52	0.42
11:Y:95:LEU:HD13	11:Y:97:MET:CE	2.49	0.42
11:K:104:TYR:CD1	11:K:104:TYR:C	2.97	0.42
7:G:68:ARG:O	7:G:68:ARG:HG3	2.20	0.42
13:M:129:TYR:O	13:M:136:THR:HA	2.19	0.42
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.67	0.42
11:Y:183:ASP:OD1	11:Y:183:ASP:N	2.52	0.42
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.92	0.42
5:E:71:LEU:C	5:E:71:LEU:HD22	2.45	0.42
14:N:135:TYR:CG	14:N:136:GLY:N	2.85	0.42
14:N:159:LEU:O	14:N:163:ILE:HG13	2.20	0.42
10:X:126:VAL:CG1	10:X:128:LEU:HG	2.50	0.42
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.45	0.42
4:R:82:GLU:OE2	11:Y:69:ARG:NH1	2.53	0.42
5:S:10:VAL:CG2	6:T:125:VAL:C	2.93	0.42
13:a:129:TYR:O	13:a:136:THR:HA	2.20	0.42
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.54	0.42
3:C:108:THR:HG21	3:C:146:TYR:HB3	2.02	0.42
14:N:14:LEU:O	14:N:175:MET:HA	2.20	0.42
14:N:163:ILE:HG23	14:N:170:GLY:HA2	2.02	0.42
8:V:5:GLY:HA3	8:V:110:LEU:HD11	2.01	0.42
11:Y:8:PHE:CE1	11:Y:13:ILE:HG12	2.54	0.42
11:Y:176:ASN:ND2	11:Y:187:TYR:OH	2.53	0.42
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.01	0.42
11:K:4:LEU:HA	11:K:100:MET:HE1	2.01	0.42
11:K:36:GLU:O	11:K:38:ASN:N	2.53	0.42
11:K:104:TYR:CE2	11:K:109:GLY:HA2	2.55	0.42
6:T:41:GLY:HA3	6:T:215:CYS:O	2.19	0.42
15:i:2:HPE:HE2	15:i:2:HPE:HB3	1.68	0.42
7:G:83:ASN:C	7:G:83:ASN:ND2	2.78	0.41
8:H:165:ASN:HD22	13:a:156:ARG:HH11	1.68	0.41
11:K:209:ASN:HD22	11:K:209:ASN:N	2.04	0.41
8:H:5:GLY:HA3	8:H:110:LEU:HD11	2.02	0.41
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.02	0.41
10:J:3:ILE:HD13	10:J:168:LEU:HD13	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:12:ILE:HG23	11:K:112:ILE:HD11	2.02	0.41
7:U:83:ASN:C	7:U:83:ASN:ND2	2.78	0.41
11:Y:98:GLY:HA3	18:Y:301:MES:H32	2.02	0.41
8:H:5:GLY:O	8:H:124:TYR:HA	2.20	0.41
14:N:19:ARG:O	14:N:33:LYS:NZ	2.49	0.41
14:N:164:LYS:O	13:a:35:ARG:HD3	2.20	0.41
2:P:6:ASP:OD2	3:Q:4:ARG:HG3	2.19	0.41
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.51	0.41
11:Y:158:LYS:HB2	11:Y:177:LEU:HD11	2.02	0.41
11:K:161:ILE:HD13	11:K:161:ILE:HA	1.91	0.41
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.01	0.41
14:b:65:LEU:HG	14:b:69:GLN:HE21	1.86	0.41
5:E:71:LEU:C	5:E:71:LEU:CD2	2.93	0.41
9:I:123:PHE:HA	9:I:128:CYS:O	2.20	0.41
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.02	0.41
10:X:184:VAL:HG22	10:X:189:ILE:HG12	2.01	0.41
14:b:14:LEU:O	14:b:175:MET:HA	2.21	0.41
15:f:1:00E:CD2	15:f:2:HPE:N	2.71	0.41
1:A:115:ALA:HB1	1:A:154:GLY:O	2.19	0.41
1:A:119:GLN:O	1:A:122:THR:HB	2.20	0.41
9:I:203:GLN:HG3	11:Y:197:PHE:CE2	2.55	0.41
11:K:30:THR:OG1	12:L:132:GLU:OE2	2.37	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41
14:b:40:LYS:HE2	14:b:179:THR:O	2.20	0.41
14:b:156:LYS:O	14:b:160:SER:HB3	2.20	0.41
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.55	0.41
10:J:139:TYR:CD2	10:J:172:MET:HE3	2.55	0.41
5:S:71:LEU:C	5:S:71:LEU:CD2	2.94	0.41
5:S:71:LEU:C	5:S:71:LEU:HD22	2.46	0.41
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.02	0.41
9:I:7:ASN:HA	9:I:29:GLY:O	2.21	0.41
11:K:209:ASN:O	9:W:37:ASN:ND2	2.53	0.41
14:N:46:SER:OG	14:N:131:SER:OG	2.20	0.41
3:Q:77:ASN:HD22	3:Q:77:ASN:N	2.18	0.41
4:R:91:HIS:HB3	4:R:99:ILE:HG21	2.03	0.41
5:S:65:CYS:SG	5:S:71:LEU:CD1	3.08	0.41
9:W:123:PHE:HA	9:W:128:CYS:O	2.20	0.41
11:Y:12:ILE:HG23	11:Y:112:ILE:HD11	2.02	0.41
11:Y:155:TYR:OH	11:Y:204:GLU:OE1	2.38	0.41
13:a:37:ASN:C	13:a:37:ASN:ND2	2.77	0.41
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:187:ARG:HA	13:a:187:ARG:HD2	1.87	0.41
14:b:163:ILE:HG23	14:b:170:GLY:HA2	2.01	0.41
3:C:77:ASN:HD22	3:C:77:ASN:N	2.19	0.41
7:G:66:ILE:HG21	7:G:108:LEU:HD21	2.02	0.41
10:J:130:TYR:OH	11:Y:209:ASN:ND2	2.51	0.41
13:M:53:ILE:HB	13:M:60:MET:HG3	2.03	0.41
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.56	0.41
13:a:48:ASN:HD22	13:a:48:ASN:N	2.13	0.41
15:d:5:A1I44:O21	18:d:101:MES:O2S	2.39	0.41
4:D:91:HIS:HB3	4:D:99:ILE:HG21	2.03	0.41
14:N:156:LYS:O	14:N:160:SER:HB3	2.21	0.41
7:U:71:GLY:HA3	7:U:224:PHE:CE2	2.55	0.41
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.56	0.41
10:X:3:ILE:HD13	10:X:168:LEU:HD13	2.02	0.41
10:X:144:LEU:O	10:X:148:TYR:HB3	2.21	0.41
5:E:80:ALA:HB2	5:E:129:VAL:HG21	2.03	0.40
7:G:68:ARG:HE	7:G:68:ARG:HB2	1.63	0.40
8:H:19:ARG:NH1	8:H:167:LEU:O	2.54	0.40
11:K:35:ILE:HD13	11:K:37:ILE:H	1.85	0.40
14:N:33:LYS:HE2	15:f:5:A1I44:C65	2.51	0.40
9:W:7:ASN:HA	9:W:29:GLY:O	2.20	0.40
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.54	0.40
11:K:140:LEU:HD12	11:K:156:LEU:HG	2.03	0.40
14:N:32:ASP:OD2	14:N:185:ARG:NH2	2.55	0.40
11:Y:104:TYR:CD1	11:Y:104:TYR:C	2.99	0.40
14:b:48:SER:HB3	14:b:51:ASP:HB2	2.04	0.40
11:K:33:LYS:O	11:K:45:MET:HG3	2.21	0.40
14:N:139:ASP:CG	14:b:164:LYS:HZ1	2.21	0.40
11:Y:5:ALA:HB2	11:Y:100:MET:HE2	1.97	0.40
14:b:51:ASP:HB3	14:b:93:LEU:HD22	2.03	0.40
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.51	0.40
6:F:117:GLN:HE21	6:F:117:GLN:HB3	1.72	0.40
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.02	0.40
11:K:86:LEU:HD13	11:K:86:LEU:C	2.46	0.40
11:Y:35:ILE:HD13	11:Y:37:ILE:H	1.86	0.40
11:Y:41:LEU:HD23	11:Y:41:LEU:HA	1.88	0.40
11:Y:83:LEU:CD2	11:Y:99:THR:HG21	2.52	0.40
13:M:119:VAL:HG11	13:M:202:LYS:HB3	2.04	0.40
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	16	44
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	16	44
3	C	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	10	32
3	Q	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	10	32
4	D	231/260 (89%)	227 (98%)	4 (2%)	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%)	235 (98%)	6 (2%)	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%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	187 (97%)	6 (3%)	0	100	100
10	X	193/198 (98%)	187 (97%)	6 (3%)	0	100	100
11	K	209/211 (99%)	204 (98%)	4 (2%)	1 (0%)	25	56
11	Y	209/211 (99%)	204 (98%)	4 (2%)	1 (0%)	25	56
12	L	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
12	Z	221/222 (100%)	218 (99%)	3 (1%)	0	100	100
13	M	231/246 (94%)	221 (96%)	10 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/246 (94%)	220 (95%)	10 (4%)	1 (0%)	30	61
14	N	193/195 (99%)	183 (95%)	7 (4%)	3 (2%)	8	27
14	b	193/195 (99%)	183 (95%)	7 (4%)	3 (2%)	8	27
15	d	1/5 (20%)	1 (100%)	0	0	100	100
15	e	1/5 (20%)	1 (100%)	0	0	100	100
15	f	1/5 (20%)	1 (100%)	0	0	100	100
15	g	1/5 (20%)	1 (100%)	0	0	100	100
15	h	1/5 (20%)	1 (100%)	0	0	100	100
15	i	1/5 (20%)	1 (100%)	0	0	100	100
All	All	6277/6638 (95%)	6095 (97%)	163 (3%)	19 (0%)	37	67

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
11	K	37	ILE
14	N	136	GLY
2	P	51	VAL
3	Q	202	GLN
11	Y	37	ILE
14	b	135	TYR
14	b	136	GLY
3	C	205	ALA
14	N	135	TYR
14	N	137	TYR
3	Q	205	ALA
13	a	36	PHE
14	b	137	TYR
3	C	239	GLN
3	Q	239	GLN
2	B	221	ASP
2	P	221	ASP

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%)	203 (97%)	6 (3%)	37	71
1	O	209/209 (100%)	203 (97%)	6 (3%)	37	71
2	B	203/216 (94%)	195 (96%)	8 (4%)	27	61
2	P	203/216 (94%)	195 (96%)	8 (4%)	27	61
3	C	212/226 (94%)	206 (97%)	6 (3%)	38	72
3	Q	212/226 (94%)	206 (97%)	6 (3%)	38	72
4	D	194/215 (90%)	186 (96%)	8 (4%)	26	59
4	R	194/215 (90%)	186 (96%)	8 (4%)	26	59
5	E	190/193 (98%)	185 (97%)	5 (3%)	41	75
5	S	190/193 (98%)	185 (97%)	5 (3%)	41	75
6	F	201/239 (84%)	192 (96%)	9 (4%)	23	55
6	T	201/239 (84%)	192 (96%)	9 (4%)	23	55
7	G	206/210 (98%)	198 (96%)	8 (4%)	27	61
7	U	206/210 (98%)	196 (95%)	10 (5%)	21	52
8	H	180/189 (95%)	171 (95%)	9 (5%)	20	51
8	V	180/189 (95%)	170 (94%)	10 (6%)	17	47
9	I	172/173 (99%)	170 (99%)	2 (1%)	67	89
9	W	172/173 (99%)	170 (99%)	2 (1%)	67	89
10	J	173/175 (99%)	165 (95%)	8 (5%)	23	55
10	X	173/175 (99%)	164 (95%)	9 (5%)	19	50
11	K	168/168 (100%)	154 (92%)	14 (8%)	9	28
11	Y	168/168 (100%)	155 (92%)	13 (8%)	10	31
12	L	185/185 (100%)	178 (96%)	7 (4%)	28	62
12	Z	186/185 (100%)	179 (96%)	7 (4%)	28	62
13	M	199/208 (96%)	186 (94%)	13 (6%)	14	40
13	a	199/208 (96%)	187 (94%)	12 (6%)	16	44
14	N	162/162 (100%)	147 (91%)	15 (9%)	7	23
14	b	162/162 (100%)	147 (91%)	15 (9%)	7	23
15	d	2/2 (100%)	2 (100%)	0	100	100
15	e	2/2 (100%)	2 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	f	2/2 (100%)	2 (100%)	0	100	100
15	g	2/2 (100%)	2 (100%)	0	100	100
15	h	2/2 (100%)	2 (100%)	0	100	100
15	i	2/2 (100%)	2 (100%)	0	100	100
All	All	5321/5548 (96%)	5083 (96%)	238 (4%)	23	55

All (238) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	29	LYS
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
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	77	ASN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	188	LEU
6	F	68	ARG
6	F	94	SER
6	F	117	GLN
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	221	ASN
7	G	26	THR
7	G	68	ARG
7	G	83	ASN
7	G	115	LEU
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
8	H	7	LYS
8	H	34	LEU
8	H	38	SER
8	H	56	THR
8	H	59	ILE
8	H	68	LEU
8	H	120	ASP
8	H	127	LEU
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	136	SER
10	J	144	LEU
10	J	172	MET
10	J	174	MET
10	J	193	ASP
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	38	ASN
11	K	67	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	73	ARG
11	K	99	THR
11	K	100	MET
11	K	134	THR
11	K	142	SER
11	K	148	LEU
11	K	181	THR
11	K	183	ASP
11	K	209	ASN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	110	ILE
12	L	130	SER
12	L	150	LEU
12	L	167	LYS
13	M	3	GLN
13	M	10	SER
13	M	29	SER
13	M	32	SER
13	M	36	PHE
13	M	37	ASN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	187	ARG
13	M	206	LEU
13	M	213	GLN
13	M	225	ILE
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	139	ASP
14	N	141	ASN
14	N	143	ARG
14	N	149	GLU
14	N	157	HIS
14	N	160	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	165	TRP
14	N	178	LEU
1	O	17	LYS
1	O	29	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
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	68	ARG
6	T	94	SER
6	T	117	GLN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	T	206	LYS
6	T	221	ASN
7	U	26	THR
7	U	58	THR
7	U	63	ILE
7	U	67	SER
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	7	LYS
8	V	13	VAL
8	V	34	LEU
8	V	38	SER
8	V	56	THR
8	V	59	ILE
8	V	68	LEU
8	V	120	ASP
8	V	127	LEU
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	67	GLU
11	Y	71	LYS
11	Y	73	ARG
11	Y	99	THR
11	Y	134	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	Y	142	SER
11	Y	181	THR
11	Y	183	ASP
11	Y	209	ASN
12	Z	23	LEU
12	Z	49	ASN
12	Z	124	SER
12	Z	130	SER
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
13	a	3	GLN
13	a	10	SER
13	a	29	SER
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
13	a	225	ILE
14	b	9	LYS
14	b	13	ILE
14	b	22	THR
14	b	35	THR
14	b	119	VAL
14	b	132	THR
14	b	135	TYR
14	b	139	ASP
14	b	141	ASN
14	b	143	ARG
14	b	149	GLU
14	b	157	HIS
14	b	160	SER
14	b	165	TRP
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (188) 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
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	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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	117	GLN
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	57	GLN
8	H	66	HIS
8	H	141	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	31	GLN
9	I	37	ASN
9	I	44	HIS
9	I	63	ASN
9	I	88	GLN
9	I	203	GLN
10	J	55	GLN
10	J	63	ASN
10	J	118	GLN
10	J	147	HIS
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	190	ASN
11	K	208	ASN
11	K	209	ASN
12	L	1	GLN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	76	HIS
12	L	79	HIS
12	L	80	ASN
12	L	152	ASN
12	L	153	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	158	ASN
12	L	197	GLN
13	M	18	ASN
13	M	26	ASN
13	M	48	ASN
13	M	108	ASN
13	M	179	ASN
13	M	213	GLN
14	N	38	HIS
14	N	69	GLN
14	N	141	ASN
14	N	145	ASN
1	O	149	GLN
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	233	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	106	GLN
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	S	147	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
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	57	GLN
8	V	141	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
8	V	200	GLN
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	147	HIS
10	X	191	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
11	Y	209	ASN
12	Z	1	GLN
12	Z	3	ASN

Continued on next page...

Continued from previous page...

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	158	ASN
12	Z	197	GLN
13	a	18	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 ⓘ

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	00E	i	1	15	9,9,10	0.51	0	10,10,12	1.19	1 (10%)
15	00E	g	1	15	9,9,10	0.78	0	10,10,12	1.16	1 (10%)
15	00E	f	1	15	9,9,10	0.49	0	10,10,12	1.38	3 (30%)
15	HPE	d	2	15	11,12,13	1.26	1 (9%)	9,14,16	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	HPE	f	2	15	11,12,13	1.65	2 (18%)	9,14,16	0.81	0
15	00E	e	1	15	9,9,10	0.75	0	10,10,12	1.27	1 (10%)
15	00E	h	1	15	9,9,10	0.77	0	10,10,12	1.20	1 (10%)
15	HPE	i	2	15	11,12,13	1.61	1 (9%)	9,14,16	0.83	0
15	HPE	g	2	15	11,12,13	1.25	1 (9%)	9,14,16	0.50	0
15	HPE	e	2	15	11,12,13	1.41	1 (9%)	9,14,16	0.78	0
15	HPE	h	2	15	11,12,13	1.43	1 (9%)	9,14,16	0.80	0
15	00E	d	1	15	9,9,10	0.78	0	10,10,12	1.17	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	00E	i	1	15	-	0/2/11/12	0/1/1/1
15	00E	g	1	15	-	0/2/11/12	0/1/1/1
15	00E	f	1	15	-	0/2/11/12	0/1/1/1
15	HPE	d	2	15	-	2/6/7/9	0/1/1/1
15	HPE	f	2	15	-	2/6/7/9	0/1/1/1
15	00E	e	1	15	-	0/2/11/12	0/1/1/1
15	00E	h	1	15	-	0/2/11/12	0/1/1/1
15	HPE	i	2	15	-	2/6/7/9	0/1/1/1
15	HPE	g	2	15	-	2/6/7/9	0/1/1/1
15	HPE	e	2	15	-	0/6/7/9	0/1/1/1
15	HPE	h	2	15	-	0/6/7/9	0/1/1/1
15	00E	d	1	15	-	0/2/11/12	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	i	2	HPE	CG-CD	-4.85	1.37	1.51
15	f	2	HPE	CG-CD	-4.73	1.37	1.51
15	h	2	HPE	CG-CD	-4.42	1.38	1.51
15	e	2	HPE	CG-CD	-4.35	1.39	1.51
15	d	2	HPE	CG-CD	-3.64	1.41	1.51
15	g	2	HPE	CG-CD	-3.60	1.41	1.51
15	f	2	HPE	CB-CA	-2.40	1.50	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	e	1	00E	CA-NB-CD2	2.95	113.77	110.48
15	h	1	00E	CA-NB-CD2	2.74	113.54	110.48
15	i	1	00E	O-C-CA	-2.51	118.80	126.39
15	g	1	00E	CA-NB-CD2	2.46	113.23	110.48
15	d	1	00E	CA-NB-CD1	2.46	113.22	110.48
15	f	1	00E	CA-NB-CD1	-2.25	107.97	110.48
15	f	1	00E	O-C-CA	-2.11	120.01	126.39
15	f	1	00E	OZ-CE2-CD2	-2.05	107.27	111.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	i	2	HPE	CE1-CD-CG-CB
15	f	2	HPE	CE2-CD-CG-CB
15	i	2	HPE	CE2-CD-CG-CB
15	f	2	HPE	CE1-CD-CG-CB
15	d	2	HPE	CE1-CD-CG-CB
15	g	2	HPE	CE1-CD-CG-CB
15	d	2	HPE	CE2-CD-CG-CB
15	g	2	HPE	CE2-CD-CG-CB

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	i	1	00E	3	0
15	f	1	00E	2	0
15	f	2	HPE	2	0
15	e	1	00E	2	0
15	h	1	00E	4	0
15	i	2	HPE	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	MES	Y	301	-	12,12,12	0.74	0	14,16,16	0.30	0
18	MES	d	101	-	12,12,12	0.79	0	14,16,16	0.40	0
18	MES	e	101	-	12,12,12	0.78	0	14,16,16	0.58	0
18	MES	a	301	-	12,12,12	0.70	0	14,16,16	0.42	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	Y	301	-	-	3/6/14/14	0/1/1/1
18	MES	d	101	-	-	2/6/14/14	0/1/1/1
18	MES	e	101	-	-	0/6/14/14	0/1/1/1
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 (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	a	301	MES	C7-C8-S-O2S
18	d	101	MES	C7-C8-S-O2S
18	a	301	MES	C7-C8-S-O3S
18	Y	301	MES	C7-C8-S-O3S
18	Y	301	MES	C7-C8-S-O1S
18	Y	301	MES	C7-C8-S-O2S
18	a	301	MES	C7-C8-S-O1S
18	d	101	MES	C7-C8-S-O1S

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	Y	301	MES	1	0
18	d	101	MES	1	0

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%)	-0.78	1 (0%) 89 85	49, 62, 92, 155	0
1	O	250/250 (100%)	-0.75	1 (0%) 89 85	54, 71, 109, 158	0
2	B	244/258 (94%)	-0.63	1 (0%) 89 85	50, 69, 112, 161	0
2	P	244/258 (94%)	-0.52	2 (0%) 82 77	55, 74, 124, 156	0
3	C	240/254 (94%)	-0.59	1 (0%) 89 85	50, 74, 128, 153	0
3	Q	240/254 (94%)	-0.48	3 (1%) 74 67	59, 83, 146, 178	0
4	D	235/260 (90%)	-0.68	1 (0%) 89 85	53, 74, 103, 145	0
4	R	235/260 (90%)	-0.66	1 (0%) 89 85	53, 75, 109, 148	0
5	E	231/234 (98%)	-0.70	0 100 100	55, 73, 104, 133	0
5	S	231/234 (98%)	-0.59	0 100 100	56, 80, 113, 139	0
6	F	243/288 (84%)	-0.74	0 100 100	46, 67, 107, 130	0
6	T	243/288 (84%)	-0.67	0 100 100	50, 74, 119, 138	0
7	G	241/252 (95%)	-0.77	0 100 100	46, 61, 91, 123	0
7	U	241/252 (95%)	-0.69	0 100 100	52, 66, 99, 124	0
8	H	221/231 (95%)	-0.82	0 100 100	47, 57, 82, 110	0
8	V	221/231 (95%)	-0.75	0 100 100	50, 62, 86, 130	0
9	I	204/205 (99%)	-0.88	0 100 100	44, 58, 82, 111	0
9	W	204/205 (99%)	-0.86	0 100 100	48, 61, 89, 111	0
10	J	195/198 (98%)	-0.77	1 (0%) 87 83	47, 61, 84, 122	0
10	X	195/198 (98%)	-0.75	1 (0%) 87 83	47, 65, 87, 129	0
11	K	211/211 (100%)	-0.81	0 100 100	47, 60, 86, 163	0
11	Y	211/211 (100%)	-0.77	2 (0%) 81 75	47, 61, 87, 168	0
12	L	222/222 (100%)	-0.68	0 100 100	48, 62, 95, 113	0
12	Z	222/222 (100%)	-0.66	1 (0%) 87 83	40, 60, 93, 110	1 (0%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.83	0 100 100	45, 62, 82, 111	0
13	a	233/246 (94%)	-0.84	1 (0%) 89 85	45, 60, 80, 107	0
14	N	195/195 (100%)	-0.72	0 100 100	44, 59, 105, 138	0
14	b	195/195 (100%)	-0.66	1 (0%) 87 83	45, 62, 108, 145	0
15	d	2/5 (40%)	-0.79	0 100 100	62, 62, 62, 62	0
15	e	2/5 (40%)	-1.32	0 100 100	49, 49, 49, 55	0
15	f	2/5 (40%)	-0.61	0 100 100	56, 56, 56, 64	0
15	g	2/5 (40%)	-0.67	0 100 100	65, 65, 65, 69	0
15	h	2/5 (40%)	-1.20	0 100 100	52, 52, 52, 58	0
15	i	2/5 (40%)	-0.58	0 100 100	57, 57, 57, 64	0
All	All	6342/6638 (95%)	-0.71	18 (0%) 90 87	40, 66, 108, 178	1 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	4.3
1	O	1	MET	3.7
12	Z	108[A]	HIS	3.6
2	P	51	VAL	3.4
10	J	1	MET	3.3
4	R	113	LEU	3.1
3	Q	50	LEU	2.8
1	A	1	MET	2.8
13	a	1	THR	2.7
11	Y	211	ILE	2.7
2	P	219	ALA	2.7
11	Y	212	GLY	2.4
3	Q	205	ALA	2.3
4	D	240	ALA	2.3
2	B	51	VAL	2.2
14	b	165	TRP	2.1
3	C	205	ALA	2.0
3	Q	51	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	00E	f	1	9/10	0.38	0.18	106,135,143,146	0
15	00E	i	1	9/10	0.52	0.17	104,135,140,143	0
15	00E	g	1	9/10	0.85	0.13	77,109,119,119	0
15	HPE	f	2	12/13	0.85	0.14	76,102,115,118	0
15	00E	e	1	9/10	0.86	0.13	84,106,113,113	0
15	00E	d	1	9/10	0.87	0.12	75,106,113,113	0
15	00E	h	1	9/10	0.88	0.11	73,100,107,109	0
15	HPE	i	2	12/13	0.90	0.14	72,102,114,115	0
15	HPE	h	2	12/13	0.94	0.08	55,68,75,75	0
15	HPE	e	2	12/13	0.96	0.08	64,68,73,75	0
15	HPE	g	2	12/13	0.96	0.07	68,71,75,76	0
15	HPE	d	2	12/13	0.97	0.06	68,73,76,77	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
18	MES	a	301	12/12	0.81	0.16	124,134,142,143	0
18	MES	d	101	12/12	0.93	0.14	71,77,90,91	0
16	MG	Z	301	1/1	0.95	0.11	95,95,95,95	0
18	MES	e	101	12/12	0.96	0.10	55,57,66,68	0
18	MES	Y	301	12/12	0.97	0.09	55,58,62,65	0
16	MG	I	301	1/1	0.97	0.13	84,84,84,84	0
16	MG	G	301	1/1	0.97	0.06	74,74,74,74	0
17	CL	G	302	1/1	0.97	0.19	30,30,30,30	0
16	MG	V	301	1/1	0.98	0.06	91,91,91,91	0
17	CL	G	303	1/1	0.99	0.03	54,54,54,54	0
17	CL	N	201	1/1	0.99	0.03	69,69,69,69	0
17	CL	U	301	1/1	0.99	0.04	57,57,57,57	0
17	CL	b	201	1/1	0.99	0.03	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.