wwPDB EM Map/Model Validation Report (i)

Sep 12, 2016 – 07:26 PM EDT

PDB ID	:	5L4G
EMDB ID:	:	EMD-4002
Title	:	The human 26S proteasome at 3.9 A
Authors	:	Schweitzer, A.; Aufderheide, A.; Rudack, T.; Beck, F.
Deposited on	:	2016-05-25
Resolution	:	4.02 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

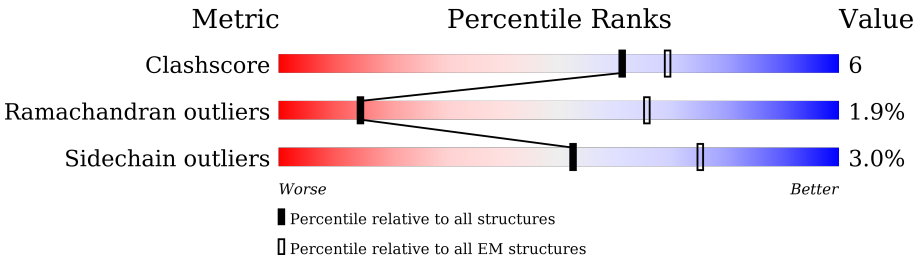
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.02 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	246	86% 13% •
1	N	246	85% 14% •
2	B	234	81% 15% •
2	O	234	83% 15% •
3	C	261	89% 6% •
3	P	261	85% 9% • •
4	D	248	86% 11% • •
4	Q	248	87% 11% •
5	E	241	85% 11% • •

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Mol	Chain	Length	Quality of chain
5	R	241	85% 11% •
6	F	263	75% 15% 10%
6	S	263	79% 11% 10%
7	G	255	82% 13% 5%
7	T	255	87% 7% 5%
8	1	241	75% 12% • 12%
8	U	241	72% 15% • 12%
9	2	201	88% 9% ••
9	V	201	88% 10% ••
10	3	205	83% 15% •
10	W	205	93% 6%
11	4	264	72% 11% 18%
11	X	264	75% 6% • 18%
12	5	263	63% 13% 24%
12	Y	263	63% 11% • 24%
13	6	239	74% 8% 17%
13	Z	239	72% 12% 16%
14	7	277	69% 9% • 21%
14	8	277	70% 8% • 21%
15	H	433	65% 24% • 9%
16	I	440	66% 19% • 14%
17	K	418	75% 17% • 6%
18	L	389	80% 17% •
19	M	439	74% 18% • 5%
20	J	406	73% 21% • •

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 135560 atoms, of which 67868 are hydrogens and 0 are deuteriums.

In the tables below, 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-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	N	244	Total	C	H	N	O	S	0	0
			3814	1206	1911	320	364	13		
1	A	244	Total	C	H	N	O	S	0	0
			3814	1206	1911	320	364	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	O	233	Total	C	H	N	O	S	0	0
			3630	1161	1812	308	343	6		
2	B	233	Total	C	H	N	O	S	0	0
			3630	1161	1812	308	343	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	P	250	Total	C	H	N	O	S	0	0
			3963	1245	1992	339	377	10		
3	C	250	Total	C	H	N	O	S	0	0
			3963	1245	1992	339	377	10		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	Q	243	Total	C	H	N	O	S	0	0
			3875	1206	1952	342	370	5		
4	D	243	Total	C	H	N	O	S	0	0
			3875	1206	1952	342	370	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	R	234	Total	C	H	N	O	S	0	0
			3563	1125	1773	295	359	11		
5	E	234	Total	C	H	N	O	S	0	0
			3563	1125	1773	295	359	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	S	238	Total	C	H	N	O	S	0	0
			3733	1172	1860	337	353	11		
6	F	238	Total	C	H	N	O	S	0	0
			3733	1172	1860	337	353	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	T	242	Total	C	H	N	O	S	0	0
			3771	1200	1877	323	360	11		
7	G	241	Total	C	H	N	O	S	0	0
			3764	1198	1874	322	359	11		

- Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	U	213	Total	C	H	N	O	S	0	0
			3308	1047	1654	284	313	10		
8	1	213	Total	C	H	N	O	S	0	0
			3308	1047	1654	284	313	10		

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	V	199	Total	C	H	N	O	S	0	0
			3197	1022	1601	272	293	9		
9	2	199	Total	C	H	N	O	S	0	0
			3197	1022	1601	272	293	9		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	W	204	Total	C	H	N	O	S	0	0
			3200	1013	1609	265	294	19		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	3	204	Total	C	H	N	O	S	0	0
			3200	1013	1609	265	294	19		

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	X	217	Total	C	H	N	O	S	0	0
			3358	1066	1667	292	321	12		
11	4	217	Total	C	H	N	O	S	0	0
			3358	1066	1667	292	321	12		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	Y	201	Total	C	H	N	O	S	0	0
			3080	982	1521	274	294	9		
12	5	201	Total	C	H	N	O	S	0	0
			3080	982	1521	274	294	9		

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	Z	200	Total	C	H	N	O	S	0	0
			2966	939	1467	256	292	12		
13	6	199	Total	C	H	N	O	S	0	0
			2956	936	1462	255	291	12		

- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	8	220	Total	C	H	N	O	S	0	0
			3338	1044	1679	283	320	12		
14	7	220	Total	C	H	N	O	S	0	0
			3338	1044	1679	283	320	12		

- Molecule 15 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	H	396	Total	C	H	N	O	S	0	0
			6283	1961	3167	549	588	18		

- Molecule 16 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	I	379	Total	C	H	N	O	S	0	0
			6043	1880	3050	510	588	15		

- Molecule 17 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	K	393	Total	C	H	N	O	S	0	0
			6302	1986	3164	537	602	13		

- Molecule 18 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	L	389	Total	C	H	N	O	S	0	0
			6271	1947	3173	552	582	17		

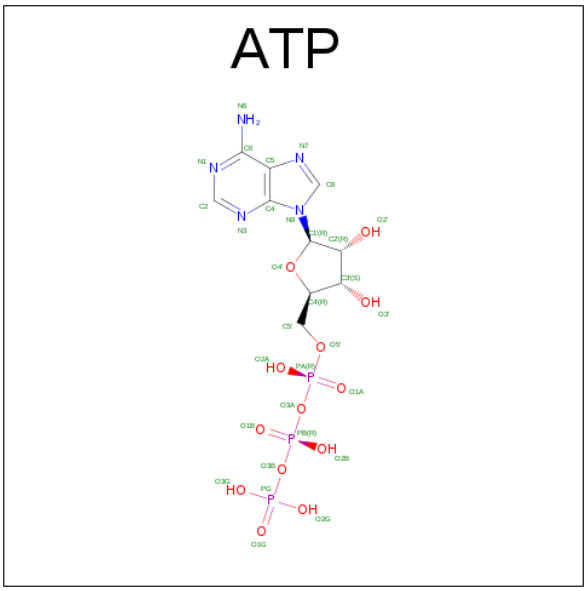
- Molecule 19 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	M	415	Total	C	H	N	O	S	0	0
			6575	2039	3322	561	635	18		

- Molecule 20 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	J	391	Total	C	H	N	O	S	0	0
			6252	1928	3178	549	579	18		

- Molecule 21 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

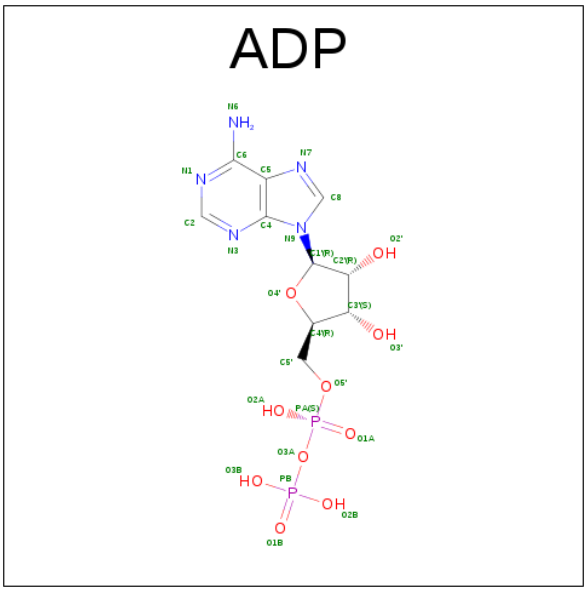


Mol	Chain	Residues	Atoms						AltConf
21	H	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
21	I	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
21	K	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
21	L	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
21	M	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
22	H	1	Total	Mg	0
			1	1	
22	I	1	Total	Mg	0
			1	1	
22	L	1	Total	Mg	0
			1	1	
22	K	1	Total	Mg	0
			1	1	
22	M	1	Total	Mg	0
			1	1	

- Molecule 23 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



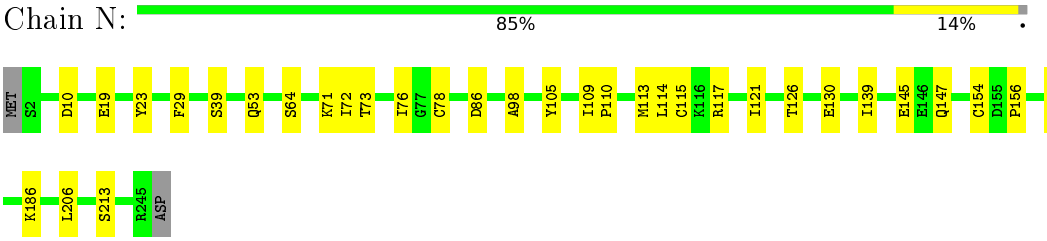
Mol	Chain	Residues	Atoms						AltConf
23	J	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

3 Residue-property plots (i)

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

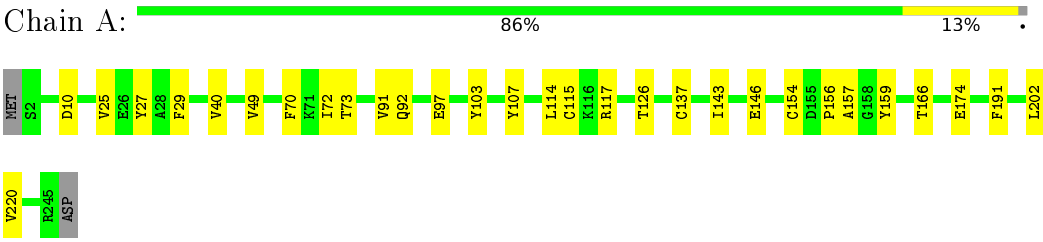
- Molecule 1: Proteasome subunit alpha type-6

Chain N:



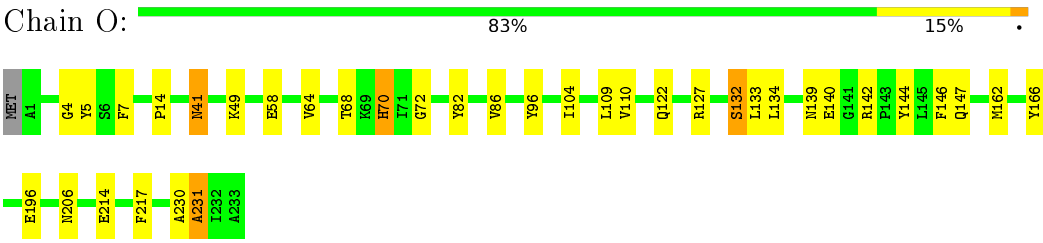
- Molecule 1: Proteasome subunit alpha type-6

Chain A:



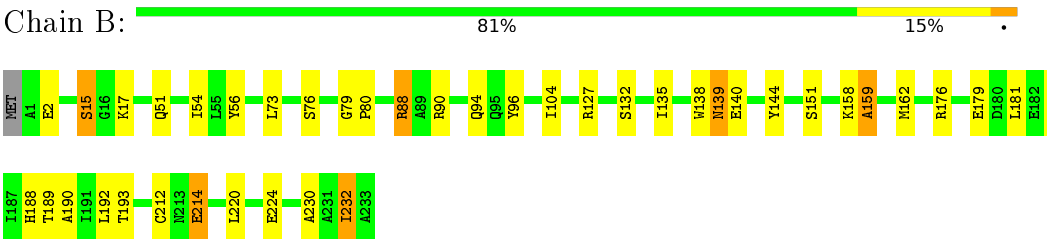
- Molecule 2: Proteasome subunit alpha type-2

Chain O:



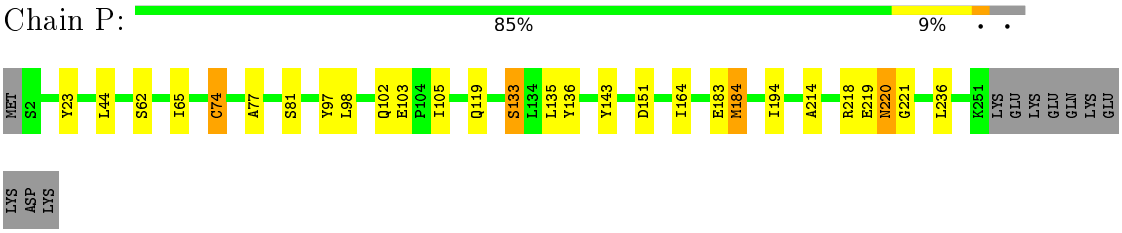
- Molecule 2: Proteasome subunit alpha type-2

Chain B:



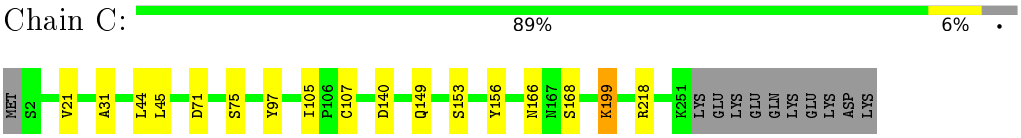
- Molecule 3: Proteasome subunit alpha type-4

Chain P:



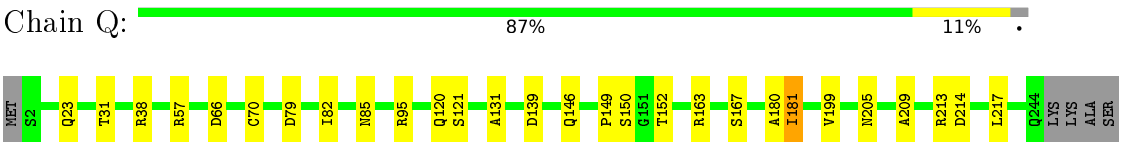
- Molecule 3: Proteasome subunit alpha type-4

Chain C:



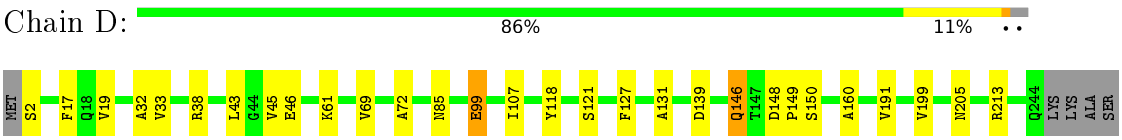
- Molecule 4: Proteasome subunit alpha type-7

Chain Q:



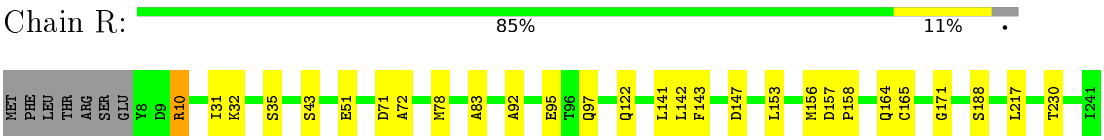
- Molecule 4: Proteasome subunit alpha type-7

Chain D:



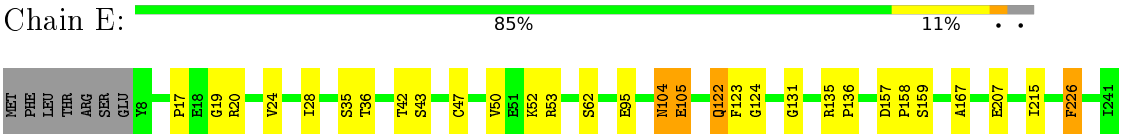
- Molecule 5: Proteasome subunit alpha type-5

Chain R:



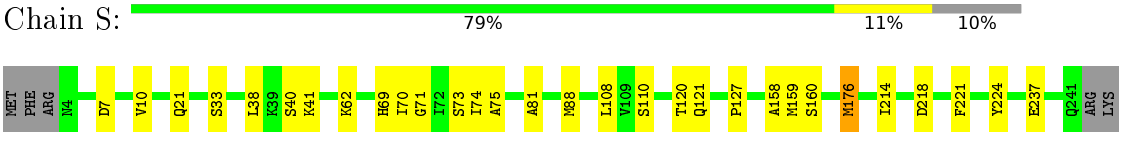
- Molecule 5: Proteasome subunit alpha type-5

Chain E:



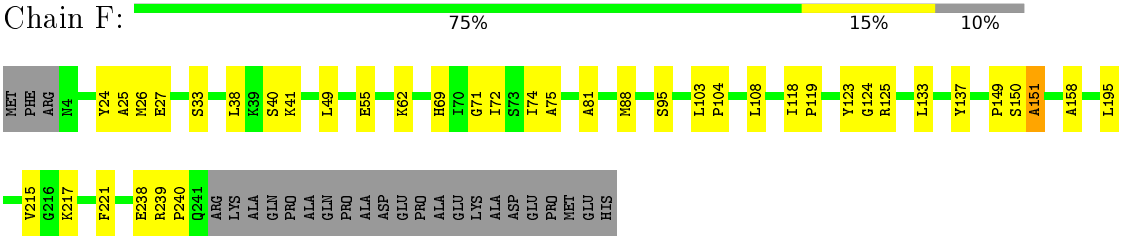
- Molecule 6: Proteasome subunit alpha type-1

Chain S:



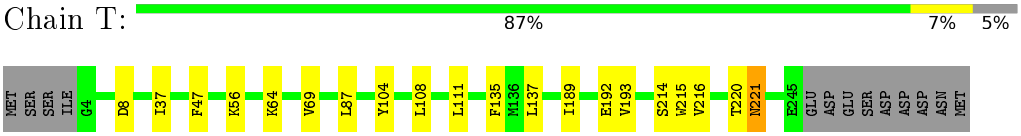
- Molecule 6: Proteasome subunit alpha type-1

Chain F:



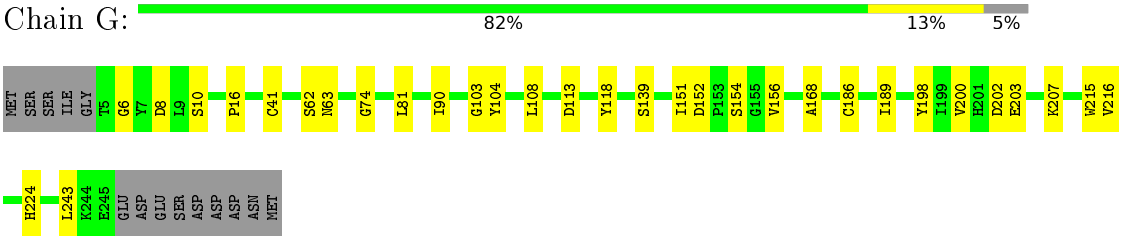
- Molecule 7: Proteasome subunit alpha type-3

Chain T:



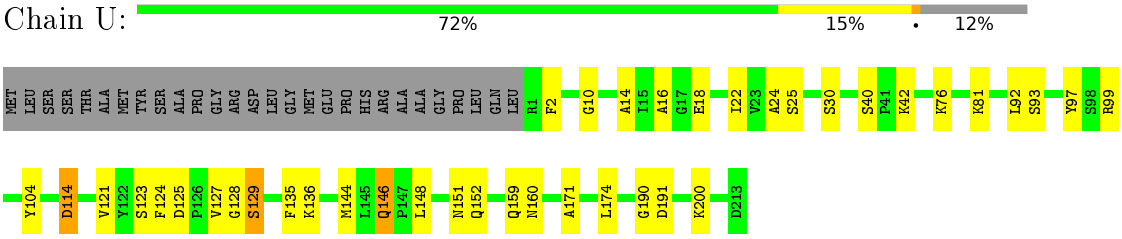
- Molecule 7: Proteasome subunit alpha type-3

Chain G:



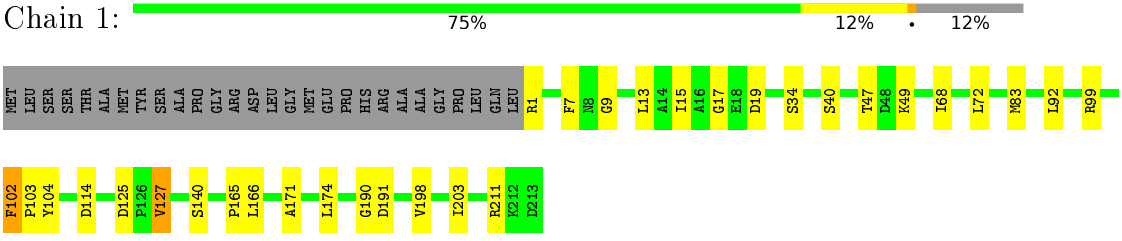
- Molecule 8: Proteasome subunit beta type-1

Chain U:



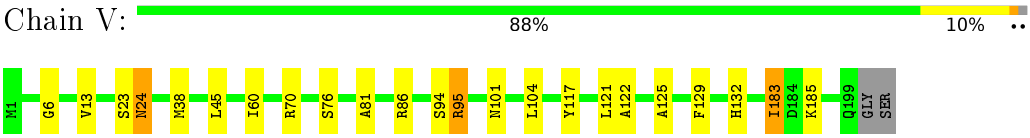
- Molecule 8: Proteasome subunit beta type-1

Chain 1:



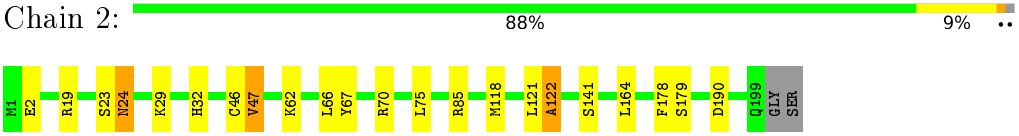
- Molecule 9: Proteasome subunit beta type-2

Chain V:



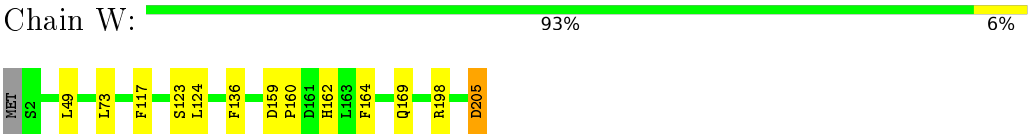
• Molecule 9: Proteasome subunit beta type-2

Chain 2:



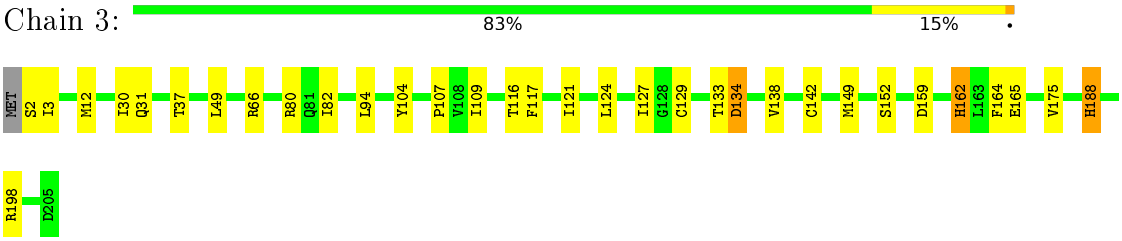
• Molecule 10: Proteasome subunit beta type-3

Chain W:



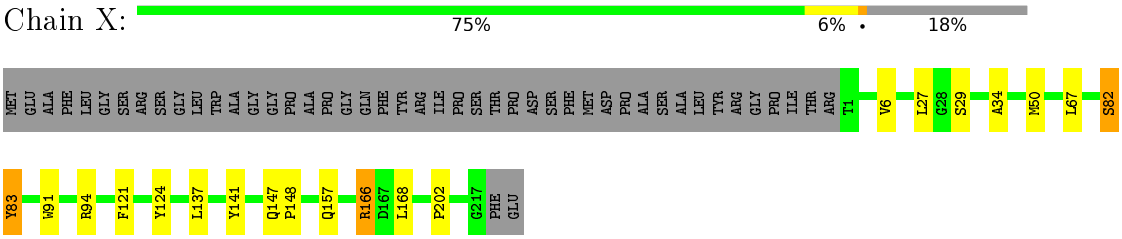
• Molecule 10: Proteasome subunit beta type-3

Chain 3:



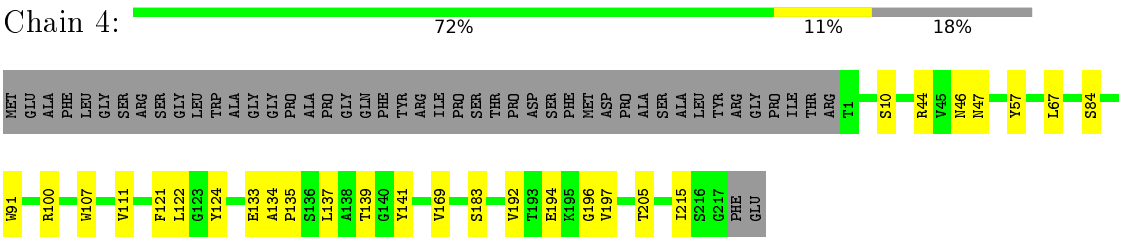
• Molecule 11: Proteasome subunit beta type-4

Chain X:



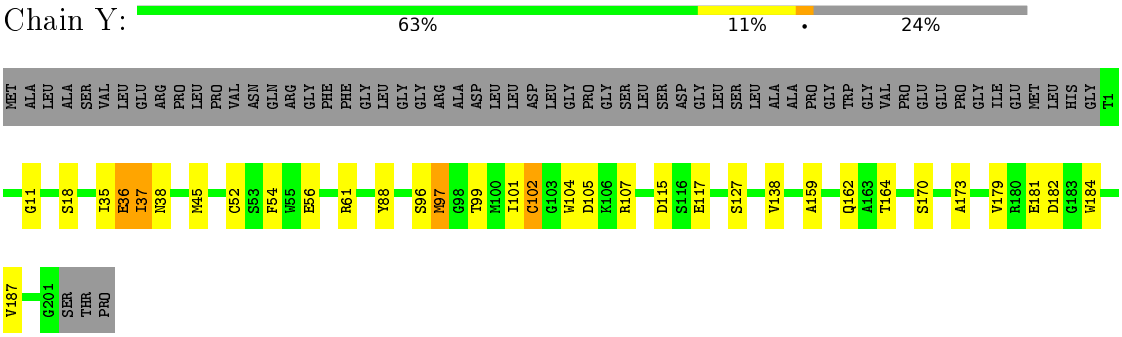
• Molecule 11: Proteasome subunit beta type-4

Chain 4:



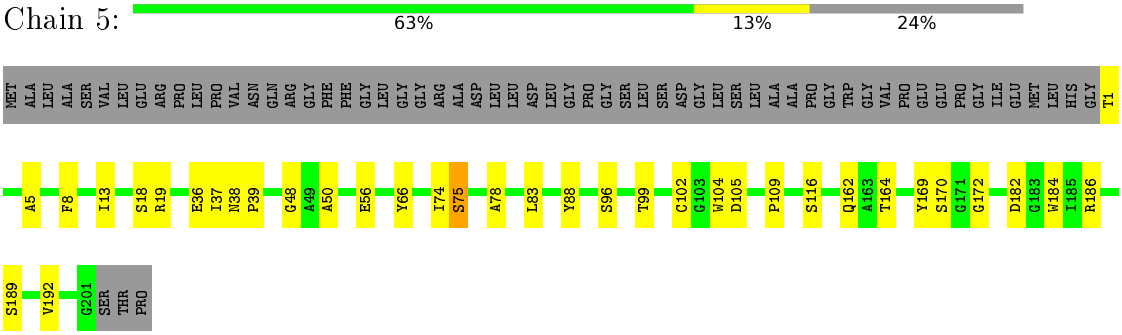
• Molecule 12: Proteasome subunit beta type-5

Chain Y:



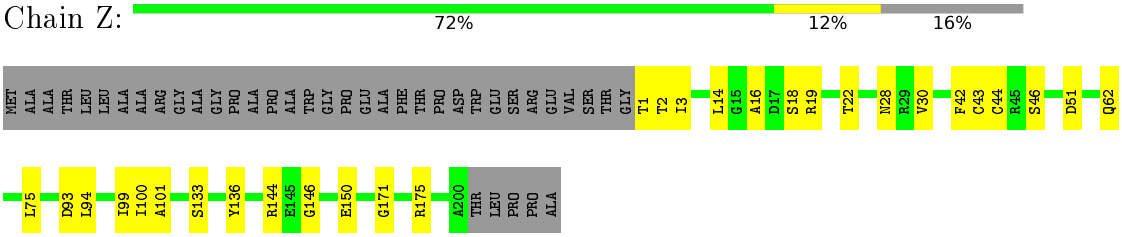
- Molecule 12: Proteasome subunit beta type-5

Chain 5:



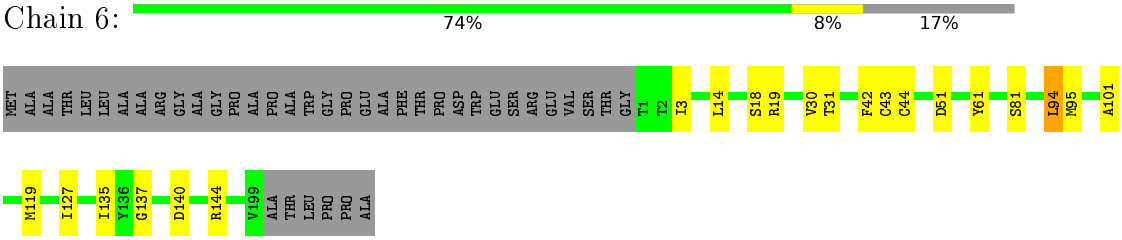
- Molecule 13: Proteasome subunit beta type-6

Chain Z:



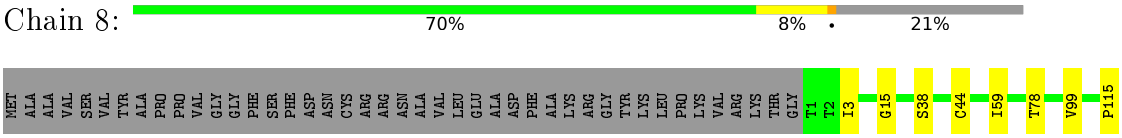
- Molecule 13: Proteasome subunit beta type-6

Chain 6:



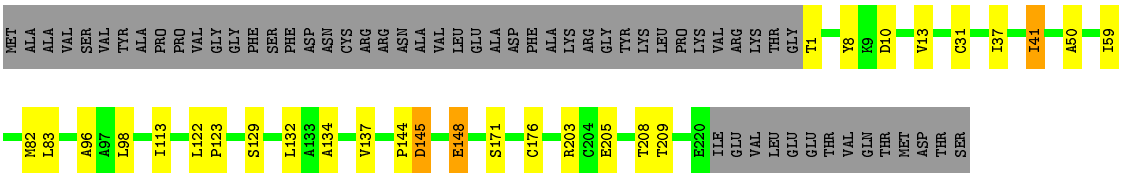
- Molecule 14: Proteasome subunit beta type-7

Chain 8:



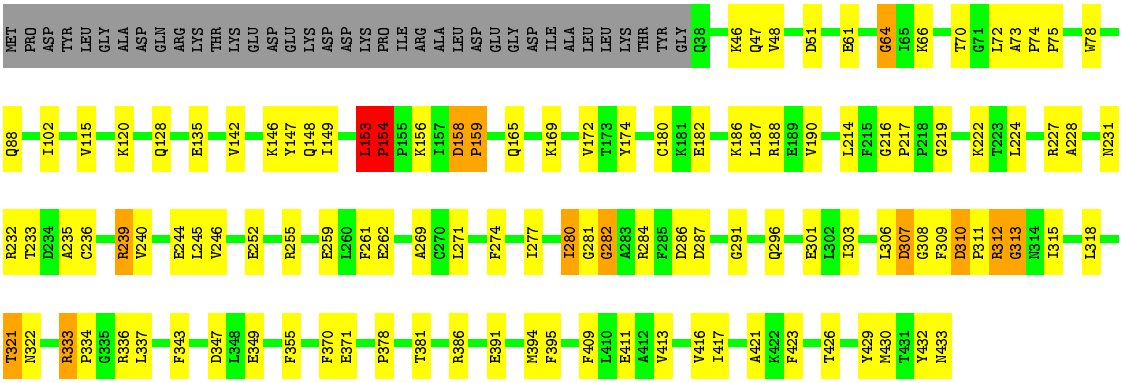
• Molecule 14: Proteasome subunit beta type-7

Chain 7:



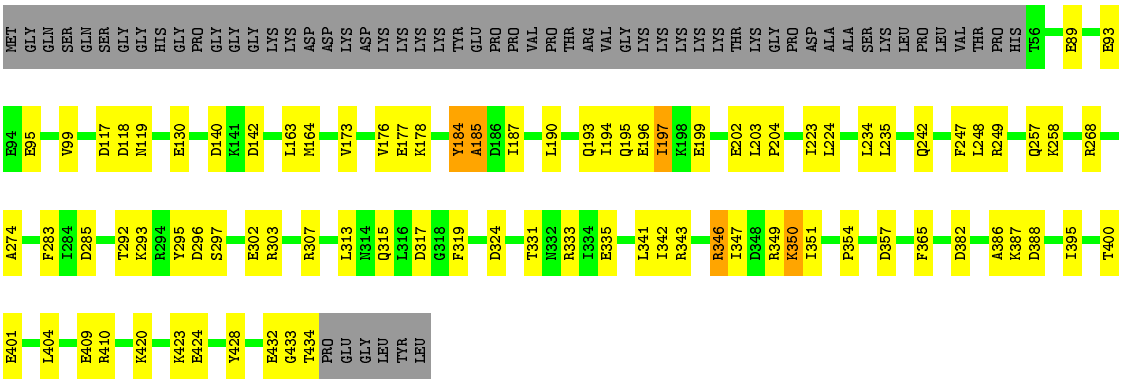
• Molecule 15: 26S protease regulatory subunit 7

Chain H:



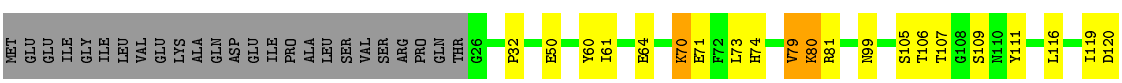
• Molecule 16: 26S protease regulatory subunit 4

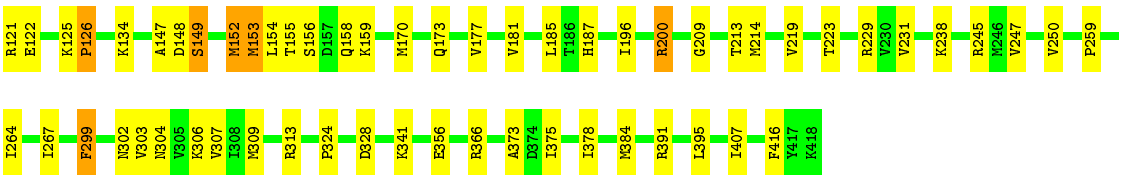
Chain I:



• Molecule 17: 26S protease regulatory subunit 6B

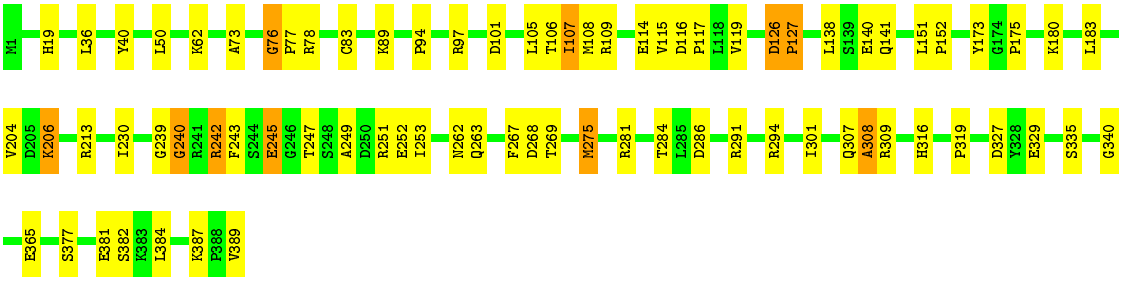
Chain K:





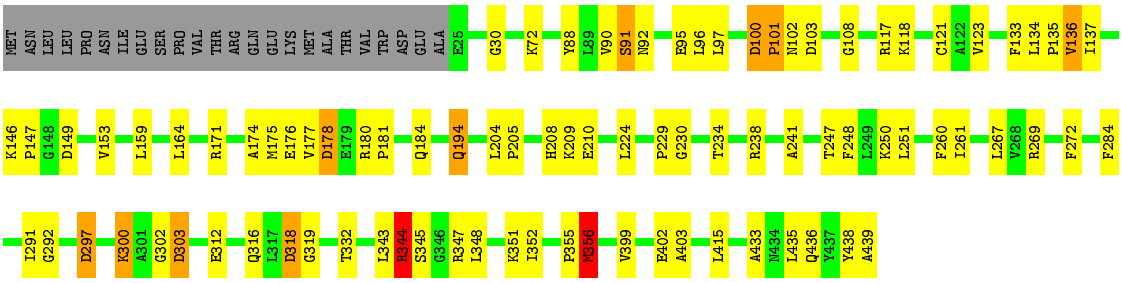
- Molecule 18: 26S protease regulatory subunit 10B

Chain L:



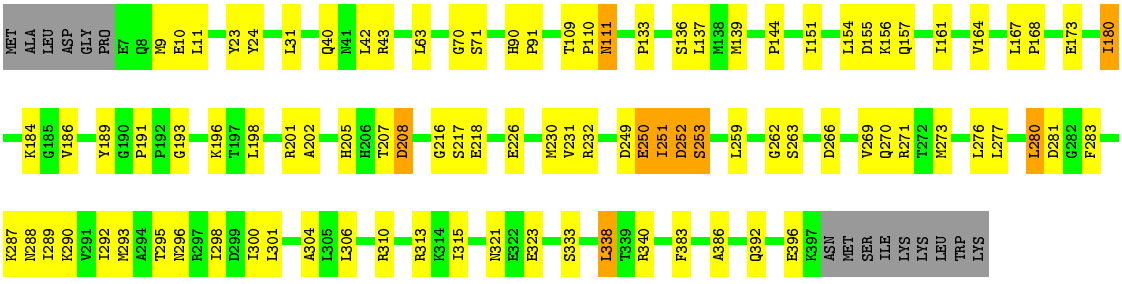
- Molecule 19: 26S protease regulatory subunit 6A

Chain M:



- Molecule 20: 26S protease regulatory subunit 8

Chain J:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	461402	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, ADP

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.43	0/1937	0.55	0/2617
1	N	0.38	0/1937	0.56	0/2617
10	3	0.42	1/1620 (0.1%)	0.57	0/2184
10	W	0.40	0/1620	0.58	0/2184
11	4	0.42	0/1724	0.61	0/2333
11	X	0.40	0/1724	0.59	0/2333
12	5	0.42	0/1590	0.59	0/2147
12	Y	0.41	0/1590	0.60	0/2147
13	6	0.40	0/1520	0.56	0/2057
13	Z	0.39	0/1525	0.60	0/2064
14	7	0.36	0/1686	0.58	0/2282
14	8	0.35	0/1686	0.58	0/2282
15	H	0.38	0/3168	0.61	2/4277 (0.0%)
16	I	0.35	0/3034	0.58	0/4089
17	K	0.37	0/3191	0.53	0/4306
18	L	0.38	0/3146	0.56	0/4233
19	M	0.38	0/3294	0.54	0/4437
2	B	0.88	6/1857 (0.3%)	0.78	9/2514 (0.4%)
2	O	0.38	0/1857	0.54	0/2514
20	J	0.39	0/3113	0.56	0/4184
3	C	0.38	0/2001	0.56	0/2694
3	P	0.36	0/2001	0.56	0/2694
4	D	0.37	0/1949	0.55	0/2626
4	Q	0.34	0/1949	0.52	0/2626
5	E	0.38	0/1818	0.56	0/2455
5	R	0.37	0/1818	0.53	0/2455
6	F	0.36	0/1908	0.56	0/2579
6	S	0.34	0/1908	0.54	0/2579
7	G	0.38	0/1925	0.55	0/2592
7	T	0.37	0/1929	0.53	0/2597
8	1	0.41	0/1684	0.58	0/2268
8	U	0.38	0/1684	0.59	0/2268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
9	2	0.43	0/1629	0.58	0/2203
9	V	0.42	0/1629	0.58	0/2203
All	All	0.41	7/68651 (0.0%)	0.57	11/92640 (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	H	0	2
16	I	0	1
17	K	0	2
2	B	0	1
20	J	0	1
7	G	0	1
7	T	0	1
All	All	0	9

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	185	ASP	CB-CG	20.70	1.95	1.51
2	B	185	ASP	CA-CB	17.41	1.92	1.53
2	B	184	GLU	CB-CG	13.19	1.77	1.52
2	B	184	GLU	C-N	8.40	1.53	1.34
2	B	185	ASP	N-CA	7.22	1.60	1.46
10	3	82	ILE	C-N	6.79	1.49	1.34
2	B	184	GLU	CA-C	5.48	1.67	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	185	ASP	N-CA-CB	12.31	132.76	110.60
2	B	184	GLU	C-N-CA	11.92	151.50	121.70
15	H	153	LEU	C-N-CD	-11.44	95.42	120.60
2	B	185	ASP	CB-CG-OD1	8.30	125.77	118.30
2	B	185	ASP	CB-CA-C	-8.00	94.41	110.40
2	B	184	GLU	N-CA-C	7.67	131.70	111.00
2	B	184	GLU	N-CA-CB	-6.22	99.41	110.60
15	H	153	LEU	C-N-CA	6.10	147.64	122.00
2	B	185	ASP	CA-CB-CG	5.40	125.27	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	185	ASP	OD1-CG-OD2	-5.29	113.24	123.30
2	B	184	GLU	CA-CB-CG	5.20	124.83	113.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	186	ALA	Peptide
7	G	215	TRP	Peptide
15	H	153	LEU	Peptide
15	H	321	THR	Peptide
16	I	195	GLN	Peptide
20	J	10	GLU	Peptide
17	K	122	GLU	Peptide
17	K	152	MET	Peptide
7	T	215	TRP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1903	1911	1911	17	0
1	N	1903	1911	1911	18	0
2	B	1818	1812	1814	46	0
2	O	1818	1812	1814	20	0
3	C	1971	1992	1992	7	0
3	P	1971	1992	1992	16	0
4	D	1923	1952	1952	15	0
4	Q	1923	1952	1952	12	0
5	E	1790	1773	1773	14	0
5	R	1790	1773	1773	13	0
6	F	1873	1860	1860	21	0
6	S	1873	1860	1860	12	0
7	G	1890	1874	1874	11	0
7	T	1894	1877	1877	9	0
8	1	1654	1654	1656	13	0
8	U	1654	1654	1656	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	2	1596	1601	1601	15	0
9	V	1596	1601	1601	14	0
10	3	1591	1609	1609	20	0
10	W	1591	1609	1609	7	0
11	4	1691	1667	1669	14	0
11	X	1691	1667	1669	9	0
12	5	1559	1521	1523	15	0
12	Y	1559	1521	1523	21	0
13	6	1494	1462	1464	10	0
13	Z	1499	1467	1469	14	0
14	7	1659	1679	1681	20	0
14	8	1659	1679	1681	12	0
15	H	3116	3167	3167	90	0
16	I	2993	3050	3050	63	0
17	K	3138	3164	3164	52	0
18	L	3098	3173	3173	52	0
19	M	3253	3322	3322	71	0
20	J	3074	3178	3178	73	0
21	H	31	12	12	2	0
21	I	31	12	12	0	0
21	K	31	12	12	5	0
21	L	31	12	12	1	0
21	M	31	12	12	4	0
22	H	1	0	0	0	0
22	I	1	0	0	0	0
22	K	1	0	0	0	0
22	L	1	0	0	0	0
22	M	1	0	0	0	0
23	J	27	12	12	2	0
All	All	67692	67868	67892	756	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 6.

All (756) 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)
2:B:184:GLU:CG	2:B:184:GLU:CB	1.77	1.54
2:B:185:ASP:CA	2:B:185:ASP:CB	1.92	1.45
2:B:185:ASP:CG	2:B:185:ASP:CB	1.95	1.35
2:B:185:ASP:O	2:B:189:THR:N	1.81	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:70:LYS:O	17:K:73:LEU:N	1.97	0.96
11:4:133:GLU:OE1	11:4:133:GLU:N	2.09	0.84
2:B:185:ASP:HB2	2:B:189:THR:HG22	1.60	0.84
20:J:277:LEU:HA	20:J:280:LEU:HD22	1.61	0.83
15:H:231:ASN:OD1	15:H:232:ARG:N	2.13	0.81
2:B:185:ASP:CB	2:B:185:ASP:C	2.50	0.80
2:B:186:ALA:O	2:B:190:ALA:HB2	1.81	0.80
2:B:186:ALA:O	2:B:190:ALA:CB	2.30	0.79
18:L:275:MET:SD	18:L:275:MET:N	2.56	0.79
15:H:146:LYS:O	15:H:148:GLN:N	2.16	0.78
2:B:232:ILE:HG12	2:B:232:ILE:O	1.84	0.78
6:F:55:GLU:N	6:F:55:GLU:OE1	2.18	0.77
2:B:185:ASP:HA	2:B:188:HIS:CB	2.18	0.74
21:K:501:ATP:O3G	18:L:294:ARG:NH2	2.20	0.74
2:B:185:ASP:HA	2:B:188:HIS:HB3	1.72	0.71
15:H:309:PHE:HD1	19:M:238:ARG:HG3	1.56	0.70
20:J:184:LYS:HE2	20:J:287:LYS:HD3	1.72	0.70
17:K:214:MET:N	21:K:501:ATP:O1A	2.23	0.70
5:E:20:ARG:NH2	19:M:438:TYR:O	2.26	0.69
15:H:347:ASP:OD1	15:H:349:GLU:N	2.26	0.67
20:J:280:LEU:O	20:J:280:LEU:HG	1.93	0.67
20:J:133:PRO:O	20:J:136:SER:N	2.27	0.66
20:J:259:LEU:HD22	20:J:300:ILE:CD1	2.25	0.66
19:M:344:ARG:NE	19:M:345:SER:O	2.29	0.66
20:J:218:GLU:N	20:J:218:GLU:OE1	2.26	0.65
2:B:181:LEU:HD13	2:B:185:ASP:OD1	1.96	0.65
19:M:194:GLN:N	19:M:194:GLN:OE1	2.30	0.65
20:J:252:ASP:CB	20:J:259:LEU:HD21	2.28	0.63
18:L:365:GLU:N	18:L:365:GLU:OE1	2.29	0.63
15:H:371:GLU:N	15:H:371:GLU:OE2	2.29	0.63
17:K:79:VAL:O	17:K:81:ARG:N	2.30	0.63
15:H:174:TYR:CD1	15:H:228:ALA:HB1	2.34	0.63
16:I:302:GLU:OE1	16:I:302:GLU:N	2.32	0.63
20:J:249:ASP:OD1	20:J:249:ASP:N	2.31	0.63
1:A:72:ILE:HG21	1:A:114:LEU:HD21	1.80	0.63
4:Q:31:THR:OG1	4:Q:163:ARG:O	2.16	0.62
10:3:2:SER:OG	10:3:3:ILE:N	2.31	0.62
19:M:269:ARG:NH1	19:M:312:GLU:OE2	2.31	0.62
16:I:317:ASP:HB2	16:I:346:ARG:CD	2.30	0.62
16:I:196:GLU:O	16:I:199:GLU:N	2.33	0.62
2:B:181:LEU:HB3	2:B:185:ASP:OD1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:8:ASP:OD1	7:T:8:ASP:N	2.35	0.60
17:K:200:ARG:HB3	17:K:306:LYS:HG3	1.84	0.60
18:L:267:PHE:O	18:L:269:THR:N	2.35	0.59
20:J:259:LEU:HD22	20:J:300:ILE:HD12	1.85	0.59
16:I:130:GLU:OE1	16:I:130:GLU:N	2.36	0.59
15:H:309:PHE:CD1	19:M:238:ARG:HG3	2.37	0.59
20:J:252:ASP:HB3	20:J:259:LEU:HD21	1.84	0.59
21:H:501:ATP:O1G	16:I:343:ARG:NH1	2.36	0.59
6:F:71:GLY:HA3	6:F:221:PHE:CZ	2.38	0.58
1:N:29:PHE:CE2	1:N:156:PRO:HD2	2.38	0.58
15:H:336:ARG:O	15:H:337:LEU:HD12	2.04	0.58
18:L:83:CYS:SG	18:L:89:LYS:HE2	2.44	0.58
18:L:106:THR:O	18:L:108:MET:N	2.35	0.58
16:I:313:LEU:HD13	16:I:341:LEU:HA	1.86	0.58
20:J:266:ASP:O	20:J:269:VAL:HG12	2.03	0.57
8:1:68:ILE:HD11	8:1:92:LEU:HD13	1.84	0.57
20:J:144:PRO:HD2	20:J:201:ARG:CZ	2.34	0.57
20:J:164:VAL:HG21	20:J:313:ARG:HE	1.69	0.57
18:L:138:LEU:O	18:L:140:GLU:N	2.38	0.57
10:3:116:THR:O	10:3:117:PHE:CD1	2.58	0.57
4:D:85:ASN:OD1	9:2:70:ARG:NH2	2.36	0.57
15:H:172:VAL:HG11	15:H:224:LEU:HD11	1.87	0.57
16:I:197:ILE:HD11	16:I:224:LEU:HD21	1.87	0.57
6:F:33:SER:H	19:M:439:ALA:HB1	1.70	0.57
20:J:251:ILE:O	20:J:253:SER:N	2.38	0.57
19:M:100:ASP:HB3	19:M:118:LYS:HG3	1.87	0.57
12:Y:11:GLY:HA2	12:Y:104:TRP:HZ3	1.68	0.57
6:F:74:ILE:HG21	6:F:81:ALA:HB1	1.86	0.56
16:I:190:LEU:O	16:I:194:ILE:HG12	2.05	0.56
3:P:65:ILE:HD13	3:P:214:ALA:HB3	1.87	0.56
13:6:137:GLY:O	13:6:140:ASP:N	2.38	0.56
20:J:277:LEU:HG	20:J:277:LEU:O	2.05	0.56
12:5:1:THR:N	12:5:169:TYR:O	2.39	0.56
14:7:208:THR:HG23	14:7:209:THR:HG23	1.87	0.56
15:H:280:ILE:O	15:H:280:ILE:HG22	2.05	0.56
16:I:317:ASP:HB2	16:I:346:ARG:HD3	1.88	0.56
5:R:92:ALA:O	5:R:95:GLU:N	2.39	0.56
18:L:206:LYS:HD3	19:M:260:PHE:HB3	1.86	0.56
18:L:175:PRO:HB3	18:L:384:LEU:HD21	1.87	0.56
6:F:24:TYR:O	6:F:27:GLU:N	2.35	0.56
18:L:381:GLU:HG3	19:M:351:LYS:CD	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:157:ASP:HB2	5:R:158:PRO:HD2	1.88	0.56
14:8:115:PRO:O	14:8:116:HIS:HB2	2.05	0.55
14:8:166:ASP:OD2	14:8:168:GLY:N	2.38	0.55
2:B:185:ASP:C	2:B:189:THR:H	2.08	0.55
1:A:27:TYR:CE1	7:G:16:PRO:HA	2.40	0.55
6:F:40:SER:OG	6:F:41:LYS:N	2.40	0.55
18:L:381:GLU:HG3	19:M:351:LYS:HD2	1.88	0.55
6:S:40:SER:OG	6:S:41:LYS:N	2.38	0.55
8:U:171:ALA:O	8:U:174:LEU:N	2.38	0.55
15:H:245:LEU:HB2	15:H:280:ILE:HD12	1.87	0.55
8:U:148:LEU:CD1	10:3:152:SER:HB3	2.36	0.55
16:I:404:LEU:HD21	20:J:313:ARG:NH2	2.22	0.55
11:4:46:ASN:OD1	11:4:47:ASN:N	2.40	0.55
15:H:252:GLU:OE2	15:H:255:ARG:NH1	2.40	0.55
20:J:202:ALA:O	20:J:205:HIS:N	2.38	0.55
15:H:426:THR:HG22	15:H:430:MET:HE2	1.90	0.54
17:K:148:ASP:O	17:K:149:SER:CB	2.55	0.54
13:Z:175:ARG:NH2	11:4:215:ILE:HD13	2.22	0.54
2:B:185:ASP:C	2:B:189:THR:HG22	2.28	0.54
7:T:108:LEU:HD11	7:T:137:LEU:HB3	1.90	0.54
10:3:164:PHE:CZ	10:3:198:ARG:HD2	2.43	0.54
7:G:168:ALA:HB1	7:G:200:VAL:HG13	1.90	0.54
20:J:269:VAL:O	20:J:273:MET:HG3	2.08	0.53
2:B:185:ASP:O	2:B:189:THR:HG22	2.08	0.53
4:D:69:VAL:HG11	4:D:107:ILE:HG21	1.89	0.53
15:H:174:TYR:CE1	15:H:228:ALA:HB1	2.43	0.53
11:X:82:SER:O	11:X:83:TYR:HB2	2.08	0.53
13:6:14:LEU:HD21	13:6:101:ALA:HB3	1.90	0.53
15:H:174:TYR:HD2	15:H:188:ARG:HH22	1.57	0.53
19:M:194:GLN:HG3	19:M:352:ILE:CG2	2.39	0.53
18:L:97:ARG:NE	18:L:114:GLU:OE2	2.41	0.53
15:H:219:GLY:O	15:H:381:THR:HB	2.09	0.53
15:H:426:THR:O	15:H:430:MET:HB2	2.09	0.53
3:P:218:ARG:NH1	3:P:221:GLY:O	2.42	0.52
7:T:189:ILE:O	7:T:192:GLU:N	2.42	0.52
15:H:156:LYS:O	15:H:159:PRO:HD2	2.08	0.52
20:J:249:ASP:O	20:J:250:GLU:C	2.48	0.52
15:H:391:GLU:HG3	15:H:416:VAL:CG2	2.39	0.52
2:O:134:LEU:CD1	2:O:162:MET:SD	2.98	0.52
6:S:218:ASP:OD1	6:S:218:ASP:N	2.35	0.52
10:3:165:GLU:HG2	14:7:208:THR:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:4:192:VAL:HG12	11:4:197:VAL:HG22	1.90	0.52
19:M:403:ALA:HB1	19:M:415:LEU:HD12	1.90	0.52
15:H:423:PHE:HE1	16:I:350:LYS:HE3	1.74	0.52
19:M:178:ASP:N	19:M:178:ASP:OD1	2.33	0.52
2:O:109:LEU:O	2:O:109:LEU:HG	2.10	0.52
11:X:27:LEU:HD11	11:X:34:ALA:HB1	1.91	0.52
20:J:277:LEU:HA	20:J:280:LEU:CD2	2.36	0.52
5:R:31:ILE:HD11	5:R:158:PRO:HD3	1.91	0.52
17:K:125:LYS:O	17:K:126:PRO:C	2.48	0.52
17:K:267:ILE:HG13	17:K:309:MET:HB3	1.90	0.52
13:6:127:ILE:HD11	13:6:135:ILE:HG13	1.91	0.51
15:H:281:GLY:O	15:H:282:GLY:O	2.27	0.51
17:K:231:VAL:HG13	18:L:262:ASN:HD22	1.74	0.51
19:M:100:ASP:O	19:M:108:GLY:HA2	2.09	0.51
12:Y:18:SER:HB3	12:Y:173:ALA:H	1.75	0.51
20:J:110:PRO:O	20:J:111:ASN:HB2	2.11	0.51
18:L:116:ASP:HB2	18:L:117:PRO:HD2	1.91	0.51
18:L:249:ALA:HA	19:M:261:ILE:HD11	1.92	0.51
2:O:230:ALA:O	2:O:231:ALA:HB3	2.11	0.51
2:B:139:ASN:HD22	2:B:140:GLU:HG2	1.76	0.51
7:G:103:GLY:O	7:G:104:TYR:HB3	2.09	0.51
9:2:121:LEU:O	9:2:122:ALA:HB3	2.11	0.51
20:J:133:PRO:O	20:J:137:LEU:N	2.42	0.51
9:V:13:VAL:HB	9:V:183:ILE:HD12	1.93	0.51
2:B:138:TRP:CE3	2:B:214:GLU:HA	2.46	0.51
6:F:26:MET:HG2	6:F:149:PRO:HD2	1.91	0.51
20:J:333:SER:HB3	20:J:338:LEU:HD11	1.92	0.51
16:I:223:ILE:HG13	16:I:347:ILE:HG21	1.93	0.51
20:J:250:GLU:O	20:J:251:ILE:O	2.28	0.51
19:M:91:SER:OG	19:M:92:ASN:N	2.43	0.51
1:A:126:THR:HG22	2:B:127:ARG:HH21	1.76	0.51
7:G:108:LEU:HD22	7:G:139:SER:HB3	1.92	0.51
2:B:185:ASP:C	2:B:188:HIS:N	2.64	0.50
16:I:333:ARG:O	16:I:335:GLU:N	2.44	0.50
1:A:159:TYR:CE2	17:K:416:PHE:CE2	2.99	0.50
10:W:205:ASP:OD2	12:5:19:ARG:NH2	2.44	0.50
18:L:126:ASP:N	18:L:127:PRO:CD	2.74	0.50
7:G:154:SER:HB2	7:G:156:VAL:HG23	1.92	0.50
16:I:177:GLU:OE1	16:I:177:GLU:N	2.44	0.50
12:Y:138:VAL:HG13	9:2:141:SER:HB3	1.92	0.50
15:H:309:PHE:CD2	19:M:250:LYS:HD3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:VAL:HG11	3:C:153:SER:HA	1.94	0.50
4:D:43:LEU:HD23	4:D:43:LEU:H	1.77	0.50
5:E:157:ASP:HB2	5:E:158:PRO:CD	2.42	0.50
5:E:17:PRO:HB3	6:F:24:TYR:CZ	2.46	0.50
15:H:74:PRO:N	15:H:75:PRO:HD2	2.26	0.50
18:L:281:ARG:HD3	18:L:387:LYS:HE2	1.94	0.50
13:6:18:SER:HB2	13:6:31:THR:H	1.76	0.50
16:I:184:TYR:O	16:I:185:ALA:CB	2.59	0.50
6:F:215:VAL:HB	6:F:221:PHE:HD1	1.77	0.50
17:K:259:PRO:HA	17:K:303:VAL:O	2.11	0.49
19:M:250:LYS:HD2	19:M:251:LEU:N	2.27	0.49
16:I:404:LEU:CD2	20:J:313:ARG:NH2	2.75	0.49
17:K:173:GLN:OE1	17:K:173:GLN:N	2.36	0.49
6:F:150:SER:O	6:F:151:ALA:HB3	2.12	0.49
4:Q:85:ASN:OD1	9:V:70:ARG:HD3	2.13	0.49
20:J:277:LEU:HD12	20:J:280:LEU:CD2	2.42	0.49
13:Z:14:LEU:HD21	13:Z:101:ALA:HB3	1.95	0.49
2:B:73:LEU:CD2	2:B:135:ILE:HG13	2.42	0.49
5:E:123:PHE:CE1	5:E:136:PRO:HG3	2.47	0.49
19:M:302:GLY:O	19:M:303:ASP:CB	2.59	0.49
19:M:343:LEU:O	19:M:344:ARG:HD3	2.13	0.49
6:S:74:ILE:HG21	6:S:81:ALA:HB1	1.94	0.49
10:3:30:ILE:O	10:3:31:GLN:HB2	2.12	0.49
2:B:181:LEU:HD22	2:B:185:ASP:OD1	2.12	0.49
2:B:185:ASP:CA	2:B:188:HIS:HB3	2.41	0.49
18:L:242:ARG:O	18:L:243:PHE:HB2	2.11	0.49
2:O:132:SER:O	2:O:162:MET:HE1	2.13	0.49
4:Q:180:ALA:O	4:Q:181:ILE:HB	2.12	0.49
15:H:277:ILE:HG13	15:H:321:THR:HG22	1.94	0.49
15:H:426:THR:HG22	15:H:430:MET:CE	2.43	0.49
16:I:258:LYS:HG2	16:I:297:SER:HB2	1.93	0.49
20:J:90:HIS:HB3	20:J:91:PRO:HD3	1.93	0.49
18:L:204:VAL:CG1	18:L:253:ILE:HD11	2.43	0.49
9:2:23:SER:O	9:2:24:ASN:CB	2.61	0.49
2:B:185:ASP:O	2:B:188:HIS:N	2.46	0.49
18:L:307:GLN:O	18:L:308:ALA:CB	2.59	0.49
1:N:160:TYR:CG	1:N:160:TYR:O	2.66	0.49
12:Y:35:ILE:HD11	12:Y:45:MET:SD	2.52	0.49
10:3:159:ASP:N	10:3:159:ASP:OD2	2.43	0.49
2:B:185:ASP:O	2:B:186:ALA:C	2.49	0.49
15:H:73:ALA:HB3	15:H:74:PRO:CD	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:264:ILE:HG12	17:K:307:VAL:CG1	2.43	0.49
20:J:251:ILE:C	20:J:253:SER:H	2.16	0.48
19:M:88:TYR:HB2	19:M:153:VAL:O	2.13	0.48
4:Q:131:ALA:O	4:Q:146:GLN:HA	2.13	0.48
7:T:47:PHE:HB2	7:T:214:SER:HB2	1.94	0.48
17:K:324:PRO:HA	17:K:328:ASP:OD2	2.13	0.48
19:M:171:ARG:HE	19:M:267:LEU:HD11	1.78	0.48
6:S:10:VAL:HG12	6:S:21:GLN:HB3	1.94	0.48
13:Z:3:ILE:HD12	13:Z:44:CYS:HB2	1.95	0.48
2:O:41:ASN:ND2	2:O:182:GLU:OE2	2.46	0.48
12:Y:104:TRP:CE2	12:Y:181:GLU:HB3	2.48	0.48
16:I:420:LYS:O	16:I:424:GLU:HG2	2.13	0.48
10:3:162:HIS:HB3	14:7:203:ARG:HH12	1.78	0.48
1:N:109:ILE:HG12	1:N:110:PRO:O	2.13	0.48
8:U:14:ALA:HA	8:U:22:ILE:O	2.13	0.48
10:3:133:THR:HG22	10:3:134:ASP:H	1.78	0.48
14:8:115:PRO:O	14:8:116:HIS:CB	2.61	0.48
4:D:19:VAL:HG11	4:D:150:SER:HA	1.96	0.48
16:I:89:GLU:O	16:I:93:GLU:HG2	2.13	0.48
20:J:189:TYR:CE1	20:J:298:ILE:HD12	2.49	0.48
2:O:96:TYR:CE1	2:O:104:ILE:HA	2.49	0.48
10:3:109:ILE:O	10:3:121:ILE:HA	2.14	0.48
15:H:246:VAL:HG21	16:I:307:ARG:HD3	1.94	0.48
15:H:227:ARG:HA	16:I:319:PHE:HE1	1.77	0.48
17:K:185:LEU:HD22	17:K:259:PRO:HB2	1.95	0.48
3:P:97:TYR:CE1	3:P:105:ILE:HA	2.49	0.48
2:B:220:LEU:HD22	2:B:224:GLU:HG2	1.94	0.48
2:B:230:ALA:CB	2:B:232:ILE:HG22	2.44	0.48
20:J:276:LEU:O	20:J:280:LEU:HB3	2.13	0.48
18:L:101:ASP:O	18:L:105:LEU:N	2.37	0.48
8:U:10:GLY:HA3	8:U:42:LYS:HE2	1.96	0.48
12:Y:138:VAL:HG11	12:Y:162:GLN:HG3	1.95	0.48
14:7:208:THR:HG23	14:7:209:THR:N	2.28	0.47
1:N:78:CYS:HA	1:N:139:ILE:O	2.14	0.47
8:1:171:ALA:O	8:1:174:LEU:N	2.47	0.47
15:H:309:PHE:HD2	19:M:250:LYS:CE	2.27	0.47
15:H:73:ALA:HB3	15:H:74:PRO:HD3	1.96	0.47
13:Z:18:SER:O	13:Z:19:ARG:HB3	2.15	0.47
10:3:107:PRO:HB2	10:3:124:LEU:HD13	1.95	0.47
15:H:182:GLU:HG3	15:H:186:LYS:HG3	1.96	0.47
4:Q:152:THR:HG23	5:R:83:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:365:PHE:HD1	16:I:395:ILE:HG23	1.80	0.47
19:M:224:LEU:HD13	19:M:348:LEU:HD13	1.95	0.47
13:6:14:LEU:HD11	13:6:42:PHE:HB2	1.95	0.47
20:J:283:PHE:HZ	20:J:289:ILE:N	2.11	0.47
2:B:185:ASP:HB2	2:B:189:THR:CG2	2.38	0.47
16:I:296:ASP:HB2	20:J:262:GLY:HA3	1.96	0.47
20:J:283:PHE:CZ	20:J:288:ASN:N	2.83	0.47
2:O:142:ARG:NH2	2:O:144:TYR:CE1	2.83	0.47
9:V:38:MET:CE	9:V:60:ILE:HG22	2.45	0.47
12:Y:96:SER:O	12:Y:97:MET:HB2	2.15	0.47
3:C:199:LYS:HD3	16:I:428:TYR:OH	2.14	0.47
17:K:106:THR:HG22	17:K:245:ARG:HD2	1.96	0.47
18:L:239:GLY:O	18:L:240:GLY:O	2.32	0.47
6:S:70:ILE:HG22	6:S:71:GLY:N	2.30	0.47
4:D:46:GLU:OE2	4:D:199:VAL:HG23	2.15	0.47
16:I:184:TYR:HH	16:I:202:GLU:CD	2.17	0.47
11:X:67:LEU:HD13	11:X:91:TRP:CZ3	2.50	0.47
5:R:164:GLN:HG2	5:R:165:CYS:N	2.30	0.47
16:I:404:LEU:HD21	20:J:313:ARG:HH21	1.80	0.47
20:J:271:ARG:HD3	20:J:304:ALA:HB3	1.95	0.47
18:L:76:GLY:O	18:L:78:ARG:N	2.48	0.47
13:Z:51:ASP:HB3	13:Z:94:LEU:HD22	1.97	0.47
15:H:395:PHE:CE1	15:H:411:GLU:HG3	2.49	0.47
17:K:313:ARG:NH2	18:L:286:ASP:OD2	2.48	0.47
2:B:185:ASP:CA	2:B:188:HIS:H	2.28	0.46
20:J:191:PRO:HA	20:J:296:ASN:OD1	2.14	0.46
1:N:10:ASP:OD1	1:N:10:ASP:N	2.42	0.46
15:H:309:PHE:CE2	19:M:284:PHE:CD2	3.03	0.46
20:J:154:LEU:O	20:J:156:LYS:N	2.47	0.46
18:L:309:ARG:NE	18:L:335:SER:O	2.48	0.46
4:Q:23:GLN:HG3	4:Q:149:PRO:HG2	1.98	0.46
1:A:70:PHE:CD2	1:A:91:VAL:HG21	2.51	0.46
18:L:141:GLN:N	18:L:141:GLN:OE1	2.44	0.46
15:H:309:PHE:CE2	19:M:250:LYS:HD3	2.51	0.46
1:N:105:TYR:HD1	14:8:78:THR:HG23	1.79	0.46
1:A:97:GLU:OE2	1:A:117:ARG:HD3	2.16	0.46
5:E:104:ASN:O	5:E:105:GLU:HB3	2.16	0.46
15:H:74:PRO:N	15:H:75:PRO:CD	2.79	0.46
20:J:196:LYS:NZ	23:J:501:ADP:O1B	2.46	0.46
20:J:70:GLY:O	20:J:71:SER:HB2	2.15	0.46
18:L:307:GLN:O	18:L:308:ALA:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:133:LEU:O	2:O:147:GLN:HA	2.15	0.46
15:H:286:ASP:OD1	15:H:287:ASP:N	2.47	0.46
16:I:163:LEU:O	16:I:163:LEU:HG	2.15	0.46
3:P:119:GLN:HG2	4:Q:82:ILE:CG1	2.45	0.46
16:I:295:TYR:O	16:I:296:ASP:HB3	2.15	0.46
17:K:341:LYS:HG3	17:K:375:ILE:HD11	1.98	0.46
4:Q:70:CYS:SG	4:Q:217:LEU:HD22	2.56	0.46
14:8:140:ASP:HB2	14:8:141:LYS:HG3	1.97	0.46
4:D:33:VAL:CG2	4:D:191:VAL:HG13	2.45	0.46
17:K:70:LYS:O	17:K:73:LEU:CA	2.62	0.46
10:3:12:MET:HG3	10:3:138:VAL:HG12	1.97	0.46
15:H:75:PRO:HA	15:H:78:TRP:CG	2.50	0.46
16:I:388:ASP:OD2	16:I:388:ASP:N	2.49	0.46
20:J:157:GLN:OE1	20:J:157:GLN:N	2.49	0.46
17:K:60:TYR:OH	17:K:64:GLU:OE1	2.27	0.46
19:M:100:ASP:N	19:M:101:PRO:CD	2.79	0.46
19:M:180:ARG:HD3	19:M:238:ARG:HG2	1.98	0.46
19:M:343:LEU:O	19:M:344:ARG:O	2.33	0.46
8:U:123:SER:CB	8:U:136:LYS:HG2	2.45	0.46
9:2:19:ARG:HD3	9:2:179:SER:HB2	1.97	0.46
8:U:148:LEU:HD11	10:3:152:SER:HB3	1.98	0.46
7:G:41:CYS:HB3	7:G:189:ILE:HG13	1.97	0.46
15:H:309:PHE:O	15:H:310:ASP:C	2.54	0.46
16:I:248:LEU:HD22	16:I:274:ALA:HB2	1.98	0.46
19:M:234:THR:CB	21:M:501:ATP:O2B	2.64	0.46
10:3:162:HIS:CG	14:7:203:ARG:HH22	2.33	0.45
5:E:42:THR:HG22	5:E:43:SER:H	1.81	0.45
6:F:49:LEU:HB2	6:F:195:LEU:HD21	1.97	0.45
15:H:240:VAL:CG2	15:H:274:PHE:CD1	2.99	0.45
1:A:49:VAL:HG22	1:A:219:VAL:HG23	1.98	0.45
16:I:117:ASP:O	16:I:119:ASN:N	2.50	0.45
16:I:387:LYS:HD2	16:I:423:LYS:HG3	1.98	0.45
5:R:97:GLN:HB3	12:Y:61:ARG:HG3	1.99	0.45
12:Y:36:GLU:HG2	12:Y:184:TRP:CZ2	2.52	0.45
5:E:207:GLU:H	5:E:207:GLU:CD	2.19	0.45
16:I:428:TYR:O	16:I:432:GLU:N	2.45	0.45
20:J:226:GLU:O	20:J:230:MET:HB2	2.17	0.45
20:J:277:LEU:HD12	20:J:280:LEU:HD22	1.99	0.45
18:L:252:GLU:OE1	18:L:253:ILE:HD12	2.16	0.45
4:Q:66:ASP:OD1	4:Q:95:ARG:NH2	2.47	0.45
12:5:88:TYR:O	12:5:88:TYR:CG	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:153:LEU:HB3	15:H:154:PRO:HB2	1.97	0.45
16:I:184:TYR:O	16:I:185:ALA:HB3	2.17	0.45
15:H:244:GLU:HB2	16:I:268:ARG:NH2	2.30	0.45
20:J:271:ARG:CD	20:J:304:ALA:HB3	2.47	0.45
5:R:147:ASP:OD2	5:R:147:ASP:N	2.49	0.45
9:V:81:ALA:HA	9:V:104:LEU:HD13	1.99	0.45
11:4:124:TYR:HB2	11:4:137:LEU:HD13	1.97	0.45
15:H:72:LEU:HA	15:H:75:PRO:HG2	1.98	0.45
20:J:164:VAL:HG21	20:J:313:ARG:NE	2.32	0.45
12:5:75:SER:HB2	12:5:78:ALA:H	1.81	0.45
16:I:173:VAL:HG13	20:J:232:ARG:HB3	1.98	0.45
20:J:186:VAL:HB	20:J:292:ILE:HD13	1.99	0.45
17:K:213:THR:CB	21:K:501:ATP:O2B	2.65	0.45
14:7:1:THR:O	14:7:129:SER:N	2.49	0.45
15:H:307:ASP:OD2	15:H:336:ARG:CZ	2.65	0.45
15:H:355:PHE:HB3	15:H:370:PHE:CD1	2.52	0.45
15:H:417:ILE:O	15:H:421:ALA:HB2	2.16	0.45
18:L:173:TYR:CZ	18:L:389:VAL:HG23	2.52	0.45
1:N:130:GLU:HG2	2:O:4:GLY:HA2	1.98	0.45
9:2:46:CYS:O	9:2:47:VAL:HB	2.17	0.45
6:F:150:SER:O	6:F:151:ALA:CB	2.63	0.45
15:H:430:MET:HG2	15:H:430:MET:O	2.17	0.45
20:J:250:GLU:HG3	20:J:295:THR:HG22	1.97	0.45
19:M:177:VAL:HG21	19:M:247:THR:HG23	1.98	0.45
12:5:75:SER:HA	12:5:105:ASP:OD1	2.16	0.45
15:H:394:MET:HG3	16:I:349:ARG:NH2	2.31	0.45
16:I:296:ASP:HB2	20:J:262:GLY:CA	2.47	0.45
19:M:234:THR:N	21:M:501:ATP:O2B	2.36	0.45
2:O:134:LEU:HD11	2:O:162:MET:SD	2.57	0.45
14:7:13:VAL:HA	14:7:176:CYS:O	2.17	0.45
14:8:3:ILE:HG21	14:8:44:CYS:HB2	1.98	0.45
2:B:185:ASP:CA	2:B:188:HIS:N	2.79	0.45
6:F:88:MET:HE3	6:F:108:LEU:HD21	1.99	0.45
6:F:238:GLU:O	6:F:240:PRO:HD3	2.17	0.45
20:J:207:THR:O	20:J:208:ASP:HB2	2.16	0.45
9:2:29:LYS:HD3	9:2:32:HIS:HB2	1.99	0.44
15:H:47:GLN:O	15:H:51:ASP:HB2	2.17	0.44
17:K:238:LYS:HD2	18:L:213:ARG:HH22	1.82	0.44
18:L:377:SER:O	18:L:381:GLU:HG2	2.18	0.44
8:U:151:ASN:C	8:U:151:ASN:OD1	2.54	0.44
13:6:51:ASP:HB3	13:6:94:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:ILE:CG1	2:B:232:ILE:O	2.62	0.44
4:D:131:ALA:O	4:D:146:GLN:HA	2.17	0.44
4:D:33:VAL:HG12	4:D:160:ALA:HB2	1.98	0.44
6:F:123:TYR:O	6:F:125:ARG:N	2.50	0.44
7:G:74:GLY:CA	7:G:224:HIS:CD2	3.00	0.44
16:I:203:LEU:HB3	16:I:204:PRO:HD3	1.99	0.44
16:I:268:ARG:HG2	16:I:315:GLN:HE22	1.81	0.44
17:K:60:TYR:O	17:K:60:TYR:CG	2.67	0.44
8:U:190:GLY:O	8:U:191:ASP:HB2	2.16	0.44
9:V:121:LEU:O	9:V:122:ALA:HB3	2.17	0.44
9:2:67:TYR:CE2	9:2:75:LEU:HD23	2.52	0.44
1:A:174:GLU:HG3	1:A:205:VAL:HG23	1.98	0.44
17:K:152:MET:O	17:K:153:MET:HB2	2.18	0.44
18:L:340:GLY:HA3	21:L:401:ATP:N7	2.32	0.44
15:H:309:PHE:HE2	19:M:284:PHE:CD2	2.35	0.44
6:S:176:MET:N	6:S:176:MET:SD	2.90	0.44
9:V:6:GLY:O	9:V:129:PHE:HA	2.17	0.44
2:B:90:ARG:O	2:B:94:GLN:HG2	2.16	0.44
6:F:24:TYR:O	6:F:25:ALA:C	2.55	0.44
15:H:303:ILE:HG23	15:H:336:ARG:NH1	2.33	0.44
20:J:321:ASN:OD1	20:J:323:GLU:N	2.49	0.44
17:K:247:VAL:O	17:K:250:VAL:HG12	2.18	0.44
3:P:136:TYR:CD1	3:P:136:TYR:N	2.86	0.44
8:1:99:ARG:O	8:1:103:PRO:HA	2.17	0.44
8:1:171:ALA:O	8:1:174:LEU:HB3	2.17	0.44
11:4:124:TYR:CE2	11:4:139:THR:HG22	2.52	0.44
14:7:122:LEU:HB3	14:7:123:PRO:HD2	2.00	0.44
5:E:53:ARG:O	5:E:53:ARG:HG2	2.17	0.44
3:P:65:ILE:HD13	3:P:214:ALA:CB	2.46	0.44
10:W:159:ASP:HB2	10:W:160:PRO:HD2	2.00	0.44
20:J:300:ILE:O	20:J:301:LEU:C	2.56	0.44
18:L:230:ILE:O	18:L:275:MET:HA	2.18	0.44
2:O:82:TYR:O	2:O:86:VAL:HG23	2.18	0.44
3:P:219:GLU:O	3:P:220:ASN:HB2	2.17	0.44
8:U:14:ALA:O	8:U:135:PHE:HA	2.17	0.44
11:X:166:ARG:NH1	11:X:166:ARG:HB2	2.33	0.44
11:4:67:LEU:CD1	11:4:91:TRP:CZ3	3.01	0.44
3:C:107:CYS:HB2	3:C:140:ASP:OD2	2.18	0.44
7:G:90:ILE:HD13	7:G:118:TYR:CE1	2.52	0.44
15:H:301:GLU:HA	15:H:301:GLU:OE1	2.17	0.44
15:H:214:LEU:HD22	15:H:343:PHE:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:J:167:LEU:HB2	20:J:168:PRO:HD3	2.00	0.44
19:M:435:LEU:HD11	19:M:438:TYR:OH	2.17	0.44
8:1:190:GLY:O	8:1:191:ASP:HB2	2.18	0.44
14:7:144:PRO:O	14:7:145:ASP:HB2	2.18	0.44
4:D:99:GLU:N	4:D:99:GLU:OE1	2.51	0.44
15:H:216:GLY:HA2	15:H:433:ASN:OD1	2.18	0.44
15:H:309:PHE:CG	19:M:180:ARG:NH2	2.86	0.44
20:J:313:ARG:HG2	20:J:315:ILE:CD1	2.47	0.44
7:T:87:LEU:HD13	7:T:135:PHE:CE1	2.53	0.44
8:U:92:LEU:HD23	8:U:124:PHE:CZ	2.53	0.44
10:W:169:GLN:OE1	10:W:169:GLN:HA	2.18	0.44
11:X:147:GLN:HB3	11:X:148:PRO:HD3	2.00	0.44
12:5:186:ARG:NH2	12:5:189:SER:HB2	2.33	0.44
5:E:28:ILE:CD1	5:E:158:PRO:HD2	2.48	0.44
15:H:417:ILE:O	15:H:421:ALA:CB	2.66	0.44
17:K:60:TYR:CE2	17:K:64:GLU:HB2	2.53	0.44
17:K:70:LYS:O	17:K:73:LEU:HB2	2.18	0.44
15:H:261:PHE:HE2	15:H:306:LEU:HD21	1.82	0.43
16:I:193:GLN:NE2	16:I:354:PRO:HD2	2.33	0.43
18:L:206:LYS:O	18:L:206:LYS:HE2	2.17	0.43
18:L:50:LEU:HD23	19:M:159:LEU:HD13	2.00	0.43
2:O:49:LYS:N	2:O:206:ASN:O	2.45	0.43
3:C:97:TYR:CE1	3:C:105:ILE:HA	2.53	0.43
15:H:245:LEU:HB2	15:H:280:ILE:CD1	2.49	0.43
15:H:311:PRO:O	15:H:312:ARG:HB3	2.18	0.43
16:I:95:GLU:O	16:I:99:VAL:HG23	2.18	0.43
17:K:105:SER:HB2	17:K:107:THR:OG1	2.18	0.43
17:K:148:ASP:O	17:K:149:SER:OG	2.32	0.43
17:K:79:VAL:HG13	17:K:116:LEU:HD11	2.00	0.43
17:K:79:VAL:O	17:K:80:LYS:C	2.55	0.43
4:Q:199:VAL:HG21	4:Q:205:ASN:HB2	1.99	0.43
11:X:124:TYR:HB2	11:X:137:LEU:HD13	1.98	0.43
8:1:99:ARG:HD3	8:1:104:TYR:CE1	2.53	0.43
14:7:8:TYR:CE2	14:7:148:GLU:HA	2.53	0.43
2:B:88:ARG:HB2	2:B:88:ARG:NH1	2.33	0.43
2:B:96:TYR:CE1	2:B:104:ILE:HA	2.53	0.43
8:U:99:ARG:HD3	8:U:104:TYR:CE2	2.53	0.43
8:U:24:ALA:O	8:U:25:SER:HB3	2.19	0.43
8:U:76:LYS:HG2	8:U:81:LYS:O	2.18	0.43
11:4:57:TYR:HD2	13:6:119:MET:SD	2.42	0.43
12:5:104:TRP:CZ3	12:5:109:PRO:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:391:ARG:NH1	17:K:395:LEU:HD12	2.33	0.43
18:L:381:GLU:HB3	19:M:343:LEU:HD13	1.99	0.43
19:M:100:ASP:HA	19:M:117:ARG:HB2	1.99	0.43
3:P:102:GLN:O	3:P:103:GLU:HB3	2.19	0.43
6:S:62:LYS:O	6:S:73:SER:HA	2.18	0.43
12:Y:115:ASP:OD2	12:Y:117:GLU:HB3	2.18	0.43
3:C:31:ALA:O	3:C:166:ASN:HB2	2.18	0.43
16:I:400:THR:HG23	20:J:180:ILE:HD11	2.00	0.43
20:J:136:SER:HA	20:J:139:MET:SD	2.58	0.43
18:L:151:LEU:HB3	18:L:152:PRO:HD3	1.99	0.43
19:M:399:VAL:O	19:M:402:GLU:N	2.51	0.43
15:H:336:ARG:NH2	21:M:501:ATP:O1G	2.51	0.43
1:N:98:ALA:HB2	1:N:114:LEU:HD13	2.01	0.43
3:P:74:CYS:HB2	3:P:135:LEU:O	2.18	0.43
6:S:71:GLY:HA3	6:S:221:PHE:CZ	2.53	0.43
7:T:220:THR:O	7:T:221:ASN:HB2	2.18	0.43
5:E:24:VAL:O	5:E:28:ILE:HG12	2.18	0.43
5:E:52:LYS:O	5:E:53:ARG:HB3	2.18	0.43
15:H:284:ARG:HA	15:H:296:GLN:OE1	2.18	0.43
15:H:303:ILE:O	15:H:307:ASP:OD2	2.36	0.43
20:J:283:PHE:HZ	20:J:289:ILE:H	1.66	0.43
19:M:146:LYS:O	19:M:147:PRO:C	2.56	0.43
9:V:23:SER:O	9:V:24:ASN:HB3	2.18	0.43
12:Y:164:THR:HG22	12:Y:170:SER:HB3	2.00	0.43
6:F:72:ILE:HA	6:F:133:LEU:O	2.18	0.43
15:H:312:ARG:O	15:H:313:GLY:O	2.37	0.43
16:I:433:GLY:O	20:J:306:LEU:HD13	2.18	0.43
2:O:5:TYR:HB3	2:O:7:PHE:CE2	2.53	0.43
8:U:114:ASP:OD1	8:U:114:ASP:N	2.52	0.43
12:Y:52:CYS:O	12:Y:56:GLU:CB	2.67	0.43
10:3:165:GLU:HG3	14:7:205:GLU:HA	2.01	0.43
14:7:59:ILE:HD12	14:7:82:MET:HB3	2.00	0.43
2:B:139:ASN:HD21	2:B:144:TYR:HE2	1.66	0.43
4:D:85:ASN:CG	9:2:70:ARG:HH12	2.22	0.43
7:G:62:SER:O	7:G:63:ASN:CG	2.57	0.43
15:H:180:CYS:SG	15:H:180:CYS:O	2.77	0.43
18:L:36:LEU:O	18:L:40:TYR:HB3	2.19	0.43
19:M:208:HIS:C	19:M:210:GLU:N	2.72	0.43
15:H:135:GLU:N	15:H:135:GLU:OE1	2.45	0.43
15:H:182:GLU:HG3	15:H:186:LYS:HE3	1.99	0.43
16:I:428:TYR:HB3	16:I:432:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:J:164:VAL:CG2	20:J:313:ARG:HE	2.32	0.43
5:R:10:ARG:HB2	5:R:10:ARG:NH1	2.34	0.43
12:Y:52:CYS:SG	12:Y:97:MET:HG3	2.59	0.43
8:1:15:ILE:HG21	8:1:166:LEU:HD21	2.01	0.43
8:1:72:LEU:HD12	8:1:83:MET:SD	2.59	0.43
11:4:134:ALA:HB1	11:4:135:PRO:HD2	1.99	0.43
14:7:134:ALA:O	14:7:137:VAL:N	2.52	0.43
1:A:107:TYR:O	1:A:107:TYR:CG	2.72	0.43
19:M:180:ARG:HB2	19:M:181:PRO:HD2	2.01	0.43
18:L:284:THR:HG22	19:M:297:ASP:HB3	2.00	0.43
6:F:33:SER:N	19:M:439:ALA:HB1	2.34	0.43
5:R:51:GLU:O	5:R:51:GLU:HG3	2.19	0.43
12:Y:102:CYS:SG	12:Y:179:VAL:HG21	2.58	0.43
12:Y:35:ILE:O	12:Y:37:ILE:N	2.52	0.43
12:5:164:THR:HG22	12:5:170:SER:HB3	2.00	0.42
14:8:170:GLY:O	14:8:171:SER:CB	2.67	0.42
1:A:40:VAL:HG23	1:A:202:LEU:HD13	2.00	0.42
4:D:118:TYR:CD2	4:D:127:PHE:CE2	3.06	0.42
6:F:137:TYR:CE1	6:F:217:LYS:HA	2.54	0.42
17:K:111:TYR:HA	20:J:71:SER:O	2.18	0.42
17:K:200:ARG:HH11	17:K:306:LYS:HE3	1.84	0.42
9:V:94:SER:O	9:V:95:ARG:CB	2.67	0.42
10:W:123:SER:O	10:W:124:LEU:HG	2.19	0.42
12:Y:101:ILE:HD13	12:Y:101:ILE:N	2.34	0.42
2:B:183:LEU:HD12	2:B:183:LEU:O	2.19	0.42
15:H:158:ASP:HB2	15:H:159:PRO:HD3	2.01	0.42
16:I:401:GLU:O	16:I:404:LEU:HB3	2.19	0.42
17:K:105:SER:C	17:K:107:THR:H	2.23	0.42
17:K:209:GLY:HA3	18:L:291:ARG:HD2	2.00	0.42
2:O:72:GLY:HA3	2:O:217:PHE:CE1	2.54	0.42
8:U:152:GLN:OE1	8:U:152:GLN:HA	2.18	0.42
9:2:164:LEU:HD22	9:2:178:PHE:CE2	2.54	0.42
14:7:132:LEU:HD12	14:7:132:LEU:H	1.85	0.42
6:F:103:LEU:HD12	6:F:104:PRO:HD2	2.00	0.42
20:J:392:GLN:HG2	20:J:396:GLU:OE2	2.19	0.42
17:K:119:ILE:O	17:K:121:ARG:N	2.52	0.42
1:N:71:LYS:HG2	1:N:73:THR:O	2.20	0.42
5:R:141:LEU:O	5:R:142:LEU:HD23	2.19	0.42
5:R:71:ASP:OD1	5:R:72:ALA:N	2.46	0.42
6:S:88:MET:HE2	6:S:108:LEU:HD21	2.01	0.42
6:S:214:ILE:HD12	6:S:224:TYR:HE2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:146:GLN:HA	8:U:146:GLN:HE21	1.84	0.42
8:U:148:LEU:O	8:U:151:ASN:HB3	2.18	0.42
2:B:189:THR:O	2:B:193:THR:HG22	2.19	0.42
16:I:140:ASP:OD1	16:I:142:ASP:N	2.45	0.42
16:I:292:THR:OG1	16:I:293:LYS:N	2.52	0.42
18:L:180:LYS:HG2	18:L:301:ILE:HD12	2.00	0.42
3:P:98:LEU:HD12	3:P:103:GLU:H	1.84	0.42
3:P:133:SER:OG	3:P:151:ASP:HA	2.19	0.42
12:5:83:LEU:HD21	12:5:99:THR:HG21	2.01	0.42
14:7:83:LEU:HB3	14:7:113:ILE:HD13	2.00	0.42
2:B:158:LYS:O	2:B:159:ALA:HB2	2.19	0.42
15:H:64:GLY:O	15:H:72:LEU:HD12	2.20	0.42
17:K:219:VAL:O	17:K:223:THR:HB	2.19	0.42
17:K:299:PHE:HE2	17:K:304:ASN:ND2	2.17	0.42
15:H:309:PHE:CG	19:M:180:ARG:CZ	3.02	0.42
7:T:37:ILE:HD11	7:T:193:VAL:HG13	2.01	0.42
8:U:159:GLN:O	8:U:160:ASN:HB2	2.20	0.42
13:Z:22:THR:HG23	13:Z:22:THR:O	2.19	0.42
8:1:19:ASP:OD1	8:1:19:ASP:N	2.53	0.42
10:3:188:HIS:N	10:3:188:HIS:ND1	2.68	0.42
14:8:59:ILE:HA	14:8:59:ILE:HD13	1.91	0.42
15:H:291:GLY:CA	16:I:303:ARG:HH12	2.32	0.42
1:N:117:ARG:O	1:N:121:ILE:HG12	2.19	0.42
3:P:183:GLU:O	3:P:184:MET:HB2	2.18	0.42
8:U:128:GLY:O	8:U:129:SER:HB3	2.18	0.42
10:W:73:LEU:O	10:W:73:LEU:HD23	2.20	0.42
13:6:3:ILE:HD12	13:6:44:CYS:HB2	2.00	0.42
16:I:173:VAL:HA	20:J:232:ARG:HG2	2.00	0.42
16:I:346:ARG:HH11	16:I:346:ARG:HB2	1.84	0.42
16:I:196:GLU:HB2	16:I:351:ILE:HD11	2.01	0.42
20:J:151:ILE:HG13	20:J:198:LEU:HD23	2.02	0.42
17:K:177:VAL:O	17:K:181:VAL:HB	2.19	0.42
17:K:213:THR:HB	21:K:501:ATP:O2B	2.19	0.42
5:R:35:SER:O	5:R:171:GLY:HA3	2.19	0.42
12:Y:88:TYR:CG	12:Y:88:TYR:O	2.72	0.42
8:1:7:PHE:CE1	8:1:9:GLY:HA2	2.54	0.42
13:Z:28:ASN:OD1	14:8:122:LEU:HD21	2.19	0.42
2:B:185:ASP:C	2:B:185:ASP:HB2	2.37	0.42
2:B:186:ALA:O	2:B:190:ALA:N	2.49	0.42
6:F:118:ILE:HB	6:F:119:PRO:HD3	2.01	0.42
15:H:190:VAL:O	15:H:190:VAL:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:263:GLN:HA	18:L:263:GLN:OE1	2.20	0.42
19:M:272:PHE:CD1	19:M:316:GLN:HB3	2.54	0.42
10:W:162:HIS:CE1	14:8:203:ARG:HH11	2.37	0.42
10:W:164:PHE:CZ	10:W:198:ARG:HD2	2.55	0.42
11:4:111:VAL:CG1	11:4:122:LEU:HD11	2.49	0.42
15:H:165:GLN:OE1	15:H:240:VAL:HA	2.18	0.42
20:J:184:LYS:HE2	20:J:287:LYS:HB3	2.02	0.42
18:L:83:CYS:HB2	18:L:107:ILE:HB	2.02	0.42
19:M:102:ASN:O	19:M:103:ASP:HB2	2.20	0.42
6:S:10:VAL:HG11	6:S:127:PRO:HD3	2.02	0.42
11:X:121:PHE:CD2	11:X:121:PHE:C	2.92	0.42
12:Y:138:VAL:HG21	12:Y:159:ALA:HA	2.02	0.42
11:4:44:ARG:HH11	11:4:47:ASN:CB	2.33	0.42
12:5:172:GLY:O	12:5:192:VAL:HG23	2.20	0.42
15:H:227:ARG:HA	16:I:319:PHE:CE1	2.55	0.42
17:K:378:ILE:HD11	17:K:407:ILE:HG13	2.02	0.42
19:M:241:ALA:HB2	19:M:248:PHE:CE2	2.55	0.42
3:P:194:ILE:HG13	3:P:236:LEU:HB3	2.01	0.42
8:U:148:LEU:HD23	8:U:148:LEU:C	2.40	0.42
9:V:94:SER:O	9:V:95:ARG:HB2	2.19	0.42
1:A:115:CYS:SG	1:A:154:CYS:HB3	2.60	0.41
2:B:185:ASP:O	2:B:188:HIS:C	2.50	0.41
7:G:198:TYR:HB3	7:G:243:LEU:HD11	2.00	0.41
16:I:223:ILE:HD11	16:I:342:ILE:HG22	2.01	0.41
17:K:209:GLY:CA	18:L:291:ARG:HD2	2.50	0.41
18:L:206:LYS:HG2	18:L:206:LYS:O	2.19	0.41
19:M:96:LEU:HA	19:M:121:CYS:O	2.20	0.41
19:M:355:PRO:O	19:M:356:MET:CB	2.68	0.41
3:P:77:ALA:HB3	3:P:164:ILE:HD12	2.02	0.41
11:X:82:SER:O	11:X:83:TYR:CB	2.68	0.41
13:Z:2:THR:O	13:Z:16:ALA:HA	2.20	0.41
1:A:114:LEU:O	1:A:114:LEU:HG	2.19	0.41
15:H:187:LEU:HD11	15:H:318:LEU:HD11	2.02	0.41
15:H:217:PRO:HD3	15:H:433:ASN:ND2	2.35	0.41
17:K:267:ILE:HG22	17:K:267:ILE:O	2.19	0.41
17:K:313:ARG:HA	18:L:242:ARG:NH2	2.35	0.41
18:L:329:GLU:CD	18:L:329:GLU:N	2.73	0.41
9:V:117:TYR:C	9:V:117:TYR:CD1	2.93	0.41
9:2:85:ARG:HG3	9:2:118:MET:HE1	2.02	0.41
4:D:43:LEU:HD12	4:D:72:ALA:HB2	2.03	0.41
5:E:95:GLU:OE1	5:E:95:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:261:PHE:CE2	15:H:306:LEU:HD21	2.55	0.41
15:H:240:VAL:HG21	15:H:274:PHE:CD1	2.55	0.41
16:I:283:PHE:CE2	16:I:285:ASP:HB2	2.55	0.41
19:M:133:PHE:CG	19:M:134:LEU:N	2.88	0.41
8:U:125:ASP:OD2	8:U:129:SER:HB3	2.21	0.41
13:Z:14:LEU:CD1	13:Z:42:PHE:HB2	2.50	0.41
13:Z:1:THR:HG23	13:Z:46:SER:HB2	2.02	0.41
11:4:107:TRP:CD1	11:4:107:TRP:O	2.73	0.41
20:J:252:ASP:HB3	20:J:259:LEU:CD2	2.49	0.41
19:M:137:ILE:HG13	19:M:159:LEU:HA	2.02	0.41
15:H:120:LYS:O	19:M:90:VAL:HG22	2.20	0.41
1:N:19:GLU:OE2	1:N:23:TYR:HE1	2.03	0.41
13:Z:99:ILE:O	13:Z:99:ILE:HG22	2.20	0.41
10:3:3:ILE:HD11	10:3:104:TYR:CG	2.55	0.41
15:H:233:THR:HG23	15:H:235:ALA:H	1.85	0.41
15:H:333:ARG:NH1	19:M:230:GLY:N	2.69	0.41
16:I:117:ASP:C	16:I:119:ASN:H	2.23	0.41
16:I:187:ILE:HG12	16:I:234:LEU:CD2	2.50	0.41
19:M:135:PRO:O	19:M:136:VAL:O	2.37	0.41
2:O:139:ASN:HB3	2:O:140:GLU:HG2	2.02	0.41
8:1:198:VAL:HG22	8:1:203:ILE:HG23	2.01	0.41
10:3:127:ILE:HD12	14:7:50:ALA:HB3	2.02	0.41
5:E:226:PHE:C	5:E:226:PHE:CD2	2.93	0.41
15:H:74:PRO:HG2	15:H:75:PRO:HD3	2.03	0.41
16:I:409:GLU:O	16:I:410:ARG:HB2	2.21	0.41
20:J:298:ILE:O	20:J:298:ILE:HG12	2.20	0.41
20:J:161:ILE:HD11	20:J:315:ILE:HD13	2.01	0.41
17:K:196:ILE:HG13	17:K:196:ILE:O	2.21	0.41
19:M:91:SER:HG	19:M:92:ASN:H	1.68	0.41
1:N:154:CYS:HB3	1:N:160:TYR:HB3	2.03	0.41
9:2:23:SER:O	9:2:24:ASN:HB3	2.21	0.41
10:3:66:ARG:NH1	10:3:94:LEU:HD11	2.36	0.41
15:H:239:ARG:HG3	16:I:319:PHE:HD2	1.85	0.41
16:I:382:ASP:O	16:I:386:ALA:HB2	2.21	0.41
20:J:193:GLY:N	23:J:501:ADP:O3B	2.52	0.41
17:K:373:ALA:HB2	21:K:501:ATP:H5'1	2.03	0.41
19:M:95:GLU:HB3	19:M:123:VAL:HB	2.03	0.41
7:T:56:LYS:HD2	7:T:56:LYS:N	2.36	0.41
8:U:16:ALA:HB2	8:U:121:VAL:HG23	2.02	0.41
1:A:29:PHE:CE2	1:A:156:PRO:HD2	2.56	0.41
3:C:149:GLN:O	3:C:156:TYR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:409:PHE:O	15:H:413:VAL:N	2.38	0.41
18:L:40:TYR:CE1	19:M:72:LYS:HB3	2.56	0.41
19:M:251:LEU:HD23	19:M:251:LEU:C	2.41	0.41
18:L:245:GLU:OE1	19:M:300:LYS:HB2	2.20	0.41
19:M:433:ALA:HB1	19:M:436:GLN:HE21	1.86	0.41
6:S:159:MET:HG3	6:S:160:SER:H	1.86	0.41
9:V:101:ASN:HB3	9:V:132:HIS:CE1	2.56	0.41
13:Z:75:LEU:N	13:Z:75:LEU:HD12	2.35	0.41
2:B:176:ARG:NH2	2:B:192:LEU:HD13	2.36	0.41
4:D:148:ASP:HB2	4:D:149:PRO:CD	2.51	0.41
5:E:36:THR:O	5:E:50:VAL:HG23	2.21	0.41
15:H:142:VAL:HG12	15:H:149:ILE:HA	2.03	0.41
16:I:184:TYR:CZ	16:I:242:GLN:HG3	2.55	0.41
2:B:56:TYR:CE1	17:K:416:PHE:CE2	3.09	0.41
18:L:247:THR:C	18:L:251:ARG:HH21	2.24	0.41
1:N:160:TYR:O	1:N:160:TYR:CD1	2.74	0.41
4:Q:209:ALA:HB1	4:Q:217:LEU:HD11	2.03	0.41
9:V:45:LEU:N	9:V:45:LEU:HD12	2.36	0.41
14:7:37:ILE:HB	14:7:41:ILE:O	2.21	0.41
1:A:191:PHE:CE2	1:A:219:VAL:HG21	2.56	0.41
1:A:25:VAL:HG11	1:A:157:ALA:HB2	2.02	0.41
16:I:319:PHE:CD1	16:I:319:PHE:O	2.74	0.41
18:L:115:VAL:HB	18:L:119:VAL:HG11	2.03	0.41
15:H:309:PHE:CD2	19:M:250:LYS:CE	3.04	0.41
2:O:110:VAL:HG21	2:O:146:PHE:CG	2.56	0.41
2:O:166:TYR:O	2:O:170:LYS:HB2	2.20	0.41
3:P:119:GLN:HG2	4:Q:82:ILE:HG13	2.03	0.41
7:T:69:VAL:HG11	7:T:111:LEU:HD21	2.02	0.41
8:U:97:TYR:CD2	12:Y:54:PHE:CD2	3.09	0.41
9:2:66:LEU:HD21	9:2:70:ARG:HH21	1.85	0.41
2:B:54:ILE:HG13	2:B:54:ILE:O	2.20	0.41
15:H:259:GLU:HA	15:H:262:GLU:OE1	2.21	0.41
15:H:423:PHE:CD1	15:H:423:PHE:O	2.74	0.41
2:O:58:GLU:N	2:O:58:GLU:CD	2.74	0.41
12:Y:105:ASP:HB3	12:Y:107:ARG:H	1.85	0.41
13:Z:100:ILE:HD12	13:Z:100:ILE:H	1.86	0.41
8:1:127:VAL:HG23	12:5:50:ALA:HB2	2.02	0.40
14:7:96:ALA:HB1	14:7:98:LEU:HD11	2.01	0.40
15:H:70:THR:OG1	15:H:75:PRO:HG3	2.21	0.40
20:J:110:PRO:O	20:J:111:ASN:CB	2.69	0.40
17:K:302:ASN:OD1	17:K:304:ASN:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:204:LEU:HB3	19:M:205:PRO:HD3	2.02	0.40
19:M:318:ASP:OD2	19:M:319:GLY:N	2.55	0.40
14:7:8:TYR:CZ	14:7:10:ASP:HB2	2.56	0.40
14:8:99:VAL:HG23	14:8:127:MET:HG3	2.02	0.40
2:B:79:GLY:N	2:B:80:PRO:CD	2.84	0.40
15:H:222:LYS:NZ	21:H:501:ATP:O2B	2.32	0.40
16:I:176:VAL:HG22	16:I:247:PHE:O	2.21	0.40
20:J:251:ILE:C	20:J:253:SER:N	2.74	0.40
17:K:71:GLU:HA	17:K:74:HIS:HB3	2.02	0.40
5:R:143:PHE:O	5:R:153:LEU:HD12	2.21	0.40
9:V:23:SER:O	9:V:24:ASN:CB	2.69	0.40
9:2:164:LEU:HD13	9:2:178:PHE:CG	2.56	0.40
9:2:2:GLU:HB2	9:2:47:VAL:HG21	2.04	0.40
12:5:36:GLU:OE2	12:5:184:TRP:CZ2	2.75	0.40
1:A:103:TYR:CD1	13:6:61:TYR:HB2	2.57	0.40
4:D:45:VAL:HG11	4:D:61:LYS:HD2	2.03	0.40
20:J:216:GLY:O	20:J:217:SER:C	2.59	0.40
20:J:263:SER:O	20:J:263:SER:OG	2.40	0.40
20:J:321:ASN:C	20:J:321:ASN:OD1	2.60	0.40
20:J:383:PHE:O	20:J:386:ALA:N	2.54	0.40
17:K:158:GLN:O	17:K:159:LYS:C	2.59	0.40
18:L:316:HIS:O	18:L:319:PRO:HD2	2.22	0.40
19:M:174:ALA:C	19:M:176:GLU:H	2.25	0.40
19:M:347:ARG:HB2	19:M:348:LEU:H	1.73	0.40
19:M:90:VAL:O	19:M:91:SER:HB2	2.21	0.40
19:M:97:LEU:HB2	19:M:121:CYS:HB3	2.04	0.40
1:N:113:MET:O	1:N:114:LEU:C	2.58	0.40
1:N:39:SER:O	1:N:167:ALA:HA	2.21	0.40
1:N:53:GLN:OE1	1:N:206:LEU:HD13	2.21	0.40
9:V:86:ARG:HA	9:V:86:ARG:NE	2.36	0.40
13:Z:14:LEU:HD11	13:Z:42:PHE:HB2	2.04	0.40
8:1:13:LEU:HD23	8:1:13:LEU:C	2.42	0.40
10:3:129:CYS:HB2	14:7:50:ALA:HB2	2.03	0.40
11:4:192:VAL:HA	11:4:196:GLY:O	2.21	0.40
12:5:48:GLY:H	12:5:96:SER:HB2	1.86	0.40
12:5:5:ALA:HA	12:5:13:ILE:O	2.21	0.40
1:A:143:ILE:HG12	1:A:220:VAL:HG22	2.02	0.40
2:B:15:SER:HB3	2:B:17:LYS:HG2	2.03	0.40
3:C:45:LEU:HD13	3:C:75:SER:HB2	2.04	0.40
15:H:271:LEU:N	15:H:271:LEU:HD12	2.36	0.40
1:N:72:ILE:HB	1:N:76:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:4:121:PHE:CE1	11:4:133:GLU:HG2	2.56	0.40
12:5:66:TYR:CD2	12:5:74:ILE:HB	2.57	0.40
13:6:127:ILE:HD11	13:6:135:ILE:CG1	2.52	0.40
14:8:15:GLY:HA2	14:8:174:ASP:O	2.22	0.40
4:D:32:ALA:O	4:D:160:ALA:HA	2.22	0.40
7:G:151:ILE:HG22	7:G:152:ASP:N	2.36	0.40
15:H:102:ILE:HD11	19:M:164:LEU:HD22	2.03	0.40
17:K:106:THR:HG22	17:K:245:ARG:CD	2.51	0.40
17:K:154:LEU:HD13	17:K:229:ARG:HB3	2.02	0.40
19:M:229:PRO:HA	21:M:501:ATP:O3G	2.21	0.40
1:N:126:THR:HG22	2:O:127:ARG:HH21	1.87	0.40
2:O:14:PRO:HA	3:P:23:TYR:CD1	2.57	0.40
11:X:6:VAL:HA	11:X:29:SER:O	2.22	0.40
12:Y:36:GLU:CG	12:Y:184:TRP:CZ2	3.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	242/246 (98%)	217 (90%)	23 (10%)	2 (1%)	24 69
1	N	242/246 (98%)	215 (89%)	25 (10%)	2 (1%)	24 69
2	B	231/234 (99%)	208 (90%)	20 (9%)	3 (1%)	15 61
2	O	231/234 (99%)	206 (89%)	21 (9%)	4 (2%)	11 56
3	C	248/261 (95%)	235 (95%)	13 (5%)	0	100 100
3	P	248/261 (95%)	230 (93%)	15 (6%)	3 (1%)	16 62
4	D	241/248 (97%)	221 (92%)	18 (8%)	2 (1%)	24 69
4	Q	241/248 (97%)	217 (90%)	20 (8%)	4 (2%)	11 56
5	E	232/241 (96%)	207 (89%)	17 (7%)	8 (3%)	5 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	R	232/241 (96%)	207 (89%)	22 (10%)	3 (1%)	15 61
6	F	236/263 (90%)	214 (91%)	17 (7%)	5 (2%)	9 52
6	S	236/263 (90%)	218 (92%)	14 (6%)	4 (2%)	11 56
7	G	239/255 (94%)	212 (89%)	24 (10%)	3 (1%)	15 61
7	T	240/255 (94%)	224 (93%)	13 (5%)	3 (1%)	15 61
8	1	211/241 (88%)	189 (90%)	17 (8%)	5 (2%)	7 50
8	U	211/241 (88%)	186 (88%)	22 (10%)	3 (1%)	14 59
9	2	197/201 (98%)	176 (89%)	18 (9%)	3 (2%)	13 58
9	V	197/201 (98%)	177 (90%)	17 (9%)	3 (2%)	13 58
10	3	202/205 (98%)	180 (89%)	21 (10%)	1 (0%)	34 76
10	W	202/205 (98%)	180 (89%)	20 (10%)	2 (1%)	19 65
11	4	215/264 (81%)	193 (90%)	21 (10%)	1 (0%)	34 76
11	X	215/264 (81%)	196 (91%)	15 (7%)	4 (2%)	10 54
12	5	199/263 (76%)	176 (88%)	19 (10%)	4 (2%)	9 54
12	Y	199/263 (76%)	178 (89%)	16 (8%)	5 (2%)	7 49
13	6	197/239 (82%)	177 (90%)	17 (9%)	3 (2%)	13 58
13	Z	198/239 (83%)	177 (89%)	19 (10%)	2 (1%)	19 65
14	7	218/277 (79%)	195 (89%)	21 (10%)	2 (1%)	21 67
14	8	218/277 (79%)	192 (88%)	24 (11%)	2 (1%)	21 67
15	H	394/433 (91%)	323 (82%)	51 (13%)	20 (5%)	2 31
16	I	377/440 (86%)	332 (88%)	41 (11%)	4 (1%)	17 64
17	K	391/418 (94%)	323 (83%)	53 (14%)	15 (4%)	4 39
18	L	387/389 (100%)	326 (84%)	45 (12%)	16 (4%)	3 37
19	M	413/439 (94%)	348 (84%)	50 (12%)	15 (4%)	4 41
20	J	389/406 (96%)	326 (84%)	52 (13%)	11 (3%)	6 47
All	All	8569/9401 (91%)	7581 (88%)	821 (10%)	167 (2%)	14 54

All (167) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	41	ASN
2	O	70	HIS
4	Q	120	GLN

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Mol	Chain	Res	Type
7	T	64	LYS
8	U	2	PHE
9	V	95	ARG
10	W	117	PHE
1	A	10	ASP
13	6	95	MET
15	H	147	TYR
15	H	154	PRO
17	K	80	LYS
17	K	126	PRO
17	K	149	SER
17	K	156	SER
18	L	107	ILE
18	L	245	GLU
18	L	308	ALA
18	L	327	ASP
19	M	101	PRO
19	M	292	GLY
19	M	344	ARG
20	J	11	LEU
20	J	251	ILE
20	J	252	ASP
1	N	147	GLN
2	O	231	ALA
3	P	184	MET
5	R	230	THR
6	S	69	HIS
6	S	121	GLN
7	T	216	VAL
9	V	24	ASN
12	Y	36	GLU
14	8	116	HIS
14	8	171	SER
2	B	159	ALA
5	E	105	GLU
6	F	151	ALA
7	G	216	VAL
9	2	24	ASN
9	2	122	ALA
12	5	37	ILE
15	H	88	GLN
15	H	282	GLY

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Mol	Chain	Res	Type
15	H	307	ASP
15	H	308	GLY
15	H	313	GLY
16	I	118	ASP
17	K	99	ASN
17	K	134	LYS
17	K	153	MET
17	K	200	ARG
18	L	240	GLY
18	L	242	ARG
19	M	297	ASP
19	M	300	LYS
19	M	303	ASP
20	J	208	ASP
20	J	231	VAL
3	P	220	ASN
4	Q	57	ARG
4	Q	181	ILE
4	Q	213	ARG
5	R	122	GLN
7	T	221	ASN
8	U	114	ASP
11	X	82	SER
11	X	202	PRO
12	Y	97	MET
2	B	179	GLU
5	E	35	SER
5	E	122	GLN
6	F	69	HIS
6	F	158	ALA
7	G	6	GLY
8	1	40	SER
8	1	114	ASP
9	2	47	VAL
12	5	38	ASN
13	6	19	ARG
15	H	64	GLY
15	H	66	LYS
15	H	128	GLN
15	H	159	PRO
15	H	169	LYS
15	H	378	PRO

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Mol	Chain	Res	Type
17	K	147	ALA
17	K	170	MET
17	K	187	HIS
18	L	76	GLY
18	L	77	PRO
18	L	382	SER
19	M	184	GLN
20	J	155	ASP
20	J	281	ASP
20	J	338	LEU
2	O	122	GLN
6	S	158	ALA
10	W	136	PHE
13	Z	171	GLY
1	A	146	GLU
4	D	205	ASN
5	E	104	ASN
5	E	131	GLY
7	G	207	LYS
14	7	145	ASP
15	H	310	ASP
15	H	432	TYR
16	I	185	ALA
16	I	357	ASP
18	L	109	ARG
18	L	268	ASP
19	M	91	SER
19	M	149	ASP
19	M	356	MET
20	J	111	ASN
20	J	250	GLU
1	N	186	LYS
3	P	143	TYR
6	S	75	ALA
8	U	129	SER
9	V	125	ALA
11	X	83	TYR
11	X	157	GLN
12	Y	38	ASN
12	Y	187	VAL
2	B	212	CYS
4	D	213	ARG

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Mol	Chain	Res	Type
6	F	75	ALA
10	3	80	ARG
11	4	10	SER
12	5	18	SER
13	6	94	LEU
15	H	269	ALA
16	I	197	ILE
17	K	120	ASP
18	L	62	LYS
18	L	73	ALA
18	L	94	PRO
19	M	30	GLY
19	M	136	VAL
19	M	175	MET
20	J	340	ARG
5	R	32	LYS
5	E	167	ALA
8	1	102	PHE
8	1	165	PRO
18	L	126	ASP
15	H	158	ASP
15	H	280	ILE
17	K	32	PRO
12	Y	37	ILE
8	1	17	GLY
15	H	334	PRO
13	Z	146	GLY
19	M	100	ASP
5	E	19	GLY
5	E	124	GLY
6	F	124	GLY
12	5	39	PRO
14	7	41	ILE
15	H	115	VAL
17	K	79	VAL
17	K	366	ARG
19	M	291	ILE
18	L	127	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	208/210 (99%)	204 (98%)	4 (2%)	65	86
1	N	208/210 (99%)	202 (97%)	6 (3%)	50	79
2	B	190/191 (100%)	178 (94%)	12 (6%)	22	61
2	O	190/191 (100%)	184 (97%)	6 (3%)	46	78
3	C	210/221 (95%)	205 (98%)	5 (2%)	57	82
3	P	210/221 (95%)	205 (98%)	5 (2%)	57	82
4	D	207/211 (98%)	200 (97%)	7 (3%)	44	77
4	Q	207/211 (98%)	200 (97%)	7 (3%)	44	77
5	E	196/203 (97%)	189 (96%)	7 (4%)	42	76
5	R	196/203 (97%)	190 (97%)	6 (3%)	47	78
6	F	204/224 (91%)	200 (98%)	4 (2%)	63	86
6	S	204/224 (91%)	197 (97%)	7 (3%)	44	77
7	G	199/212 (94%)	192 (96%)	7 (4%)	43	76
7	T	199/212 (94%)	198 (100%)	1 (0%)	92	96
8	1	178/199 (89%)	169 (95%)	9 (5%)	29	68
8	U	178/199 (89%)	170 (96%)	8 (4%)	34	71
9	2	170/171 (99%)	168 (99%)	2 (1%)	78	90
9	V	170/171 (99%)	167 (98%)	3 (2%)	66	87
10	3	173/174 (99%)	165 (95%)	8 (5%)	33	70
10	W	173/174 (99%)	171 (99%)	2 (1%)	78	90
11	4	179/215 (83%)	172 (96%)	7 (4%)	39	74
11	X	179/215 (83%)	174 (97%)	5 (3%)	51	79
12	5	156/202 (77%)	149 (96%)	7 (4%)	34	71
12	Y	156/202 (77%)	152 (97%)	4 (3%)	54	81
13	6	155/181 (86%)	151 (97%)	4 (3%)	54	81
13	Z	155/181 (86%)	147 (95%)	8 (5%)	29	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	7	181/228 (79%)	178 (98%)	3 (2%)	68 88
14	8	181/228 (79%)	173 (96%)	8 (4%)	35 71
15	H	341/372 (92%)	329 (96%)	12 (4%)	43 76
16	I	336/385 (87%)	325 (97%)	11 (3%)	45 78
17	K	344/366 (94%)	336 (98%)	8 (2%)	58 83
18	L	341/341 (100%)	337 (99%)	4 (1%)	78 90
19	M	357/379 (94%)	350 (98%)	7 (2%)	63 86
20	J	339/352 (96%)	322 (95%)	17 (5%)	30 68
All	All	7270/7879 (92%)	7049 (97%)	221 (3%)	52 78

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	64	SER
1	N	86	ASP
1	N	115	CYS
1	N	145	GLU
1	N	166	THR
1	N	213	SER
2	O	64	VAL
2	O	68	THR
2	O	70	HIS
2	O	132	SER
2	O	196	GLU
2	O	214	GLU
3	P	44	LEU
3	P	62	SER
3	P	74	CYS
3	P	81	SER
3	P	133	SER
4	Q	38	ARG
4	Q	79	ASP
4	Q	121	SER
4	Q	139	ASP
4	Q	150	SER
4	Q	167	SER
4	Q	214	ASP
5	R	10	ARG
5	R	43	SER

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Mol	Chain	Res	Type
5	R	78	MET
5	R	156	MET
5	R	188	SER
5	R	217	LEU
6	S	7	ASP
6	S	33	SER
6	S	38	LEU
6	S	110	SER
6	S	120	THR
6	S	176	MET
6	S	237	GLU
7	T	104	TYR
8	U	18	GLU
8	U	30	SER
8	U	40	SER
8	U	93	SER
8	U	127	VAL
8	U	144	MET
8	U	146	GLN
8	U	200	LYS
9	V	76	SER
9	V	183	ILE
9	V	185	LYS
10	W	49	LEU
10	W	205	ASP
11	X	50	MET
11	X	94	ARG
11	X	141	TYR
11	X	166	ARG
11	X	168	LEU
12	Y	99	THR
12	Y	102	CYS
12	Y	127	SER
12	Y	182	ASP
13	Z	30	VAL
13	Z	43	CYS
13	Z	62	GLN
13	Z	93	ASP
13	Z	133	SER
13	Z	136	TYR
13	Z	144	ARG
13	Z	150	GLU

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Mol	Chain	Res	Type
14	8	38	SER
14	8	127	MET
14	8	129	SER
14	8	143	ARG
14	8	182	LYS
14	8	186	LEU
14	8	194	LYS
14	8	213	THR
1	A	73	THR
1	A	92	GLN
1	A	137	CYS
1	A	166	THR
2	B	2	GLU
2	B	15	SER
2	B	51	GLN
2	B	76	SER
2	B	88	ARG
2	B	132	SER
2	B	139	ASN
2	B	151	SER
2	B	162	MET
2	B	185	ASP
2	B	214	GLU
2	B	232	ILE
3	C	44	LEU
3	C	71	ASP
3	C	168	SER
3	C	199	LYS
3	C	218	ARG
4	D	2	SER
4	D	17	PHE
4	D	38	ARG
4	D	99	GLU
4	D	121	SER
4	D	139	ASP
4	D	146	GLN
5	E	47	CYS
5	E	62	SER
5	E	122	GLN
5	E	135	ARG
5	E	159	SER
5	E	215	ILE

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Mol	Chain	Res	Type
5	E	226	PHE
6	F	38	LEU
6	F	62	LYS
6	F	95	SER
6	F	239	ARG
7	G	8	ASP
7	G	10	SER
7	G	81	LEU
7	G	113	ASP
7	G	186	CYS
7	G	202	ASP
7	G	203	GLU
8	1	1	ARG
8	1	34	SER
8	1	47	THR
8	1	49	LYS
8	1	102	PHE
8	1	125	ASP
8	1	127	VAL
8	1	140	SER
8	1	211	ARG
9	2	62	LYS
9	2	190	ASP
10	3	37	THR
10	3	49	LEU
10	3	134	ASP
10	3	142	CYS
10	3	149	MET
10	3	162	HIS
10	3	175	VAL
10	3	188	HIS
11	4	84	SER
11	4	100	ARG
11	4	141	TYR
11	4	169	VAL
11	4	183	SER
11	4	194	GLU
11	4	205	THR
12	5	8	PHE
12	5	56	GLU
12	5	75	SER
12	5	102	CYS

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Mol	Chain	Res	Type
12	5	116	SER
12	5	162	GLN
12	5	182	ASP
13	6	30	VAL
13	6	43	CYS
13	6	81	SER
13	6	144	ARG
14	7	31	CYS
14	7	148	GLU
14	7	171	SER
15	H	46	LYS
15	H	48	VAL
15	H	61	GLU
15	H	154	PRO
15	H	236	CYS
15	H	239	ARG
15	H	312	ARG
15	H	315	ILE
15	H	322	ASN
15	H	333	ARG
15	H	386	ARG
15	H	429	TYR
16	I	164	MET
16	I	178	LYS
16	I	184	TYR
16	I	235	LEU
16	I	249	ARG
16	I	257	GLN
16	I	324	ASP
16	I	331	THR
16	I	346	ARG
16	I	350	LYS
16	I	434	THR
17	K	50	GLU
17	K	61	ILE
17	K	70	LYS
17	K	109	SER
17	K	155	THR
17	K	299	PHE
17	K	356	GLU
17	K	384	MET
18	L	19	HIS

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Mol	Chain	Res	Type
18	L	183	LEU
18	L	206	LYS
18	L	275	MET
19	M	178	ASP
19	M	194	GLN
19	M	209	LYS
19	M	318	ASP
19	M	332	THR
19	M	344	ARG
19	M	356	MET
20	J	9	MET
20	J	23	TYR
20	J	24	TYR
20	J	31	LEU
20	J	40	GLN
20	J	42	LEU
20	J	43	ARG
20	J	63	LEU
20	J	109	THR
20	J	173	GLU
20	J	180	ILE
20	J	253	SER
20	J	270	GLN
20	J	280	LEU
20	J	290	LYS
20	J	293	MET
20	J	310	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
17	K	257	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
21	ATP	H	501	22	26,33,33	0.83	1 (3%)	26,52,52	2.29	4 (15%)
21	ATP	I	501	22	26,33,33	0.90	1 (3%)	26,52,52	2.14	4 (15%)
23	ADP	J	501	-	24,29,29	1.02	2 (8%)	23,45,45	1.79	1 (4%)
21	ATP	K	501	22	26,33,33	1.11	1 (3%)	26,52,52	1.89	7 (26%)
21	ATP	L	401	22	26,33,33	0.98	1 (3%)	26,52,52	2.13	4 (15%)
21	ATP	M	501	22	26,33,33	1.00	0	26,52,52	2.03	3 (11%)

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
21	ATP	H	501	22	-	0/18/38/38	0/3/3/3
21	ATP	I	501	22	-	0/18/38/38	0/3/3/3
23	ADP	J	501	-	-	0/12/32/32	0/3/3/3
21	ATP	K	501	22	-	0/18/38/38	0/3/3/3
21	ATP	L	401	22	-	0/18/38/38	0/3/3/3
21	ATP	M	501	22	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	H	501	ATP	C5-C4	2.11	1.45	1.40
23	J	501	ADP	O4'-C1'	2.32	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	I	501	ATP	C5-C4	2.47	1.46	1.40
21	L	401	ATP	C5-C4	2.79	1.46	1.40
21	K	501	ATP	C5-C4	2.86	1.46	1.40
23	J	501	ADP	C5-C4	2.99	1.47	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	H	501	ATP	N3-C2-N1	-10.19	120.86	128.87
21	I	501	ATP	N3-C2-N1	-9.35	121.53	128.87
21	L	401	ATP	N3-C2-N1	-9.32	121.55	128.87
21	M	501	ATP	N3-C2-N1	-7.68	122.84	128.87
23	J	501	ADP	N3-C2-N1	-7.00	123.37	128.87
21	K	501	ATP	N3-C2-N1	-5.27	124.73	128.87
21	K	501	ATP	C1'-N9-C4	-4.00	122.34	126.81
21	K	501	ATP	O2'-C2'-C1'	-3.20	101.61	111.61
21	H	501	ATP	C1'-N9-C4	-2.39	124.14	126.81
21	I	501	ATP	O3G-PG-O2G	2.07	115.02	107.44
21	K	501	ATP	O2B-PB-O3A	2.08	114.18	105.27
21	I	501	ATP	N6-C6-N1	2.10	122.05	118.52
21	K	501	ATP	O2B-PB-O3B	2.11	114.30	105.27
21	L	401	ATP	O3G-PG-O2G	2.13	115.25	107.44
21	L	401	ATP	N6-C6-N1	2.25	122.29	118.52
21	K	501	ATP	C2'-C1'-N9	2.26	119.52	113.47
21	L	401	ATP	C2-N1-C6	2.33	122.92	118.77
21	H	501	ATP	C2-N1-C6	2.33	122.93	118.77
21	I	501	ATP	C2-N1-C6	2.41	123.07	118.77
21	H	501	ATP	N6-C6-N1	2.59	122.86	118.52
21	M	501	ATP	O3G-PG-O2G	2.69	117.32	107.44
21	K	501	ATP	O3G-PG-O2G	2.87	117.99	107.44
21	M	501	ATP	N6-C6-N1	4.18	125.53	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	H	501	ATP	2	0
23	J	501	ADP	2	0
21	K	501	ATP	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	L	401	ATP	1	0
21	M	501	ATP	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.