



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:45 AM UTC

PDB ID : 3MG8 / pdb_00003mg8
Title : Structure of yeast 20S open-gate proteasome with Compound 16
Authors : Sintchak, M.D.
Deposited on : 2010-04-05
Resolution : 2.59 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

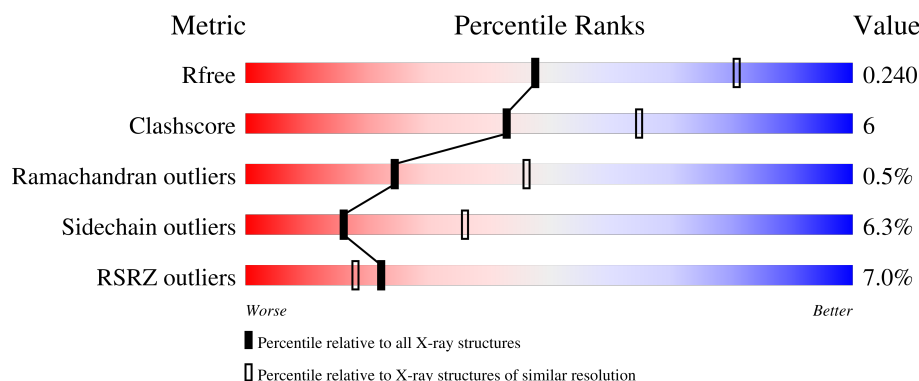
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	6% 88% 12%
1	O	250	9% 85% 13%
2	B	245	10% 77% 16%
2	P	245	11% 76% 18%
3	C	243	19% 84% 14%

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Mol	Chain	Length	Quality of chain
3	Q	243	
4	D	250	
4	R	250	
5	E	234	
5	S	234	
6	F	248	
6	T	248	
7	G	252	
7	U	252	
8	H	222	
8	V	222	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	241	
12	Z	241	
13	1	266	
13	M	266	
14	2	196	
14	N	196	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49429 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 component Y7.

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 component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	0
			1829	1158	303	365	3			
2	P	235	Total	C	N	O	S	0	0	0
			1829	1158	303	365	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
4	R	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	237	Total	C	N	O	S	0	0	0
			1848	1175	323	346	4			
6	T	237	Total	C	N	O	S	0	0	0
			1848	1175	323	346	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

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

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called Proteasome component PUP3.

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 component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

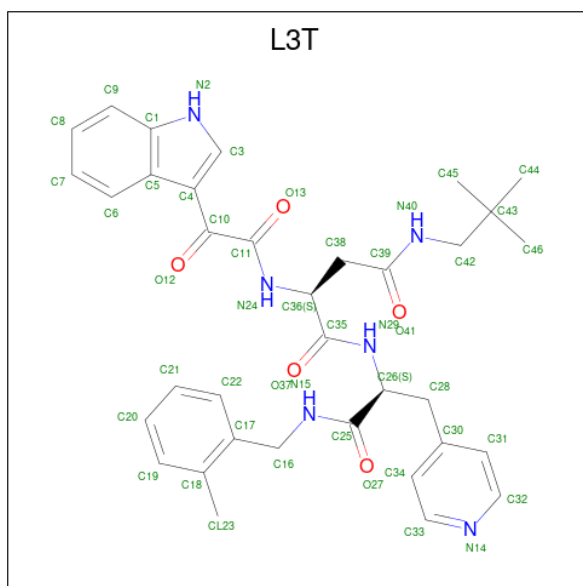
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	F	2	Total	Mg	0	0
			2	2		
15	G	1	Total	Mg	0	0
			1	1		

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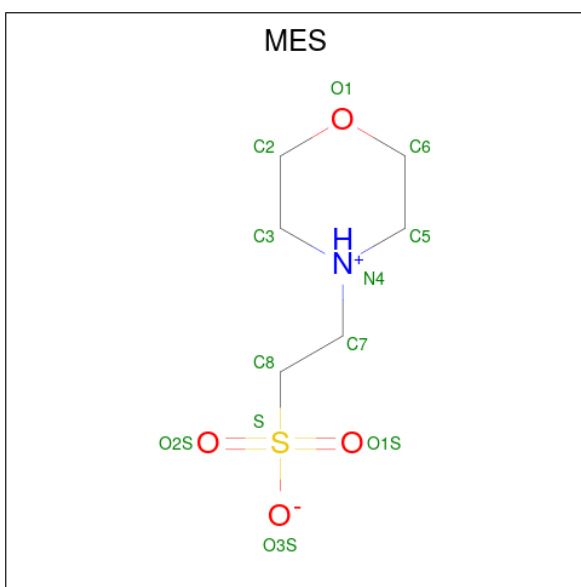
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	1	Total	Mg	0	0
			1	1		
15	I	2	Total	Mg	0	0
			2	2		
15	K	1	Total	Mg	0	0
			1	1		
15	L	2	Total	Mg	0	0
			2	2		
15	N	1	Total	Mg	0	0
			1	1		

- Molecule 16 is N-(2,2-dimethylpropyl)-N 2 -[1H-indol-3-yl(oxo)acetyl]-L-asparaginyln-N-(2-methylbenzyl)-3-pyridin-4-yl-L-alaninamide (CCD ID: L3T) (formula: $C_{35}H_{40}N_6O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	K	1	Total	C	N	O	0	0
			46	35	6	5		
16	Y	1	Total	C	N	O	0	0
			46	35	6	5		

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

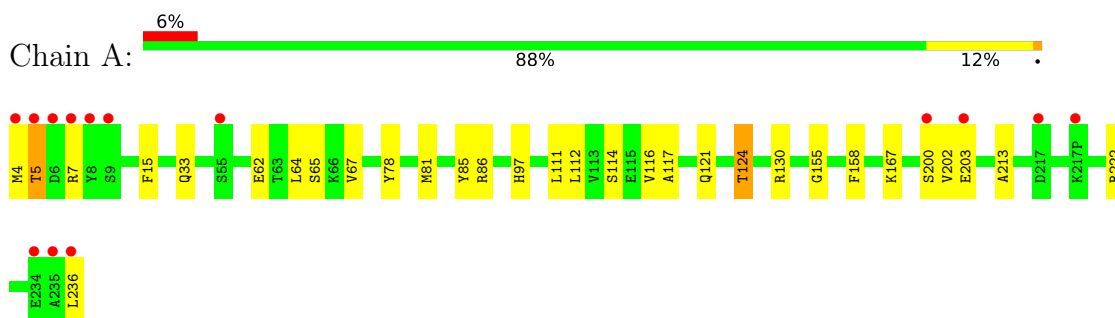
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	K	2	Total	O	0	0
			2	2		
18	L	3	Total	O	0	0
			3	3		

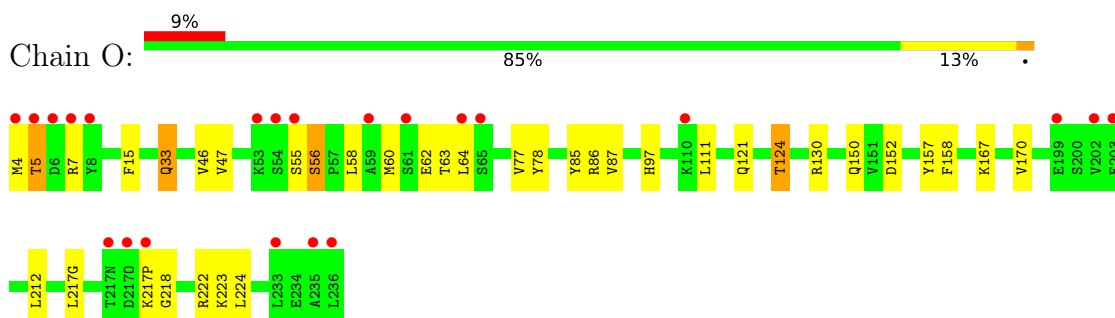
3 Residue-property plots

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

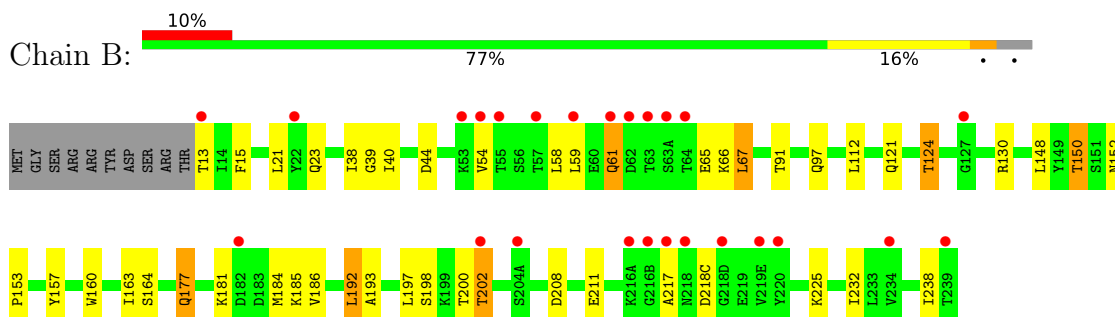
• Molecule 1: Proteasome component Y7



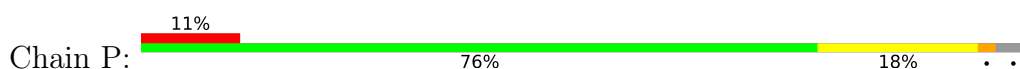
• Molecule 1: Proteasome component Y7

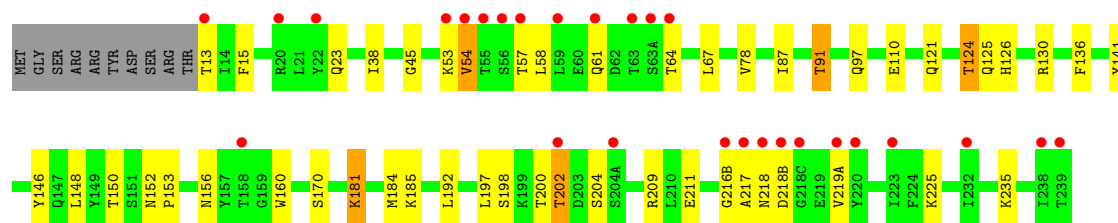


• Molecule 2: Proteasome component Y13

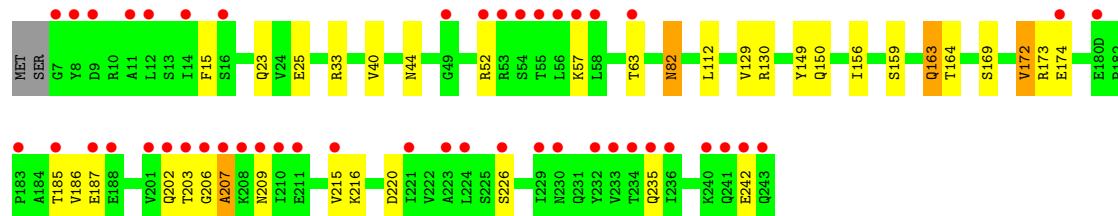
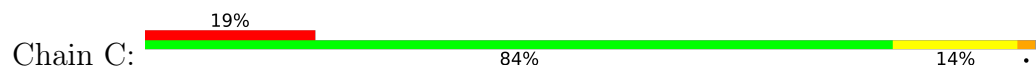


• Molecule 2: Proteasome component Y13

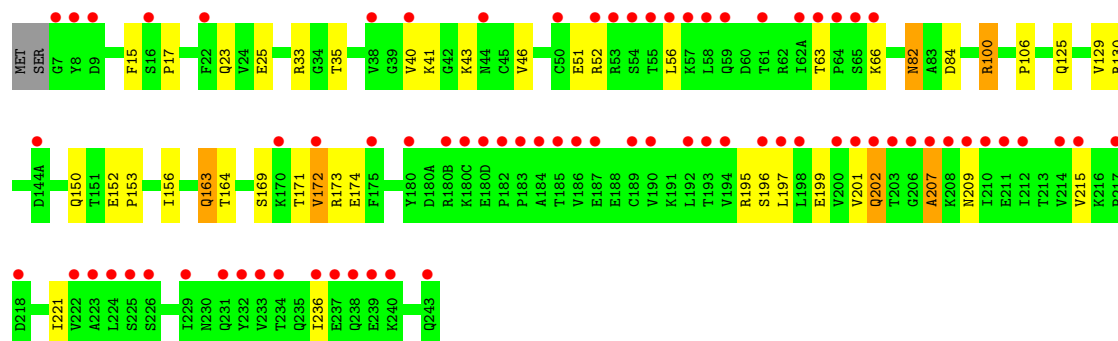
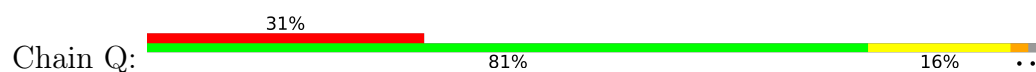




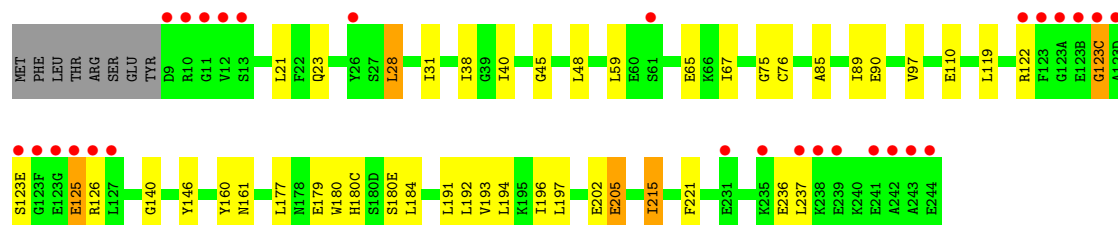
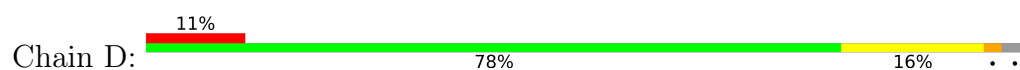
• Molecule 3: Proteasome component PRE6



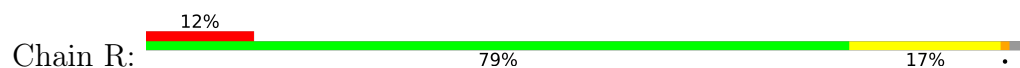
• Molecule 3: Proteasome component PRE6

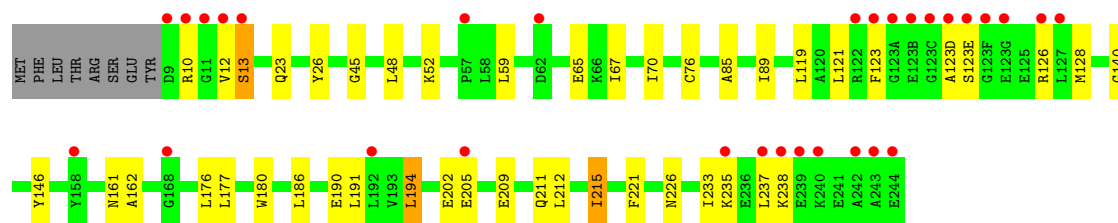


• Molecule 4: Proteasome component PUP2

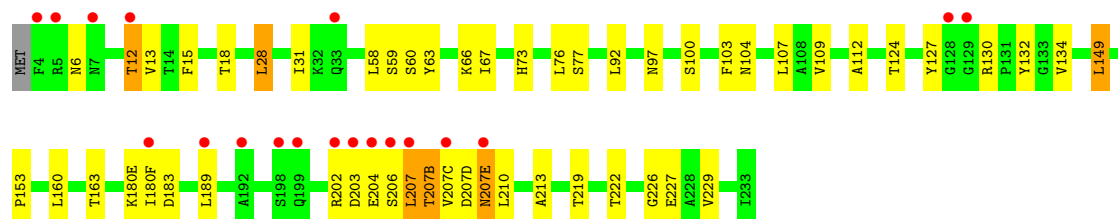
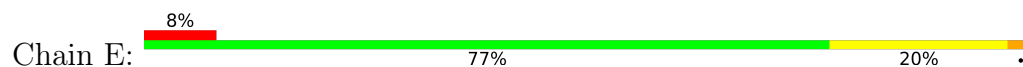


• Molecule 4: Proteasome component PUP2

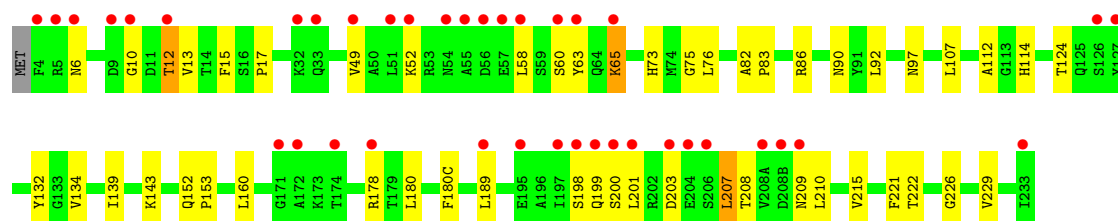
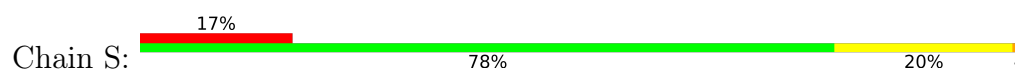




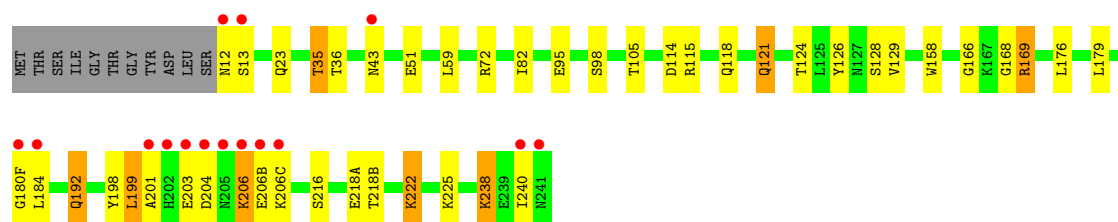
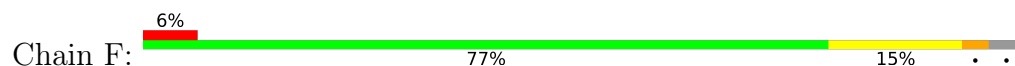
• Molecule 5: Proteasome component PRE5



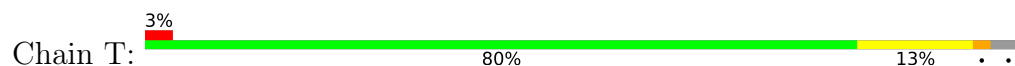
• Molecule 5: Proteasome component PRE5

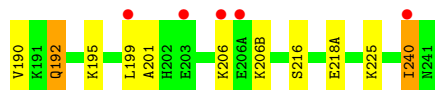


• Molecule 6: Proteasome component C1

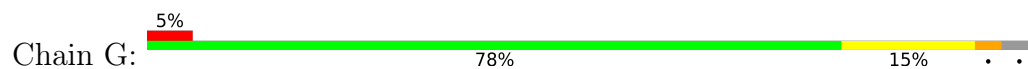


• Molecule 6: Proteasome component C1

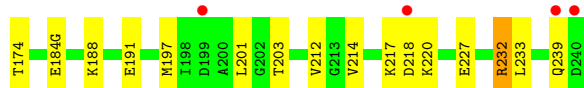
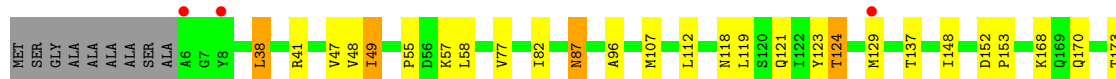
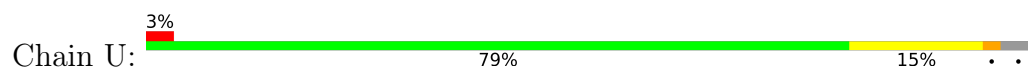




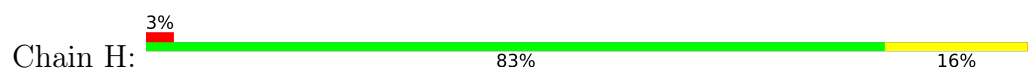
• Molecule 7: Proteasome component C7-alpha



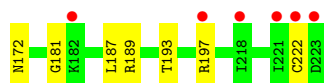
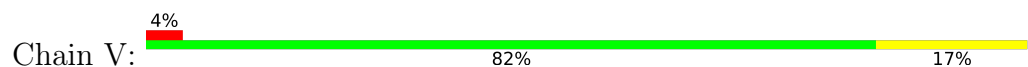
• Molecule 7: Proteasome component C7-alpha



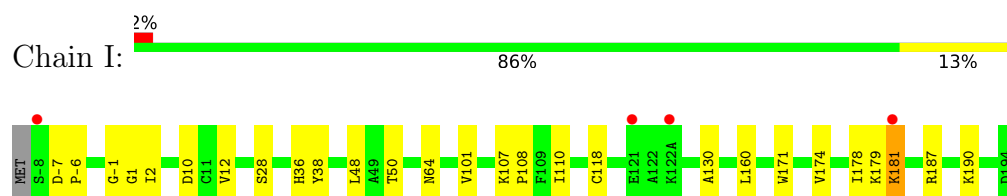
• Molecule 8: Proteasome component PUP1



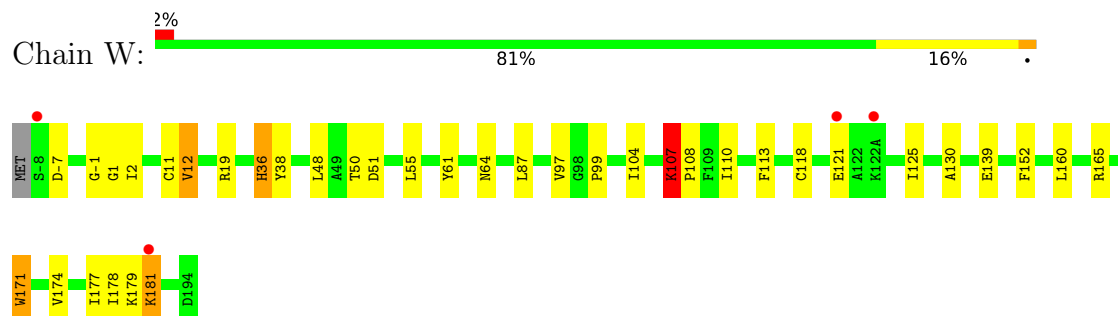
• Molecule 8: Proteasome component PUP1



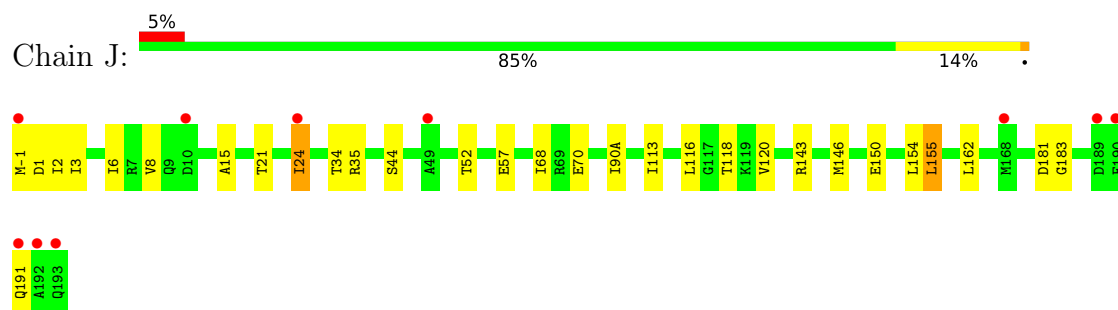
• Molecule 9: Proteasome component PUP3



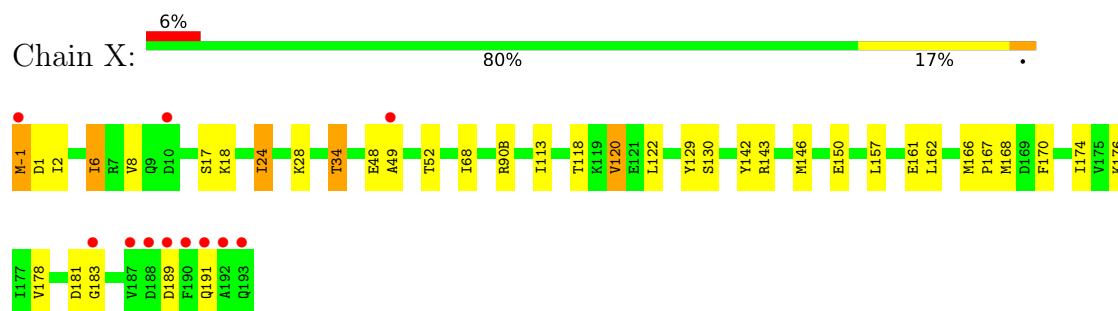
- Molecule 9: Proteasome component PUP3



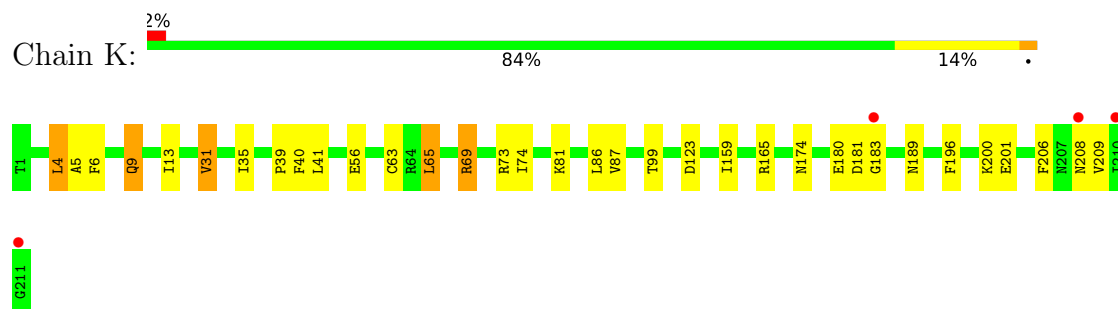
- Molecule 10: Proteasome component C11



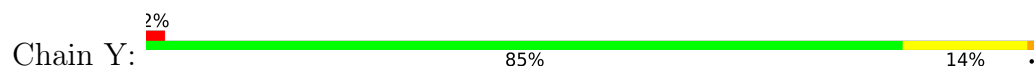
- Molecule 10: Proteasome component C11



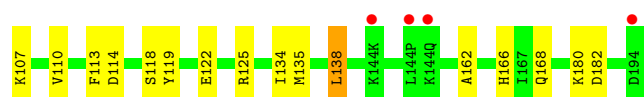
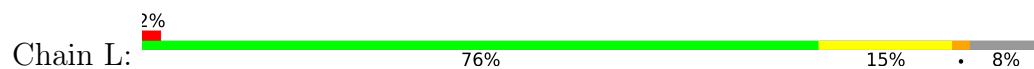
- Molecule 11: Proteasome component PRE2



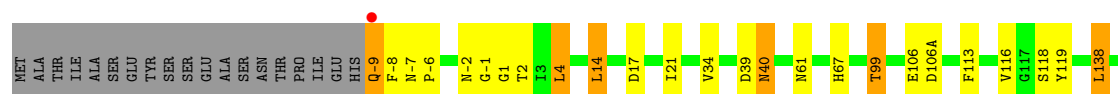
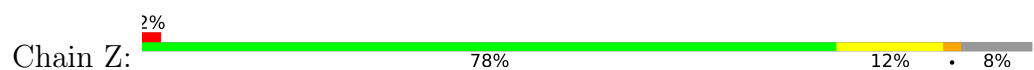
- Molecule 11: Proteasome component PRE2



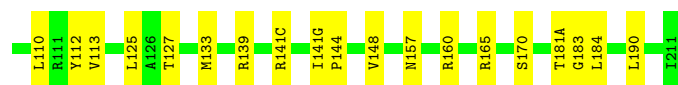
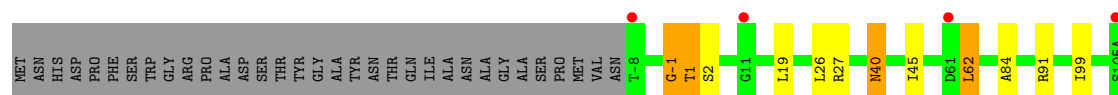
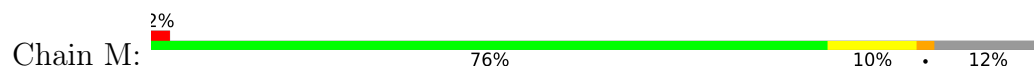
- Molecule 12: Proteasome component C5



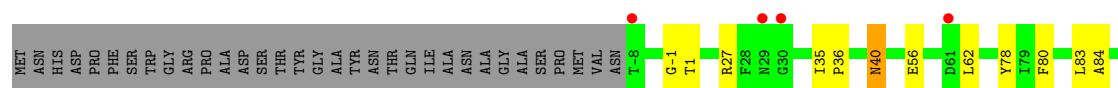
- Molecule 12: Proteasome component C5

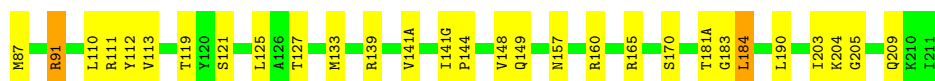


- Molecule 13: Proteasome component PRE4

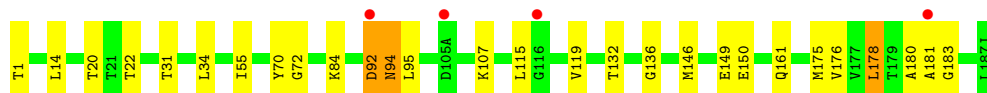
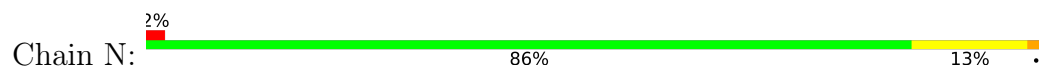


- Molecule 13: Proteasome component PRE4

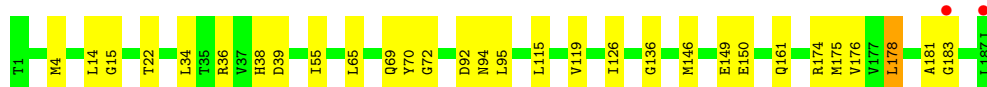
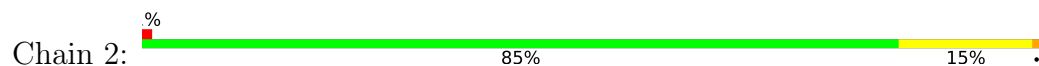




- Molecule 14: Proteasome component PRE3



- Molecule 14: Proteasome component PRE3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.33Å 299.19Å 145.67Å 90.00° 113.13° 90.00°	Depositor
Resolution (Å)	49.88 – 2.59 49.88 – 2.59	Depositor EDS
% Data completeness (in resolution range)	95.2 (49.88-2.59) 95.2 (49.88-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.224 , 0.252 (Not available) , 0.240	Depositor DCC
R_{free} test set	6368 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 25.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	49429	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, L3T, MES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/1951	0.79	0/2639
1	O	0.51	0/1951	0.81	2/2639 (0.1%)
2	B	0.51	0/1857	0.83	1/2513 (0.0%)
2	P	0.51	0/1857	0.81	0/2513
3	C	0.50	0/1918	0.82	0/2591
3	Q	0.51	0/1918	0.81	1/2591 (0.0%)
4	D	0.52	0/1883	0.80	1/2529 (0.0%)
4	R	0.51	0/1884	0.81	0/2532
5	E	0.48	0/1819	0.80	1/2451 (0.0%)
5	S	0.47	0/1821	0.79	2/2457 (0.1%)
6	F	0.54	1/1885 (0.1%)	0.83	0/2540
6	T	0.52	0/1886	0.83	1/2543 (0.0%)
7	G	0.55	1/1956 (0.1%)	0.78	0/2643
7	U	0.53	1/1958 (0.1%)	0.81	0/2649
8	H	0.52	0/1714	0.80	0/2320
8	V	0.51	0/1714	0.78	0/2320
9	I	0.51	0/1608	0.80	0/2165
9	W	0.96	1/1609 (0.1%)	0.85	3/2168 (0.1%)
10	J	0.51	0/1611	0.80	0/2167
10	X	0.51	0/1611	0.80	1/2167 (0.0%)
11	K	0.50	0/1680	0.79	0/2271
11	Y	0.49	0/1680	0.78	0/2271
12	L	0.49	0/1793	0.79	1/2414 (0.0%)
12	Z	0.50	0/1793	0.80	1/2414 (0.0%)
13	1	0.53	0/1852	0.81	1/2504 (0.0%)
13	M	1.13	1/1853 (0.1%)	0.87	3/2507 (0.1%)
14	2	0.52	0/1538	0.78	1/2078 (0.0%)
14	N	1.14	1/1539 (0.1%)	0.84	3/2081 (0.1%)
All	All	0.59	6/50139 (0.0%)	0.81	23/67677 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	-1	GLY	C-N	43.30	1.94	1.33
14	N	92	ASP	C-N	39.67	1.86	1.33
9	W	36	HIS	C-N	32.10	1.90	1.33
6	F	82	ILE	CA-CB	8.25	1.58	1.54
7	G	82	ILE	CA-CB	6.39	1.58	1.53
7	U	82	ILE	CA-CB	5.80	1.57	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	-1	GLY	O-C-N	-17.68	99.72	122.70
14	N	92	ASP	O-C-N	-12.78	105.30	122.43
9	W	36	HIS	O-C-N	-7.02	115.19	123.41
5	E	202	ARG	N-CA-C	-6.30	106.13	113.88
13	M	2	SER	N-CA-C	6.14	118.22	110.24
14	N	92	ASP	CA-C-N	5.84	131.37	122.37
14	N	92	ASP	C-N-CA	5.84	131.37	122.37
4	D	236	GLU	N-CA-C	5.81	117.61	111.28
9	W	107	LYS	CA-C-N	5.59	125.52	119.76
9	W	107	LYS	C-N-CA	5.59	125.52	119.76
13	1	27	ARG	N-CA-C	5.53	118.15	111.40
6	T	107	ILE	N-CA-C	5.45	114.29	108.95
3	Q	125	GLN	N-CA-C	5.42	117.82	110.88
1	O	152	ASP	CA-C-N	5.38	126.56	119.84
1	O	152	ASP	C-N-CA	5.38	126.56	119.84
10	X	49	ALA	N-CA-C	5.36	120.22	111.37
12	L	119	TYR	N-CA-C	5.28	117.21	109.24
14	2	115	LEU	N-CA-C	5.24	117.39	111.11
2	B	238	ILE	N-CA-C	-5.22	108.19	113.47
13	M	27	ARG	N-CA-C	5.11	117.63	111.40
5	S	152	GLN	CA-C-N	5.05	124.71	119.56
5	S	152	GLN	C-N-CA	5.05	124.71	119.56
12	Z	116	VAL	N-CA-C	5.03	116.95	112.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1925	23	0
1	O	1915	0	1925	24	0
2	B	1829	0	1828	28	0
2	P	1829	0	1828	28	0
3	C	1891	0	1899	19	0
3	Q	1891	0	1899	32	0
4	D	1862	0	1832	25	0
4	R	1862	0	1833	20	0
5	E	1795	0	1793	31	0
5	S	1795	0	1795	32	0
6	F	1848	0	1842	24	0
6	T	1848	0	1843	26	0
7	G	1921	0	1907	33	0
7	U	1921	0	1909	28	0
8	H	1685	0	1686	24	0
8	V	1685	0	1686	22	0
9	I	1581	0	1574	24	0
9	W	1581	0	1574	30	0
10	J	1585	0	1591	20	0
10	X	1585	0	1591	26	0
11	K	1644	0	1594	28	0
11	Y	1644	0	1594	21	0
12	L	1757	0	1712	24	0
12	Z	1757	0	1712	28	0
13	1	1824	0	1833	30	0
13	M	1824	0	1833	25	0
14	2	1512	0	1478	17	0
14	N	1512	0	1478	16	0
15	F	2	0	0	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	2	0	0	0	0
15	N	1	0	0	0	0
16	K	46	0	40	4	0
16	Y	46	0	40	2	0
17	K	12	0	13	0	0
17	Y	12	0	13	1	0
18	K	2	0	0	0	0
18	L	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	49429	0	49100	615	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 (615) 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)
13:M:-1:GLY:C	13:M:1:THR:H1	1.31	1.36
14:N:92:ASP:C	14:N:94:ASN:N	1.86	1.30
9:W:36:HIS:C	9:W:38:TYR:N	1.89	1.29
13:1:-1:GLY:C	13:1:1:THR:H1	1.37	1.28
13:M:-1:GLY:C	13:M:1:THR:N	1.94	1.22
2:P:200:THR:O	2:P:202:THR:N	1.71	1.22
13:1:-1:GLY:C	13:1:1:THR:N	2.02	1.18
9:I:-1:GLY:C	9:I:1:GLY:N	2.04	1.16
9:W:-1:GLY:C	9:W:1:GLY:N	2.04	1.15
14:2:70:TYR:C	14:2:72:GLY:N	2.06	1.13
14:N:70:TYR:C	14:N:72:GLY:N	2.09	1.11
13:1:141(G):ILE:C	13:1:144:PRO:N	2.10	1.10
13:M:141(G):ILE:C	13:M:144:PRO:N	2.09	1.10
8:H:91:GLN:C	8:H:93:GLY:N	2.14	1.06
7:G:96:ALA:HA	7:G:107:MET:HE2	1.37	1.01
7:U:96:ALA:HA	7:U:107:MET:HE2	1.42	1.01
9:I:36:HIS:C	9:I:38:TYR:N	2.21	0.99
9:I:-1:GLY:C	9:I:1:GLY:H1	1.71	0.97
12:Z:-1:GLY:C	12:Z:1:GLY:N	2.23	0.96
2:B:200:THR:C	2:B:202:THR:N	2.22	0.95
8:V:187:LEU:C	8:V:189:ARG:N	2.24	0.95
7:G:218:ASP:C	7:G:220:LYS:N	2.24	0.95
8:H:187:LEU:C	8:H:189:ARG:N	2.24	0.94
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.33	0.94
9:W:-1:GLY:C	9:W:1:GLY:H1	1.72	0.92
9:W:-1:GLY:C	9:W:1:GLY:H3	1.71	0.91
9:I:-1:GLY:C	9:I:1:GLY:H3	1.73	0.90
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.37	0.87
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.58	0.85
9:W:179:LYS:C	9:W:181:LYS:N	2.35	0.84
6:F:35:THR:HG21	6:F:51:GLU:O	1.79	0.83
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.40	0.83
6:T:192:GLN:NE2	6:T:195:LYS:HE3	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:207:LEU:HA	5:E:207(E):ASN:HD22	1.45	0.82
12:L:180:LYS:C	12:L:182:ASP:N	2.38	0.82
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.24	0.82
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.44	0.82
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.44	0.80
1:O:124:THR:CG2	2:P:130:ARG:HH21	1.94	0.80
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.30	0.79
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.30	0.79
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.95	0.79
3:C:15:PHE:H	4:D:23:GLN:HE22	1.29	0.79
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.32	0.78
11:K:31:VAL:HG11	16:K:213:L3T:C21	2.14	0.78
12:Z:-1:GLY:C	12:Z:1:GLY:H1	1.88	0.78
5:E:15:PHE:H	6:F:23:GLN:HE22	1.31	0.78
3:C:163:GLN:NE2	3:C:164:THR:H	1.82	0.77
13:M:141(C):ARG:HG3	13:M:141(C):ARG:HH11	1.48	0.77
1:O:15:PHE:H	2:P:23:GLN:HE22	1.33	0.77
12:Z:-1:GLY:C	12:Z:1:GLY:CA	2.56	0.77
6:T:192:GLN:HE22	6:T:195:LYS:HE3	1.49	0.77
13:M:-1:GLY:C	13:M:1:THR:H2	1.91	0.77
4:D:202:GLU:C	4:D:205:GLU:N	2.43	0.77
7:G:38:LEU:HD23	7:G:197:MET:HE3	1.67	0.76
8:V:91:GLN:C	8:V:93:GLY:N	2.43	0.76
12:Z:180:LYS:C	12:Z:182:ASP:N	2.43	0.76
10:J:181:ASP:C	10:J:183:GLY:N	2.43	0.76
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.99	0.76
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.48	0.76
14:2:92:ASP:C	14:2:94:ASN:N	2.44	0.76
7:G:184(M):SER:HA	7:G:186:TRP:N	2.01	0.76
11:K:31:VAL:HG11	16:K:213:L3T:H21	1.68	0.75
11:K:40:PHE:HA	11:K:183:GLY:N	2.00	0.75
12:L:-1:GLY:C	12:L:1:GLY:N	2.45	0.75
14:2:146:MET:HE2	14:2:150:GLU:HB3	1.69	0.74
11:K:181:ASP:C	11:K:183:GLY:CA	2.60	0.74
2:B:13:THR:O	3:C:130:ARG:HD3	1.87	0.74
12:L:4:LEU:HD13	12:L:138:LEU:HD21	1.68	0.74
14:2:92:ASP:O	14:2:94:ASN:N	2.20	0.74
13:M:40:ASN:H	13:M:40:ASN:HD22	1.35	0.73
2:P:121:GLN:O	2:P:124:THR:HB	1.87	0.73
3:C:163:GLN:HE21	3:C:164:THR:H	1.33	0.73
12:L:-1:GLY:C	12:L:1:GLY:H3	1.96	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.37	0.72
11:Y:174:ASN:ND2	11:Y:189:ASN:HD22	1.87	0.72
7:U:96:ALA:CA	7:U:107:MET:HE2	2.18	0.72
7:U:121:GLN:O	7:U:124:THR:HB	1.90	0.72
9:W:36:HIS:CA	9:W:38:TYR:N	2.52	0.72
12:Z:4:LEU:HD13	12:Z:138:LEU:HD21	1.72	0.71
2:B:181:LYS:O	2:B:184:MET:HG3	1.91	0.71
11:K:181:ASP:C	11:K:183:GLY:HA2	2.16	0.71
12:Z:-1:GLY:C	12:Z:1:GLY:HA3	2.15	0.71
12:Z:-1:GLY:O	12:Z:1:GLY:HA3	1.91	0.71
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.73	0.71
6:F:168:GLY:HA3	6:F:201:ALA:HB1	1.73	0.70
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.36	0.70
7:U:218:ASP:C	7:U:220:LYS:N	2.49	0.70
10:X:146:MET:HE2	10:X:150:GLU:HB3	1.73	0.70
10:J:24:ILE:HD11	10:X:129:TYR:HB3	1.73	0.70
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.74	0.70
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.55	0.70
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.74	0.70
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.40	0.70
8:H:202:LYS:HE3	12:Z:150:GLU:OE2	1.91	0.70
11:Y:196:PHE:HZ	11:Y:209:VAL:HG21	1.57	0.70
7:G:107:MET:HE3	7:G:112:LEU:HD13	1.74	0.69
5:S:52:LYS:HB2	5:S:63:TYR:HB3	1.73	0.69
6:T:35:THR:HG21	6:T:51:GLU:O	1.91	0.69
11:K:181:ASP:C	11:K:183:GLY:HA3	2.17	0.69
6:T:199:LEU:C	6:T:201:ALA:N	2.51	0.69
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.40	0.69
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.75	0.68
12:Z:179:THR:HG1	12:Z:182:ASP:N	1.90	0.68
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.42	0.68
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.42	0.68
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.93	0.67
7:U:107:MET:HE3	7:U:112:LEU:HD13	1.76	0.67
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.41	0.66
13:1:181(A):THR:O	13:1:183:GLY:N	2.28	0.66
8:H:91:GLN:O	8:H:93:GLY:N	2.26	0.66
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.26	0.66
11:Y:181:ASP:C	11:Y:183:GLY:N	2.54	0.66
5:E:12:THR:HG21	5:E:124:THR:HA	1.77	0.66
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:50:ALA:HB2	9:I:118:CYS:HB2	1.78	0.66
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.78	0.66
13:1:-1:GLY:C	13:1:1:THR:H2	1.99	0.66
11:K:181:ASP:O	11:K:183:GLY:HA2	1.96	0.65
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.77	0.65
7:U:87:ASN:C	7:U:87:ASN:HD22	2.03	0.65
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.44	0.65
3:Q:171:THR:O	3:Q:174:GLU:HB3	1.97	0.65
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.44	0.65
5:S:60:SER:C	5:S:63:TYR:N	2.55	0.65
2:B:67:LEU:HD22	2:B:211:GLU:HB3	1.79	0.65
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.62	0.65
4:D:122:ARG:HA	4:D:126:ARG:HD3	1.78	0.64
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.62	0.64
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.62	0.64
4:R:12:VAL:HG23	4:R:13:SER:H	1.63	0.64
11:Y:31:VAL:HG21	16:Y:212:L3T:H21	1.78	0.64
9:I:179:LYS:C	9:I:181:LYS:N	2.56	0.63
9:I:36:HIS:CA	9:I:38:TYR:N	2.61	0.63
3:Q:33:ARG:NH1	3:Q:33:ARG:HB2	2.13	0.63
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.44	0.63
4:R:233:ILE:C	4:R:235:LYS:N	2.57	0.63
7:U:184(G):GLU:HG2	7:U:188:LYS:HB2	1.78	0.63
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.96	0.62
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.29	0.62
10:X:181:ASP:C	10:X:183:GLY:N	2.58	0.62
2:P:97:GLN:HE21	9:W:61:TYR:HA	1.64	0.62
5:E:180(E):LYS:O	5:E:183:ASP:N	2.33	0.62
6:F:35:THR:CG2	6:F:51:GLU:O	2.46	0.62
3:Q:100:ARG:HH11	3:Q:106:PRO:HG3	1.65	0.62
13:1:-1:GLY:CA	13:1:1:THR:H1	2.11	0.62
10:X:28:LYS:HE3	11:Y:121:LYS:O	1.98	0.62
13:1:-1:GLY:CA	13:1:1:THR:N	2.62	0.61
13:1:112:TYR:HE1	13:1:127:THR:HG22	1.64	0.61
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.13	0.61
4:D:179:GLU:HB3	4:D:192:LEU:HD21	1.81	0.61
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.82	0.61
1:A:200:SER:O	1:A:202:VAL:HA	2.00	0.61
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.49	0.61
3:C:163:GLN:HE21	3:C:164:THR:N	1.99	0.60
1:A:7:ARG:CG	6:F:128:SER:HB3	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:96:ALA:CA	7:G:107:MET:HE2	2.22	0.60
12:L:166:HIS:HD2	12:L:168:GLN:H	1.47	0.60
10:X:-1:MET:HE3	10:X:-1:MET:HA	1.83	0.60
3:Q:163:GLN:HE21	3:Q:163:GLN:HA	1.65	0.60
10:X:2:ILE:HG12	10:X:130:SER:HB3	1.84	0.60
7:G:121:GLN:O	7:G:124:THR:HB	2.02	0.60
14:2:181:ALA:C	14:2:183:GLY:N	2.60	0.60
2:B:121:GLN:O	2:B:124:THR:HB	2.02	0.59
5:S:73:HIS:HE1	5:S:107:LEU:O	1.84	0.59
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	1.99	0.59
5:E:207:LEU:HA	5:E:207(E):ASN:ND2	2.14	0.59
4:D:180(E):SER:C	4:D:184:LEU:N	2.60	0.59
6:F:199:LEU:C	6:F:201:ALA:N	2.61	0.59
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.34	0.59
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.99	0.59
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.84	0.59
5:S:132:TYR:O	5:S:153:PRO:HB3	2.02	0.59
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.68	0.59
10:J:-1:MET:HA	10:J:1:ASP:N	2.18	0.59
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	1.99	0.59
7:U:184(G):GLU:HG2	7:U:188:LYS:CB	2.33	0.58
6:T:12:ASN:C	6:T:14:VAL:H	2.11	0.58
9:I:179:LYS:O	9:I:181:LYS:N	2.37	0.58
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.85	0.58
13:M:-1:GLY:CA	13:M:1:THR:H1	2.13	0.58
13:M:-1:GLY:CA	13:M:1:THR:N	2.66	0.58
14:N:181:ALA:O	14:N:183:GLY:N	2.37	0.58
1:O:55:SER:O	1:O:56:SER:HB3	2.03	0.58
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.69	0.58
4:R:123(D):ALA:HB3	4:R:126:ARG:HG3	1.86	0.58
1:A:7:ARG:HG2	6:F:128:SER:HB3	1.86	0.58
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.86	0.58
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.84	0.58
5:S:180:LEU:HA	5:S:180(C):PHE:CE2	2.39	0.58
5:E:60:SER:C	5:E:63:TYR:N	2.62	0.57
1:A:121:GLN:O	1:A:124:THR:HB	2.04	0.57
6:T:35:THR:CG2	6:T:51:GLU:O	2.52	0.57
1:A:15:PHE:H	2:B:23:GLN:HE22	1.51	0.57
4:D:123(C):GLY:HA2	4:D:126:ARG:H	1.70	0.57
10:J:-1:MET:HA	10:J:1:ASP:H3	1.69	0.57
3:C:163:GLN:HE21	3:C:163:GLN:HA	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:40:ASN:HD22	13:M:40:ASN:N	1.99	0.57
5:E:180(F):ILE:C	5:E:183:ASP:N	2.63	0.57
14:N:146:MET:HE2	14:N:150:GLU:HB3	1.85	0.57
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.05	0.57
2:B:15:PHE:H	3:C:23:GLN:HE22	1.53	0.57
5:S:139:ILE:HD12	5:S:215:VAL:HG12	1.87	0.56
9:I:36:HIS:HA	9:I:38:TYR:N	2.20	0.56
10:J:146:MET:HE2	10:J:150:GLU:HB3	1.88	0.56
4:R:186:LEU:O	4:R:190:GLU:HG3	2.06	0.56
5:S:134:VAL:O	5:S:153:PRO:HG3	2.06	0.56
8:V:187:LEU:O	8:V:189:ARG:N	2.38	0.56
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.14	0.56
5:S:15:PHE:H	6:T:23:GLN:HE22	1.54	0.56
13:M:133:MET:HE1	13:M:165:ARG:HG3	1.88	0.56
10:J:15:ALA:HB2	10:J:155:LEU:HD11	1.87	0.56
7:U:107:MET:CE	7:U:112:LEU:HD13	2.36	0.56
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.71	0.55
1:O:7:ARG:HG2	6:T:128:SER:HB3	1.88	0.55
2:P:54:VAL:HA	2:P:209:ARG:HH12	1.70	0.55
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.06	0.55
8:V:128:GLY:O	8:V:131:SER:HB3	2.07	0.55
5:E:207(B):THR:H	5:E:207(E):ASN:HD22	1.54	0.55
7:G:218:ASP:C	7:G:220:LYS:CA	2.80	0.55
10:J:2:ILE:HD13	10:J:162:LEU:HD13	1.88	0.55
11:K:31:VAL:CG1	16:K:213:L3T:H21	2.35	0.55
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.02	0.55
13:M:181(A):THR:O	13:M:183:GLY:N	2.40	0.55
1:O:121:GLN:O	1:O:124:THR:HB	2.06	0.55
11:Y:196:PHE:CZ	11:Y:209:VAL:HG21	2.38	0.55
11:Y:208:ASN:H	11:Y:208:ASN:HD22	1.53	0.55
3:Q:84:ASP:CG	3:Q:130:ARG:HH22	2.15	0.54
6:T:186:ALA:O	6:T:190:VAL:HG23	2.07	0.54
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.04	0.54
10:J:181:ASP:O	10:J:183:GLY:HA3	2.07	0.54
14:N:181:ALA:HB3	14:N:183:GLY:HA3	1.89	0.54
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.55	0.54
5:E:73:HIS:HE1	5:E:107:LEU:O	1.90	0.54
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.90	0.54
9:W:12:VAL:HG23	9:W:178:ILE:HB	1.88	0.54
6:F:13:SER:HB2	7:G:130:ARG:HB3	1.90	0.54
6:F:179:LEU:HD11	6:F:192:GLN:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:10:ASP:HB3	9:I:181:LYS:HE2	1.89	0.54
5:S:17:PRO:HA	6:T:26:TYR:CD1	2.43	0.54
5:S:86:ARG:O	5:S:90:ASN:HB2	2.08	0.53
8:H:165:ASN:ND2	13:1:139:ARG:HH11	2.03	0.53
14:N:70:TYR:C	14:N:72:GLY:CA	2.79	0.53
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.56	0.53
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.90	0.53
10:J:146:MET:HE1	10:J:154:LEU:HD13	1.90	0.53
3:Q:33:ARG:HB2	3:Q:33:ARG:HH11	1.72	0.53
13:1:112:TYR:CE1	13:1:127:THR:HG22	2.42	0.53
13:1:133:MET:HE1	13:1:165:ARG:HG3	1.90	0.53
6:T:43:ASN:HD22	6:T:44:ASP:N	2.07	0.53
6:F:218(B):THR:HB	6:F:222:LYS:HE3	1.91	0.53
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.39	0.53
13:M:165:ARG:HD3	8:V:139:GLU:OE1	2.09	0.53
8:V:197:ARG:HH21	9:W:139:GLU:HG3	1.74	0.52
11:Y:31:VAL:CG2	16:Y:212:L3T:H21	2.39	0.52
13:1:35:ILE:HG12	13:1:56:GLU:HG2	1.90	0.52
12:L:9:GLU:O	12:L:107:LYS:HA	2.09	0.52
10:X:-1:MET:HA	10:X:-1:MET:CE	2.40	0.52
1:A:7:ARG:HD2	5:E:127:TYR:CD2	2.45	0.52
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.19	0.52
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.92	0.52
4:D:21:LEU:HD21	5:E:130:ARG:HD3	1.92	0.52
12:L:43:MET:HG3	12:L:101:ILE:HG22	1.92	0.52
13:M:157:ASN:ND2	13:M:160:ARG:HH11	2.01	0.52
2:P:97:GLN:NE2	9:W:61:TYR:HA	2.24	0.52
5:E:207(E):ASN:O	5:E:210:LEU:N	2.43	0.52
3:Q:163:GLN:NE2	3:Q:164:THR:H	2.07	0.52
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.89	0.52
3:C:203:THR:HA	3:C:206:GLY:N	2.24	0.52
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.23	0.52
5:E:207:LEU:HD23	5:E:207:LEU:H	1.74	0.52
8:H:172:ASN:HD22	8:H:193:THR:HA	1.74	0.52
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.40	0.52
11:K:39:PRO:O	11:K:183:GLY:N	2.43	0.52
11:K:165:ARG:HH22	11:K:208:ASN:HD22	1.56	0.52
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.91	0.52
1:O:217(G):LEU:HD13	1:O:218:GLY:HA2	1.91	0.52
5:S:12:THR:HG21	5:S:124:THR:HA	1.93	0.51
5:S:207:LEU:HD12	5:S:210:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:50:ALA:HB2	9:W:118:CYS:HB2	1.92	0.51
12:Z:-1:GLY:C	12:Z:1:GLY:H3	2.14	0.51
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.92	0.51
12:L:-1:GLY:O	12:L:1:GLY:HA3	2.10	0.51
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.20	0.51
10:X:24:ILE:HG12	10:X:24:ILE:O	2.08	0.51
13:1:-1:GLY:O	13:1:1:THR:N	2.23	0.51
4:D:123(C):GLY:HA2	4:D:125:GLU:HA	1.92	0.51
1:O:97:HIS:HD2	8:V:61:SER:OG	1.93	0.51
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.93	0.51
6:F:198:TYR:HB3	6:F:240:ILE:HD12	1.92	0.51
7:U:168:LYS:HD3	7:U:201:LEU:HD22	1.93	0.51
6:F:203:GLU:O	6:F:206:LYS:HG3	2.11	0.51
7:G:184(M):SER:CA	7:G:186:TRP:N	2.73	0.51
9:I:12:VAL:HG23	9:I:178:ILE:HB	1.92	0.51
6:T:114:ASP:O	6:T:118:GLN:HG2	2.10	0.51
2:P:87:ILE:O	2:P:91:THR:HG23	2.11	0.51
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.38	0.51
8:V:91:GLN:O	8:V:93:GLY:N	2.44	0.51
13:1:111:ARG:HH11	13:1:121:SER:HB2	1.74	0.51
4:D:140:GLY:HA2	4:D:215:ILE:HG12	1.93	0.51
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.46	0.51
1:O:5:THR:HB	1:O:7:ARG:HH21	1.76	0.50
6:T:216:SER:HB3	6:T:218(A):GLU:HB2	1.91	0.50
5:E:31:ILE:HD11	5:E:153:PRO:HD3	1.91	0.50
14:N:149:GLU:CD	14:N:149:GLU:H	2.19	0.50
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.58	0.50
5:S:60:SER:HA	5:S:63:TYR:N	2.26	0.50
11:K:200:LYS:HG3	11:K:206:PHE:HB2	1.93	0.50
11:Y:200:LYS:HG3	11:Y:206:PHE:HB2	1.92	0.50
9:I:190:LYS:HZ2	11:Y:197:TRP:CD1	2.29	0.50
9:W:36:HIS:HA	9:W:38:TYR:N	2.26	0.50
7:G:109:CYS:HB2	7:G:140:SER:OG	2.11	0.50
10:X:-1:MET:HE2	10:X:1:ASP:H1	1.77	0.50
14:2:34:LEU:HD13	14:2:176:VAL:HG23	1.94	0.50
1:O:58:LEU:HD12	7:U:173:THR:HG23	1.92	0.50
14:2:181:ALA:O	14:2:183:GLY:N	2.45	0.50
5:E:204:GLU:HG3	5:E:206:SER:O	2.12	0.49
3:Q:152:GLU:HB2	3:Q:153:PRO:HD2	1.93	0.49
6:T:176:LEU:HB3	7:U:58:LEU:HD21	1.94	0.49
12:L:135:MET:HE2	9:W:165:ARG:NH2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:110:ILE:HD12	9:W:125:ILE:HG12	1.93	0.49
2:P:45:GLY:HA2	2:P:146:TYR:CE1	2.46	0.49
12:L:180:LYS:O	12:L:182:ASP:N	2.44	0.49
7:U:123:TYR:CE1	7:U:129:MET:HE2	2.47	0.49
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.42	0.49
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.17	0.49
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.94	0.49
4:D:97:VAL:HG11	11:K:65:LEU:HD22	1.94	0.49
8:V:35:HIS:HB2	8:V:56:THR:HG21	1.94	0.49
14:N:34:LEU:HD13	14:N:176:VAL:HG23	1.95	0.49
7:G:123:TYR:CE1	7:G:129:MET:HE3	2.47	0.49
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.94	0.49
4:R:162:ALA:HB1	4:R:176:LEU:HD22	1.95	0.49
4:D:85:ALA:O	4:D:89:ILE:HG12	2.13	0.49
14:N:181:ALA:O	14:N:183:GLY:CA	2.61	0.49
3:C:163:GLN:HE21	3:C:163:GLN:CA	2.26	0.49
4:D:38:ILE:HD12	4:D:197:LEU:HG	1.95	0.48
2:B:150:THR:HG22	2:B:160:TRP:HE1	1.77	0.48
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.95	0.48
9:I:1:GLY:C	9:I:1:GLY:CA	2.86	0.48
10:X:1:MET:HE2	10:X:1:ASP:N	2.28	0.48
12:Z:180:LYS:O	12:Z:182:ASP:N	2.45	0.48
13:1:141(A):VAL:HG23	13:1:141(A):VAL:O	2.12	0.48
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.28	0.48
4:R:85:ALA:O	4:R:89:ILE:HG12	2.14	0.48
4:R:123:PHE:HA	4:R:128:MET:HB3	1.94	0.48
2:B:184:MET:HE1	2:B:192:LEU:HD12	1.95	0.48
5:E:207:LEU:HD12	5:E:210:LEU:HD13	1.96	0.48
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.96	0.48
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.62	0.48
8:H:105:ASP:HB2	8:H:105(A):PRO:CD	2.43	0.48
6:T:12:ASN:OD1	6:T:124:THR:HA	2.14	0.48
4:D:192:LEU:O	4:D:196:ILE:HG13	2.14	0.48
2:P:181:LYS:O	2:P:184:MET:HG3	2.14	0.48
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.95	0.48
11:K:31:VAL:CG1	16:K:213:L3T:C21	2.89	0.48
10:X:120:VAL:HG13	10:X:122:LEU:HG	1.94	0.48
3:C:207:ALA:C	3:C:209:ASN:H	2.22	0.48
4:D:180(C):HIS:CE1	4:D:180(E):SER:HB2	2.49	0.48
7:G:87:ASN:C	7:G:87:ASN:HD22	2.22	0.48
7:G:233:LEU:O	7:G:236:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:156:ASN:OD1	3:Q:82:ASN:HB2	2.14	0.48
13:1:36:PRO:HB3	13:1:184:LEU:HD11	1.94	0.48
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.96	0.48
4:D:123(C):GLY:HA2	4:D:126:ARG:N	2.28	0.47
13:1:157:ASN:HD22	13:1:160:ARG:NH1	2.09	0.47
3:Q:215:VAL:HG12	3:Q:221:ILE:HG12	1.95	0.47
5:S:60:SER:CA	5:S:63:TYR:N	2.77	0.47
11:Y:200:LYS:HE3	11:Y:206:PHE:O	2.14	0.47
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.95	0.47
11:K:196:PHE:HZ	11:K:209:VAL:HG21	1.79	0.47
1:A:67:VAL:HG11	1:A:213:ALA:HB2	1.95	0.47
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.96	0.47
9:W:-1:GLY:O	9:W:1:GLY:N	2.43	0.47
10:X:2:ILE:HD13	10:X:162:LEU:HD13	1.96	0.47
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.96	0.47
1:A:78:TYR:HB3	1:A:85:TYR:CD1	2.50	0.47
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.49	0.47
6:F:114:ASP:O	6:F:118:GLN:HG2	2.15	0.47
8:H:105:ASP:HB2	8:H:105(A):PRO:HD2	1.96	0.47
10:J:143:ARG:O	10:J:146:MET:HG3	2.15	0.47
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.95	0.47
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.95	0.47
9:W:55:LEU:HD11	9:W:97:VAL:HG21	1.95	0.47
14:2:14:LEU:O	14:2:175:MET:HA	2.15	0.47
14:2:65:LEU:HG	14:2:69:GLN:HE21	1.80	0.47
1:A:112:LEU:O	1:A:116:VAL:HG23	2.15	0.47
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.44	0.47
8:V:172:ASN:HD22	8:V:193:THR:HA	1.80	0.47
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.44	0.47
3:C:164:THR:HG21	3:C:172:VAL:HG22	1.98	0.47
12:L:-2:ASN:HA	12:L:21:ILE:O	2.15	0.47
8:V:105:ASP:HB2	8:V:105(A):PRO:CD	2.45	0.46
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.51	0.46
9:W:-1:GLY:C	9:W:1:GLY:CA	2.87	0.46
11:Y:181:ASP:O	11:Y:183:GLY:HA3	2.15	0.46
7:G:191:GLU:HG3	7:G:232:ARG:HG3	1.97	0.46
9:W:11:CYS:HA	9:W:104:ILE:HD11	1.97	0.46
6:F:166:GLY:O	6:F:169:ARG:HB3	2.15	0.46
6:F:216:SER:HB3	6:F:218(A):GLU:HB2	1.97	0.46
9:I:48:LEU:HG	9:I:50:THR:HG22	1.96	0.46
4:R:121:LEU:HD21	5:S:83:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:MET:HE1	7:G:21:LEU:HD11	1.97	0.46
8:H:187:LEU:O	8:H:189:ARG:N	2.47	0.46
9:W:107:LYS:HA	9:W:108:PRO:HD3	1.85	0.46
4:D:21:LEU:HD21	5:E:130:ARG:CD	2.45	0.46
12:L:-1:GLY:C	12:L:1:GLY:CA	2.89	0.46
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.81	0.46
13:1:83:LEU:O	13:1:87:MET:HG2	2.15	0.46
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.51	0.46
8:H:3:ILE:HG13	8:H:100:ILE:HD12	1.98	0.46
9:I:36:HIS:O	9:I:38:TYR:N	2.49	0.46
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.51	0.46
5:S:207:LEU:HA	5:S:209:ASN:HD22	1.81	0.46
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.51	0.46
1:A:111:LEU:O	1:A:114:SER:HB3	2.16	0.46
11:Y:1:THR:HB	17:Y:213:MES:O1S	2.16	0.46
10:J:24:ILE:CD1	10:X:129:TYR:HB3	2.44	0.45
10:J:113:ILE:HA	10:J:118:THR:O	2.15	0.45
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.99	0.45
2:P:67:LEU:HD22	2:P:211:GLU:HB3	1.98	0.45
1:A:97:HIS:HD2	8:H:61:SER:OG	1.98	0.45
7:U:38:LEU:C	7:U:38:LEU:HD12	2.40	0.45
11:Y:33:LYS:HA	11:Y:45:MET:HE3	1.98	0.45
2:B:163:ILE:HG13	2:B:164:SER:N	2.31	0.45
1:O:212:LEU:HD22	1:O:224:LEU:HD12	1.98	0.45
11:K:86:LEU:C	11:K:86:LEU:HD13	2.41	0.45
5:E:67:ILE:HG21	5:E:213:ALA:HB2	1.98	0.45
2:P:202:THR:HG22	2:P:204:SER:H	1.80	0.45
5:S:198:SER:C	5:S:200:SER:H	2.25	0.45
8:H:84:LYS:HG3	8:H:85:GLN:N	2.31	0.45
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.47	0.45
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.52	0.45
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.51	0.45
5:S:143:LYS:HE3	13:1:78:TYR:OH	2.17	0.45
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.17	0.45
3:Q:82:ASN:N	3:Q:82:ASN:HD22	2.15	0.45
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.99	0.45
14:2:4:MET:HB3	14:2:126:ILE:HG22	1.99	0.45
6:F:158:TRP:CZ3	7:G:64:VAL:HA	2.52	0.44
10:X:181:ASP:O	10:X:183:GLY:HA3	2.16	0.44
2:P:38:ILE:HD12	2:P:197:LEU:HG	1.99	0.44
5:S:208:THR:OG1	5:S:209:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:99:PRO:HD2	9:W:113:PHE:HB2	1.99	0.44
13:1:1:GLY:HA2	13:1:1:THR:N	2.32	0.44
13:M:45:ILE:HG12	13:M:99:ILE:HG12	2.00	0.44
1:O:60:MET:HE3	1:O:63:THR:HG21	1.98	0.44
5:E:132:TYR:O	5:E:153:PRO:HB3	2.18	0.44
7:U:77:VAL:HG12	7:U:137:THR:HB	1.98	0.44
7:U:191:GLU:HG3	7:U:232:ARG:HG3	1.99	0.44
9:W:107:LYS:HB3	9:W:107:LYS:HE2	1.46	0.44
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.82	0.44
5:E:103:PHE:HE2	13:M:62:LEU:HD21	1.82	0.44
2:B:44:ASP:OD2	2:B:44:ASP:N	2.51	0.44
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.98	0.44
1:O:7:ARG:CG	6:T:128:SER:HB3	2.47	0.44
7:U:87:ASN:C	7:U:87:ASN:ND2	2.67	0.44
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.00	0.44
8:V:35:HIS:CB	8:V:56:THR:HG21	2.48	0.44
13:1:112:TYR:O	13:1:119:THR:HA	2.18	0.44
7:G:184(M):SER:C	7:G:188:LYS:H	2.26	0.44
11:K:6:PHE:HA	11:K:123:ASP:O	2.18	0.44
2:P:216(B):GLY:O	2:P:218:ASN:N	2.51	0.44
3:Q:35:THR:HB	3:Q:51:GLU:HG3	2.00	0.44
8:H:172:ASN:ND2	8:H:193:THR:HA	2.33	0.44
10:J:90(A):ILE:HG12	10:J:116:LEU:HD23	1.99	0.44
11:K:4:LEU:HD13	11:K:159:ILE:HD11	1.99	0.44
12:L:114:ASP:OD1	12:L:118:SER:HB3	2.18	0.44
8:V:197:ARG:NH2	9:W:139:GLU:HG3	2.32	0.44
14:2:15:GLY:HA2	14:2:174:ARG:O	2.18	0.44
8:H:165:ASN:HD22	13:1:139:ARG:NH1	2.10	0.43
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.99	0.43
10:X:6:ILE:HD11	10:X:142:TYR:CD1	2.53	0.43
13:1:84:ALA:HA	13:1:113:VAL:HG21	2.00	0.43
5:E:160:LEU:HD13	5:E:163:THR:HB	2.00	0.43
1:A:200:SER:C	1:A:202:VAL:N	2.76	0.43
2:B:112:LEU:HD23	2:B:112:LEU:C	2.43	0.43
11:K:5:ALA:HA	11:K:13:ILE:O	2.18	0.43
13:M:112:TYR:HE1	13:M:127:THR:HG22	1.82	0.43
14:N:180:ALA:O	14:N:181:ALA:C	2.62	0.43
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.30	0.43
7:U:41:ARG:HG3	7:U:148:ILE:HD12	2.01	0.43
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.18	0.43
12:L:122:GLU:OE1	12:L:125:ARG:NH2	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:12:ASN:C	6:T:14:VAL:N	2.77	0.43
10:X:113:ILE:HA	10:X:118:THR:O	2.18	0.43
6:F:192:GLN:HE21	6:F:192:GLN:HA	1.83	0.43
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.67	0.43
13:1:205:GLY:HA3	13:1:209:GLN:HB3	2.00	0.43
5:E:109:VAL:HG12	5:E:149:LEU:HD22	2.01	0.43
5:S:198:SER:HA	5:S:201:LEU:HD12	2.00	0.43
6:T:12:ASN:ND2	6:T:126:TYR:O	2.52	0.43
9:W:152:PHE:HD1	9:W:177:ILE:HD11	1.82	0.43
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.18	0.43
3:Q:169:SER:HA	3:Q:172:VAL:HG13	2.00	0.43
4:R:67:ILE:HD12	4:R:211:GLN:HE21	1.83	0.43
10:X:143:ARG:O	10:X:146:MET:HG3	2.18	0.43
2:B:150:THR:O	2:B:157:TYR:HA	2.19	0.43
12:L:134:ILE:HD11	12:L:162:ALA:HB2	2.01	0.43
1:O:33:GLN:H	1:O:33:GLN:HG2	1.69	0.43
9:W:19:ARG:HB2	9:W:171:TRP:HB2	2.00	0.43
10:X:24:ILE:HD13	11:Y:132:THR:HG21	2.00	0.43
12:Z:-9:GLN:HE21	12:Z:-8:PHE:H	1.67	0.43
3:C:216:LYS:HB2	3:C:220:ASP:HB3	2.01	0.43
7:G:218:ASP:C	7:G:220:LYS:HA	2.43	0.43
10:J:-1:MET:HG3	10:J:1:ASP:HB2	2.01	0.43
12:L:114:ASP:CG	12:L:118:SER:HB3	2.44	0.43
2:P:141:TYR:CD1	2:P:219(A):VAL:HG21	2.54	0.43
8:H:223:ASP:N	8:H:223:ASP:OD2	2.52	0.42
13:M:40:ASN:N	13:M:40:ASN:ND2	2.67	0.42
5:S:226:GLY:O	5:S:229:VAL:HG22	2.19	0.42
6:T:95:GLU:HG2	6:T:115:ARG:CG	2.49	0.42
8:V:105:ASP:HB2	8:V:105(A):PRO:HD2	2.01	0.42
9:W:48:LEU:HG	9:W:50:THR:HG22	2.01	0.42
1:A:117:ALA:HB1	1:A:155:GLY:O	2.19	0.42
8:H:124:TYR:HB2	8:H:138:LEU:HD13	2.00	0.42
6:T:43:ASN:HD22	6:T:44:ASP:H	1.67	0.42
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.50	0.42
4:R:202:GLU:O	4:R:205:GLU:N	2.52	0.42
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.55	0.42
12:L:-7:ASN:ND2	12:L:-5:TYR:H	2.16	0.42
5:E:66:LYS:O	5:E:77:SER:HA	2.19	0.42
6:F:180(F):GLY:O	6:F:184:LEU:N	2.51	0.42
10:J:3:ILE:HD12	10:J:44:SER:HB2	2.01	0.42
3:Q:207:ALA:C	3:Q:209:ASN:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:209:GLU:HG3	4:R:226:ASN:HB3	2.01	0.42
6:T:126:TYR:HB2	6:T:129:VAL:HG22	2.01	0.42
11:Y:208:ASN:H	11:Y:208:ASN:ND2	2.17	0.42
12:Z:-9:GLN:HE21	12:Z:-8:PHE:N	2.18	0.42
10:J:57:GLU:OE1	11:K:81:LYS:NZ	2.48	0.42
2:P:78:VAL:HG22	2:P:136:PHE:HE2	1.84	0.42
10:X:178:VAL:HA	10:X:183:GLY:O	2.19	0.42
11:Y:87:VAL:CG1	11:Y:115:SER:HA	2.50	0.42
2:B:40:ILE:HD12	2:B:193:ALA:HB2	2.02	0.42
2:B:61:GLN:OE1	2:B:208:ASP:HA	2.20	0.42
3:C:169:SER:HA	3:C:172:VAL:HG13	2.01	0.42
6:F:121:GLN:HE21	6:F:121:GLN:HB3	1.70	0.42
8:H:100:ILE:HG13	8:H:127:LEU:HD12	2.01	0.42
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	2.02	0.42
3:Q:152:GLU:HB2	3:Q:153:PRO:CD	2.50	0.42
4:R:70:ILE:HD11	4:R:76:CYS:HB2	2.01	0.42
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.85	0.42
8:V:41:ILE:HG12	8:V:76:VAL:HG22	2.01	0.42
10:X:18:LYS:HD3	10:X:174:ILE:HG13	2.02	0.42
7:G:152:ASP:HB2	7:G:153:PRO:HD2	2.01	0.42
8:H:38:SER:HB2	8:H:39:PRO:HD2	2.01	0.42
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.83	0.42
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.55	0.42
14:2:38:HIS:O	14:2:39:ASP:C	2.63	0.42
5:E:226:GLY:O	5:E:229:VAL:HG22	2.20	0.42
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.19	0.42
6:T:206:LYS:C	6:T:206(B):LYS:H	2.28	0.42
9:W:51:ASP:OD2	10:X:90(B):ARG:NH2	2.53	0.42
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	2.00	0.42
5:E:134:VAL:O	5:E:153:PRO:HG3	2.20	0.42
3:C:82:ASN:HD22	3:C:82:ASN:N	2.17	0.41
1:O:78:TYR:HB3	1:O:85:TYR:CD1	2.55	0.41
13:1:40:ASN:H	13:1:40:ASN:HD22	1.68	0.41
2:P:148:LEU:HB3	2:P:160:TRP:O	2.19	0.41
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.86	0.41
10:J:181:ASP:C	10:J:183:GLY:CA	2.94	0.41
12:L:99:THR:HG23	12:L:113:PHE:HB2	2.02	0.41
6:F:126:TYR:HE1	7:G:129:MET:SD	2.44	0.41
13:M:141(C):ARG:HH11	13:M:141(C):ARG:CG	2.25	0.41
1:O:217(P):LYS:N	1:O:217(P):LYS:HE3	2.36	0.41
12:Z:39:ASP:OD2	12:Z:67:HIS:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:77:VAL:CG1	7:G:137:THR:HB	2.50	0.41
8:H:104:VAL:HG13	8:H:178:MET:HB3	2.03	0.41
2:P:125:GLN:HG3	3:Q:130:ARG:HG3	2.01	0.41
4:R:10:ARG:HD2	5:S:10:GLY:HA2	2.01	0.41
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.55	0.41
7:G:87:ASN:C	7:G:87:ASN:ND2	2.79	0.41
7:G:238:GLU:O	7:G:239:GLN:HB2	2.20	0.41
4:R:140:GLY:HA2	4:R:215:ILE:HG12	2.02	0.41
13:1:80:PHE:CZ	13:1:111:ARG:HG2	2.55	0.41
9:I:28:SER:CB	10:J:120:VAL:HG21	2.49	0.41
9:I:101:VAL:O	9:I:110:ILE:HA	2.20	0.41
1:O:77:VAL:HG22	1:O:78:TYR:H	1.85	0.41
5:S:114:HIS:HB3	6:T:86:ARG:NH2	2.36	0.41
7:U:47:VAL:HG22	7:U:214:VAL:HG22	2.01	0.41
4:D:90:GLU:OE2	11:K:69:ARG:NH1	2.53	0.41
5:E:28:LEU:HD12	5:E:153:PRO:HD2	2.03	0.41
3:Q:41:LYS:HA	3:Q:46:VAL:HA	2.02	0.41
7:U:49:ILE:HG13	7:U:212:VAL:HG22	2.02	0.41
9:W:181:LYS:N	9:W:181:LYS:HD2	2.36	0.41
12:Z:99:THR:HG23	12:Z:113:PHE:HB2	2.02	0.41
5:E:100:SER:O	5:E:104:ASN:HA	2.21	0.41
6:F:238:LYS:HB2	6:F:238:LYS:HE3	1.89	0.41
8:H:101:VAL:HG13	8:H:111:PHE:HB2	2.03	0.41
9:I:-7:ASP:HA	9:I:-6:PRO:HD3	1.94	0.41
14:N:14:LEU:O	14:N:175:MET:HA	2.21	0.41
1:O:150:GLN:O	1:O:157:TYR:HA	2.21	0.41
5:S:65:LYS:HE2	5:S:65:LYS:HB3	1.83	0.41
2:B:39:GLY:C	2:B:148:LEU:HD21	2.46	0.41
4:D:28:LEU:HA	4:D:31:ILE:HD12	2.02	0.41
11:K:63:CYS:SG	11:K:74:ILE:HG21	2.61	0.41
12:L:7:ALA:HB2	12:L:110:VAL:HG23	2.02	0.41
11:Y:97:MET:HG2	11:Y:115:SER:HB3	2.02	0.41
11:K:35:ILE:HG21	11:K:56:GLU:HB3	2.03	0.40
2:P:78:VAL:HG22	2:P:136:PHE:CE2	2.56	0.40
3:Q:163:GLN:NE2	3:Q:173:ARG:HE	2.13	0.40
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	2.03	0.40
12:Z:144(J):ASN:OD1	12:Z:144(J):ASN:C	2.63	0.40
2:B:177:GLN:HE21	2:B:177:GLN:HB2	1.64	0.40
10:J:21:THR:HG21	10:X:167:PRO:HB3	2.03	0.40
2:P:53:LYS:O	2:P:54:VAL:C	2.64	0.40
6:T:199:LEU:HD12	6:T:240:ILE:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:38:SER:HB2	8:V:39:PRO:HD2	2.03	0.40
10:X:166:MET:HA	10:X:167:PRO:HD3	1.88	0.40
6:F:12:ASN:OD1	6:F:124:THR:HA	2.22	0.40
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.56	0.40
5:S:82:ALA:N	5:S:83:PRO:CD	2.85	0.40
8:V:14:ILE:HD11	8:V:42:TRP:HB3	2.03	0.40
9:W:87:LEU:HD11	9:W:99:PRO:HG2	2.02	0.40
11:Y:4:LEU:HD13	11:Y:159:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/250 (98%)	239 (97%)	5 (2%)	2 (1%)	16	34
1	O	246/250 (98%)	234 (95%)	11 (4%)	1 (0%)	30	51
2	B	231/245 (94%)	222 (96%)	6 (3%)	3 (1%)	9	21
2	P	231/245 (94%)	219 (95%)	9 (4%)	3 (1%)	9	21
3	C	235/243 (97%)	229 (97%)	5 (2%)	1 (0%)	30	51
3	Q	235/243 (97%)	226 (96%)	7 (3%)	2 (1%)	14	30
4	D	232/250 (93%)	219 (94%)	11 (5%)	2 (1%)	14	30
4	R	234/250 (94%)	220 (94%)	13 (6%)	1 (0%)	30	51
5	E	223/234 (95%)	214 (96%)	7 (3%)	2 (1%)	14	30
5	S	227/234 (97%)	215 (95%)	10 (4%)	2 (1%)	14	30
6	F	231/248 (93%)	223 (96%)	8 (4%)	0	100	100
6	T	233/248 (94%)	225 (97%)	7 (3%)	1 (0%)	30	51
7	G	235/252 (93%)	227 (97%)	7 (3%)	1 (0%)	30	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	U	239/252 (95%)	233 (98%)	4 (2%)	2 (1%)	16	34
8	H	216/222 (97%)	209 (97%)	7 (3%)	0	100	100
8	V	216/222 (97%)	209 (97%)	5 (2%)	2 (1%)	14	30
9	I	196/205 (96%)	192 (98%)	4 (2%)	0	100	100
9	W	198/205 (97%)	191 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	186 (96%)	6 (3%)	1 (0%)	24	46
10	X	193/198 (98%)	184 (95%)	8 (4%)	1 (0%)	24	46
11	K	208/212 (98%)	201 (97%)	5 (2%)	2 (1%)	12	28
11	Y	208/212 (98%)	201 (97%)	7 (3%)	0	100	100
12	L	216/241 (90%)	210 (97%)	6 (3%)	0	100	100
12	Z	216/241 (90%)	209 (97%)	7 (3%)	0	100	100
13	1	225/266 (85%)	219 (97%)	6 (3%)	0	100	100
13	M	227/266 (85%)	217 (96%)	9 (4%)	1 (0%)	30	51
14	2	188/196 (96%)	184 (98%)	4 (2%)	0	100	100
14	N	190/196 (97%)	184 (97%)	6 (3%)	0	100	100
All	All	6168/6524 (94%)	5941 (96%)	197 (3%)	30 (0%)	24	46

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54	VAL
3	C	207	ALA
5	E	6	ASN
7	G	239	GLN
2	P	54	VAL
2	P	217	ALA
3	Q	202	GLN
5	S	203	ASP
1	A	5	THR
2	B	217	ALA
11	K	9	GLN
13	M	1	THR
2	P	218(B)	ASP
3	Q	207	ALA
5	S	6	ASN
1	A	167	LYS
2	B	218(C)	ASP

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Mol	Chain	Res	Type
5	E	203	ASP
11	K	180	GLU
4	D	123(E)	SER
8	V	171	SER
6	T	240	ILE
4	D	123(C)	GLY
4	R	123(E)	SER
7	U	239	GLN
1	O	56	SER
10	X	8	VAL
10	J	8	VAL
7	U	55	PRO
8	V	181	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	198 (95%)	11 (5%)	20	43
1	O	209/209 (100%)	194 (93%)	15 (7%)	13	30
2	B	195/204 (96%)	180 (92%)	15 (8%)	12	27
2	P	195/204 (96%)	178 (91%)	17 (9%)	9	21
3	C	213/215 (99%)	191 (90%)	22 (10%)	7	15
3	Q	213/215 (99%)	200 (94%)	13 (6%)	17	37
4	D	198/206 (96%)	184 (93%)	14 (7%)	13	31
4	R	198/206 (96%)	186 (94%)	12 (6%)	17	37
5	E	192/193 (100%)	176 (92%)	16 (8%)	10	23
5	S	192/193 (100%)	180 (94%)	12 (6%)	16	36
6	F	196/205 (96%)	176 (90%)	20 (10%)	7	15
6	T	196/205 (96%)	182 (93%)	14 (7%)	13	31
7	G	207/210 (99%)	191 (92%)	16 (8%)	12	27
7	U	207/210 (99%)	194 (94%)	13 (6%)	16	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	181/181 (100%)	170 (94%)	11 (6%)	17	37
8	V	181/181 (100%)	172 (95%)	9 (5%)	22	46
9	I	172/173 (99%)	168 (98%)	4 (2%)	44	71
9	W	172/173 (99%)	164 (95%)	8 (5%)	23	48
10	J	175/175 (100%)	166 (95%)	9 (5%)	21	45
10	X	175/175 (100%)	163 (93%)	12 (7%)	14	32
11	K	169/169 (100%)	159 (94%)	10 (6%)	18	38
11	Y	169/169 (100%)	159 (94%)	10 (6%)	18	38
12	L	185/201 (92%)	176 (95%)	9 (5%)	22	47
12	Z	185/201 (92%)	175 (95%)	10 (5%)	20	42
13	1	199/224 (89%)	189 (95%)	10 (5%)	22	46
13	M	199/224 (89%)	193 (97%)	6 (3%)	36	64
14	2	162/162 (100%)	157 (97%)	5 (3%)	35	63
14	N	162/162 (100%)	151 (93%)	11 (7%)	14	32
All	All	5306/5454 (97%)	4972 (94%)	334 (6%)	16	36

All (334) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	5	THR
1	A	33	GLN
1	A	62	GLU
1	A	64	LEU
1	A	65	SER
1	A	124	THR
1	A	158	PHE
1	A	203	GLU
1	A	222	ARG
1	A	236	LEU
2	B	58	LEU
2	B	59	LEU
2	B	61	GLN
2	B	67	LEU
2	B	91	THR
2	B	124	THR
2	B	150	THR

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Mol	Chain	Res	Type
2	B	177	GLN
2	B	185	LYS
2	B	186	VAL
2	B	192	LEU
2	B	198	SER
2	B	202	THR
2	B	225	LYS
2	B	232	ILE
3	C	25	GLU
3	C	33	ARG
3	C	40	VAL
3	C	44	ASN
3	C	52	ARG
3	C	57	LYS
3	C	63	THR
3	C	82	ASN
3	C	112	LEU
3	C	129	VAL
3	C	150	GLN
3	C	156	ILE
3	C	163	GLN
3	C	172	VAL
3	C	174	GLU
3	C	185	THR
3	C	187	GLU
3	C	202	GLN
3	C	215	VAL
3	C	226	SER
3	C	235	GLN
3	C	242	GLU
4	D	28	LEU
4	D	48	LEU
4	D	59	LEU
4	D	65	GLU
4	D	76	CYS
4	D	110	GLU
4	D	119	LEU
4	D	125	GLU
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	205	GLU

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Mol	Chain	Res	Type
4	D	215	ILE
4	D	237	LEU
5	E	12	THR
5	E	13	VAL
5	E	18	THR
5	E	28	LEU
5	E	58	LEU
5	E	76	LEU
5	E	149	LEU
5	E	189	LEU
5	E	207	LEU
5	E	207(B)	THR
5	E	207(C)	VAL
5	E	207(D)	ASP
5	E	207(E)	ASN
5	E	219	THR
5	E	222	THR
5	E	227	GLU
6	F	35	THR
6	F	36	THR
6	F	43	ASN
6	F	59	LEU
6	F	72	ARG
6	F	98	SER
6	F	105	THR
6	F	121	GLN
6	F	129	VAL
6	F	169	ARG
6	F	176	LEU
6	F	192	GLN
6	F	199	LEU
6	F	204	ASP
6	F	206	LYS
6	F	206(B)	GLU
6	F	206(C)	LYS
6	F	222	LYS
6	F	225	LYS
6	F	238	LYS
7	G	33	GLN
7	G	38	LEU
7	G	49	ILE
7	G	54	VAL

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Mol	Chain	Res	Type
7	G	87	ASN
7	G	119	LEU
7	G	124	THR
7	G	169	GLN
7	G	171	GLU
7	G	184	ASN
7	G	184(G)	GLU
7	G	184(H)	GLU
7	G	184(M)	SER
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	13	VAL
8	H	34	LEU
8	H	55	VAL
8	H	63	ILE
8	H	68	LEU
8	H	84	LYS
8	H	101	VAL
8	H	144	GLN
8	H	182	LYS
8	H	197	ARG
8	H	200	LYS
9	I	160	LEU
9	I	171	TRP
9	I	174	VAL
9	I	181	LYS
10	J	6	ILE
10	J	24	ILE
10	J	34	THR
10	J	35	ARG
10	J	52	THR
10	J	68	ILE
10	J	70	GLU
10	J	155	LEU
10	J	191	GLN
11	K	4	LEU
11	K	9	GLN
11	K	31	VAL
11	K	41	LEU
11	K	65	LEU
11	K	69	ARG

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Mol	Chain	Res	Type
11	K	73	ARG
11	K	87	VAL
11	K	99	THR
11	K	201	GLU
12	L	-9	GLN
12	L	4	LEU
12	L	14	LEU
12	L	25	SER
12	L	40	ASN
12	L	58	ARG
12	L	62	SER
12	L	99	THR
12	L	138	LEU
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	148	VAL
13	M	184	LEU
13	M	190	LEU
14	N	1	THR
14	N	20	THR
14	N	22	THR
14	N	31	THR
14	N	84	LYS
14	N	94	ASN
14	N	107	LYS
14	N	115	LEU
14	N	119	VAL
14	N	132	THR
14	N	178	LEU
1	O	4	MET
1	O	5	THR
1	O	33	GLN
1	O	46	VAL
1	O	47	VAL
1	O	62	GLU
1	O	64	LEU
1	O	87	VAL
1	O	111	LEU
1	O	124	THR
1	O	158	PHE
1	O	167	LYS

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Mol	Chain	Res	Type
1	O	170	VAL
1	O	222	ARG
1	O	223	LYS
2	P	13	THR
2	P	57	THR
2	P	58	LEU
2	P	61	GLN
2	P	64	THR
2	P	91	THR
2	P	110	GLU
2	P	124	THR
2	P	150	THR
2	P	170	SER
2	P	181	LYS
2	P	185	LYS
2	P	192	LEU
2	P	198	SER
2	P	202	THR
2	P	225	LYS
2	P	235	LYS
3	Q	25	GLU
3	Q	40	VAL
3	Q	43	LYS
3	Q	56	LEU
3	Q	63	THR
3	Q	66	LYS
3	Q	82	ASN
3	Q	100	ARG
3	Q	150	GLN
3	Q	156	ILE
3	Q	163	GLN
3	Q	172	VAL
3	Q	199	GLU
4	R	13	SER
4	R	48	LEU
4	R	52	LYS
4	R	59	LEU
4	R	65	GLU
4	R	119	LEU
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU

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Mol	Chain	Res	Type
4	R	215	ILE
4	R	237	LEU
4	R	238	LYS
5	S	12	THR
5	S	13	VAL
5	S	49	VAL
5	S	58	LEU
5	S	65	LYS
5	S	76	LEU
5	S	160	LEU
5	S	178	ARG
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU
5	S	222	THR
6	T	25	GLU
6	T	35	THR
6	T	36	THR
6	T	43	ASN
6	T	63	LYS
6	T	72	ARG
6	T	95	GLU
6	T	98	SER
6	T	127	ASN
6	T	169	ARG
6	T	176	LEU
6	T	187	ARG
6	T	192	GLN
6	T	225	LYS
7	U	38	LEU
7	U	48	VAL
7	U	49	ILE
7	U	57	LYS
7	U	87	ASN
7	U	119	LEU
7	U	124	THR
7	U	197	MET
7	U	203	THR
7	U	217	LYS
7	U	227	GLU
7	U	232	ARG
7	U	233	LEU

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Mol	Chain	Res	Type
8	V	13	VAL
8	V	34	LEU
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	144	GLN
8	V	149	GLU
8	V	153	LYS
8	V	222	CYS
9	W	-7	ASP
9	W	12	VAL
9	W	107	LYS
9	W	121	GLU
9	W	160	LEU
9	W	171	TRP
9	W	174	VAL
9	W	181	LYS
10	X	-1	MET
10	X	6	ILE
10	X	24	ILE
10	X	34	THR
10	X	48	GLU
10	X	52	THR
10	X	68	ILE
10	X	120	VAL
10	X	157	LEU
10	X	168	MET
10	X	189	ASP
10	X	191	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	41	LEU
11	Y	65	LEU
11	Y	69	ARG
11	Y	87	VAL
11	Y	145	ASP
11	Y	146	LEU
11	Y	156	LYS
11	Y	210	ILE
12	Z	-9	GLN
12	Z	2	THR
12	Z	4	LEU

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Mol	Chain	Res	Type
12	Z	14	LEU
12	Z	40	ASN
12	Z	99	THR
12	Z	106	GLU
12	Z	106(A)	ASP
12	Z	118	SER
12	Z	138	LEU
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	148	VAL
13	1	149	GLN
13	1	170	SER
13	1	184	LEU
13	1	190	LEU
13	1	203	ILE
13	1	204	LYS
14	2	22	THR
14	2	36	ARG
14	2	119	VAL
14	2	149	GLU
14	2	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (198) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
2	B	23	GLN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	82	ASN
3	C	121	GLN
3	C	150	GLN
3	C	163	GLN
3	C	235	GLN
4	D	23	GLN
4	D	108	ASN

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Mol	Chain	Res	Type
4	D	147	GLN
4	D	150	HIS
4	D	180(C)	HIS
4	D	199	GLN
4	D	226	ASN
5	E	6	ASN
5	E	7	ASN
5	E	64	GLN
5	E	73	HIS
5	E	104	ASN
5	E	121	GLN
5	E	125	GLN
5	E	152	GLN
5	E	185	ASN
5	E	207(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	192	GLN
7	G	33	GLN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
8	H	22	GLN
8	H	30	ASN
8	H	66	HIS
8	H	86	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
10	J	54	GLN
10	J	62	ASN
10	J	85	GLN
10	J	112	GLN

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Mol	Chain	Res	Type
10	J	186	GLN
11	K	9	GLN
11	K	85	ASN
11	K	131	GLN
11	K	141	ASN
11	K	174	ASN
11	K	189	ASN
11	K	207	ASN
11	K	208	ASN
12	L	-7	ASN
12	L	27	ASN
12	L	40	ASN
12	L	61	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	123	GLN
12	L	144(B)	ASN
12	L	144(I)	ASN
12	L	166	HIS
12	L	168	GLN
13	M	-7	GLN
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	105	GLN
13	M	149	GLN
13	M	157	ASN
13	M	181	ASN
14	N	69	GLN
14	N	141	ASN
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
2	P	95	HIS
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	147	GLN
2	P	173	GLN
2	P	177	GLN

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Mol	Chain	Res	Type
3	Q	23	GLN
3	Q	44	ASN
3	Q	82	ASN
3	Q	120	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	179	ASN
3	Q	209	ASN
3	Q	241	GLN
4	R	23	GLN
4	R	99	HIS
4	R	108	ASN
4	R	150	HIS
4	R	161	ASN
4	R	199	GLN
4	R	211	GLN
4	R	226	ASN
5	S	33	GLN
5	S	73	HIS
5	S	95	GLN
5	S	104	ASN
5	S	121	GLN
5	S	125	GLN
5	S	156	ASN
5	S	170	GLN
5	S	185	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	147	HIS
6	T	192	GLN
6	T	205	ASN
6	T	241	ASN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN

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Mol	Chain	Res	Type
7	U	170	GLN
7	U	178	ASN
7	U	182	HIS
8	V	30	ASN
8	V	35	HIS
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
8	V	220	ASN
9	W	29	ASN
9	W	56	ASN
9	W	64	ASN
9	W	81	GLN
10	X	9	GLN
10	X	36	GLN
10	X	54	GLN
10	X	62	ASN
10	X	77	GLN
10	X	85	GLN
10	X	96	GLN
10	X	112	GLN
10	X	141	HIS
10	X	186	GLN
10	X	191	GLN
10	X	193	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	174	ASN
11	Y	189	ASN
11	Y	207	ASN
11	Y	208	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70	HIS
12	Z	70(A)	ASN
12	Z	141	GLN
12	Z	144(B)	ASN

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Mol	Chain	Res	Type
12	Z	144(C)	GLN
12	Z	166	HIS
13	1	-7	GLN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN
13	1	191	GLN
14	2	38	HIS
14	2	69	GLN
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 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
17	MES	Y	213	-	12,12,12	2.40	1 (8%)	15,16,16	1.29	0
17	MES	K	214	-	12,12,12	2.30	1 (8%)	15,16,16	1.19	1 (6%)
16	L3T	K	213	-	49,49,49	2.11	4 (8%)	67,68,68	1.48	15 (22%)
16	L3T	Y	212	-	49,49,49	2.06	5 (10%)	67,68,68	1.57	12 (17%)

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
17	MES	Y	213	-	-	0/6/14/14	0/1/1/1
17	MES	K	214	-	-	3/6/14/14	0/1/1/1
16	L3T	K	213	-	-	0/43/43/43	0/4/4/4
16	L3T	Y	212	-	-	3/43/43/43	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	213	L3T	CL23-C18	12.78	1.74	1.51
16	Y	212	L3T	CL23-C18	12.33	1.74	1.51
17	Y	213	MES	C8-S	-8.10	1.66	1.77
17	K	214	MES	C8-S	-7.74	1.66	1.77
16	Y	212	L3T	C4-C10	3.96	1.53	1.45
16	Y	212	L3T	C5-C4	-3.91	1.38	1.45
16	K	213	L3T	C4-C10	3.85	1.53	1.45
16	K	213	L3T	C5-C4	-3.69	1.39	1.45
16	K	213	L3T	C3-C4	-2.69	1.34	1.38
16	Y	212	L3T	C3-C4	-2.45	1.34	1.38
16	Y	212	L3T	C1-N2	-2.10	1.34	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	212	L3T	C4-C10-C11	6.03	125.31	119.11
16	K	213	L3T	C5-C4-C3	5.38	109.12	106.15
16	Y	212	L3T	C5-C4-C3	4.93	108.87	106.15
16	K	213	L3T	C4-C10-C11	3.57	122.79	119.11
17	K	214	MES	O3S-S-C8	2.96	111.79	106.00
16	K	213	L3T	C9-C1-C5	-2.81	119.47	122.19
16	K	213	L3T	C33-N14-C32	2.81	123.29	116.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	212	L3T	C9-C1-C5	-2.76	119.52	122.19
16	Y	212	L3T	C6-C5-C1	2.74	121.68	118.84
16	K	213	L3T	C1-C5-C4	-2.70	104.89	106.62
16	Y	212	L3T	C33-N14-C32	2.69	123.01	116.86
16	Y	212	L3T	C25-C26-N29	-2.67	103.89	111.11
16	K	213	L3T	C4-C3-N2	-2.56	108.48	110.22
16	Y	212	L3T	C1-C5-C4	-2.40	105.08	106.62
16	Y	212	L3T	C34-C33-N14	-2.37	119.56	123.60
16	Y	212	L3T	C36-C35-N29	-2.33	111.65	116.63
16	K	213	L3T	C36-C35-N29	-2.31	111.69	116.63
16	Y	212	L3T	C4-C3-N2	-2.30	108.66	110.22
16	K	213	L3T	C6-C5-C1	2.28	121.20	118.84
16	K	213	L3T	C16-C17-C22	-2.23	116.05	120.98
16	K	213	L3T	C34-C33-N14	-2.22	119.80	123.60
16	Y	212	L3T	C17-C16-N15	-2.17	108.78	113.15
16	K	213	L3T	C30-C28-C26	-2.14	107.66	113.36
16	K	213	L3T	C31-C32-N14	-2.12	119.99	123.60
16	K	213	L3T	O13-C11-C10	-2.09	119.28	121.92
16	Y	212	L3T	O12-C10-C4	-2.05	118.09	122.48
16	K	213	L3T	C38-C36-C35	-2.05	105.73	110.57
16	K	213	L3T	C25-C26-N29	-2.02	105.65	111.11

There are no chirality outliers.

All (6) torsion outliers are listed below:

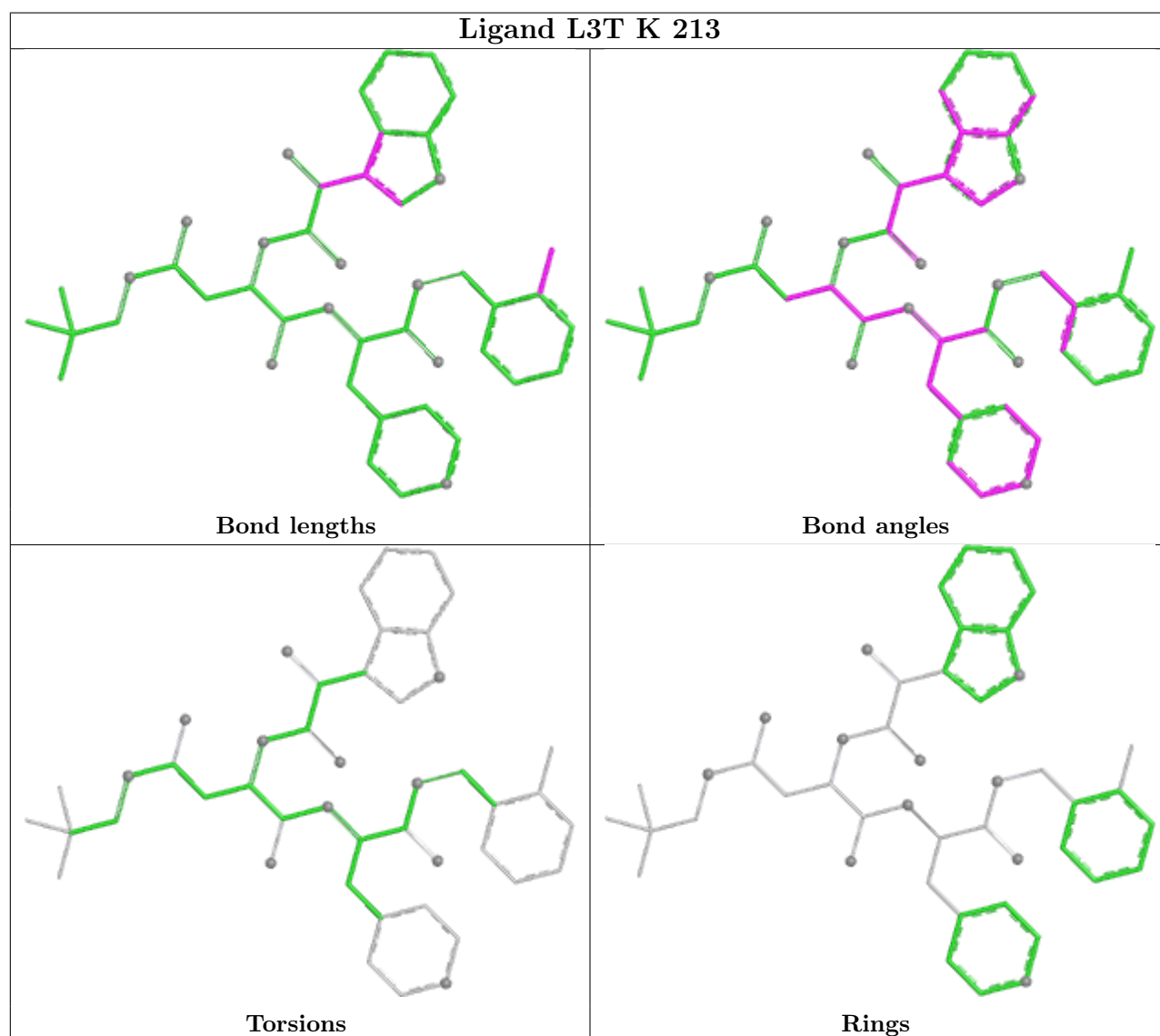
Mol	Chain	Res	Type	Atoms
17	K	214	MES	C7-C8-S-O2S
17	K	214	MES	C7-C8-S-O3S
16	Y	212	L3T	O12-C10-C4-C3
17	K	214	MES	C7-C8-S-O1S
16	Y	212	L3T	O12-C10-C4-C5
16	Y	212	L3T	C11-C10-C4-C3

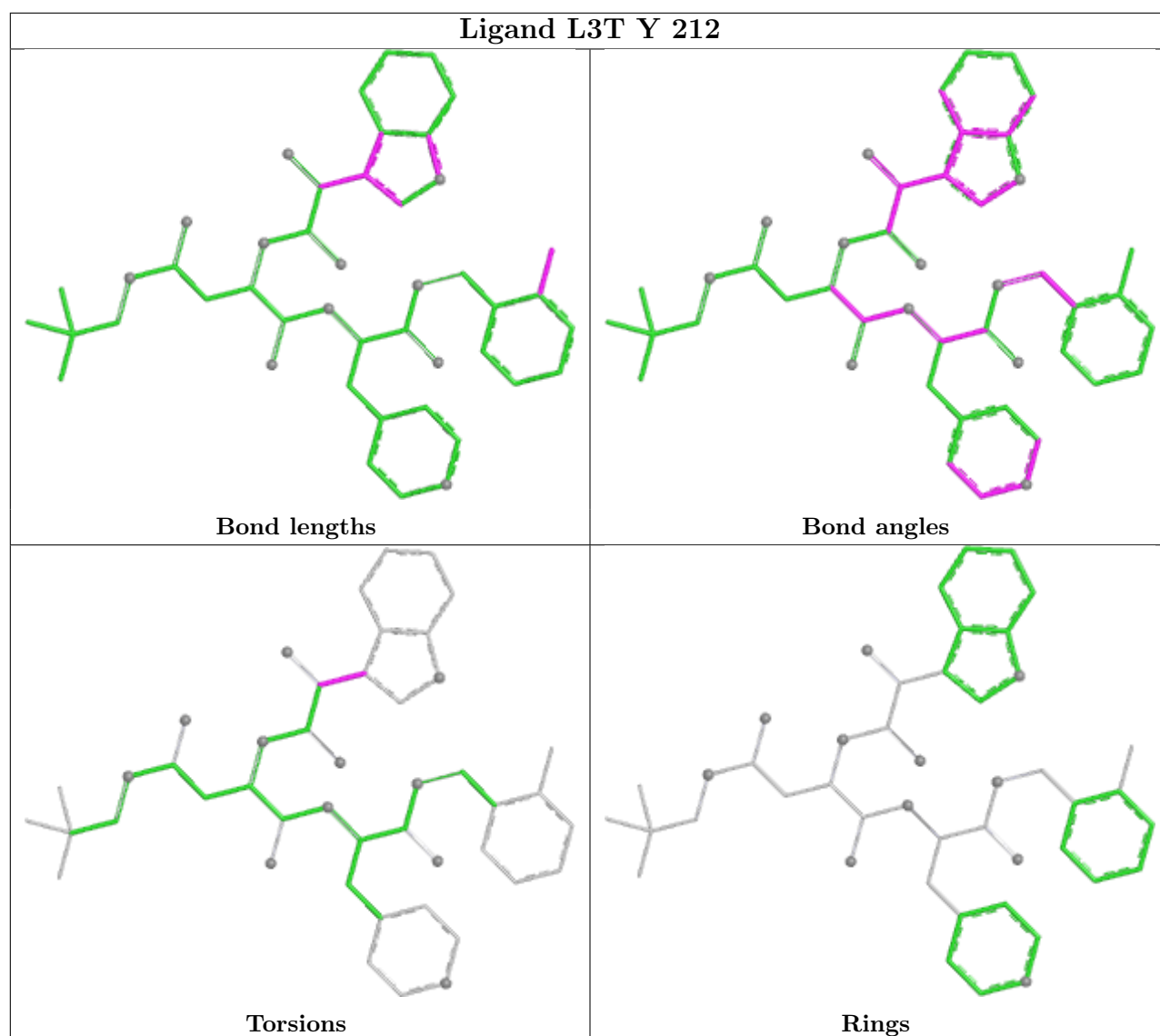
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	213	MES	1	0
16	K	213	L3T	4	0
16	Y	212	L3T	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	4
5	E	4
4	R	3
14	N	3
13	1	3

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Mol	Chain	Number of breaks
13	M	3
7	G	3
14	2	3
9	I	3
9	W	3
3	C	2
10	J	2
10	X	2
3	Q	2
6	F	2
5	S	2
12	L	2
8	V	2
12	Z	2
8	H	2
11	K	1
2	P	1
1	O	1
1	A	1
11	Y	1
6	T	1
7	U	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	123(G):GLU	C	125:GLU	N	4.17
1	R	123(G):GLU	C	125:GLU	N	4.03
1	C	203:THR	C	206:GLY	N	3.88
1	J	-1:MET	C	1:ASP	N	3.79
1	K	181:ASP	C	183:GLY	N	3.66
1	X	-1:MET	C	1:ASP	N	3.62
1	Q	180(D):GLU	C	182:PRO	N	3.35
1	F	180(F):GLY	C	184:LEU	N	3.23
1	S	204:GLU	C	206:SER	N	3.20
1	E	204:GLU	C	206:SER	N	3.18
1	Q	203:THR	C	206:GLY	N	3.16
1	D	233:ILE	C	235:LYS	N	3.10
1	C	180(D):GLU	C	182:PRO	N	3.07
1	N	181:ALA	C	183:GLY	N	3.04
1	1	181(A):THR	C	183:GLY	N	2.93
1	P	200:THR	C	202:THR	N	2.87

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	202:GLU	C	205:GLU	N	2.86
1	M	181(A):THR	C	183:GLY	N	2.85
1	E	207(E):ASN	C	210:LEU	N	2.84
1	G	180(D):ILE	C	184:ASN	N	2.83
1	O	200:SER	C	202:VAL	N	2.83
1	G	184(M):SER	C	186:TRP	N	2.81
1	A	200:SER	C	202:VAL	N	2.76
1	E	180(F):ILE	C	183:ASP	N	2.63
1	E	60:SER	C	63:TYR	N	2.62
1	F	199:LEU	C	201:ALA	N	2.61
1	D	180(E):SER	C	184:LEU	N	2.60
1	2	181:ALA	C	183:GLY	N	2.60
1	X	181:ASP	C	183:GLY	N	2.58
1	R	233:ILE	C	235:LYS	N	2.57
1	I	179:LYS	C	181:LYS	N	2.56
1	S	60:SER	C	63:TYR	N	2.55
1	Y	181:ASP	C	183:GLY	N	2.54
1	T	199:LEU	C	201:ALA	N	2.51
1	U	218:ASP	C	220:LYS	N	2.49
1	L	-1:GLY	C	1:GLY	N	2.45
1	2	92:ASP	C	94:ASN	N	2.44
1	D	202:GLU	C	205:GLU	N	2.43
1	J	181:ASP	C	183:GLY	N	2.43
1	V	91:GLN	C	93:GLY	N	2.43
1	Z	180:LYS	C	182:ASP	N	2.43
1	L	180:LYS	C	182:ASP	N	2.38
1	W	179:LYS	C	181:LYS	N	2.35
1	G	218:ASP	C	220:LYS	N	2.24
1	H	187:LEU	C	189:ARG	N	2.24
1	V	187:LEU	C	189:ARG	N	2.24
1	Z	-1:GLY	C	1:GLY	N	2.23
1	B	200:THR	C	202:THR	N	2.22
1	I	36:HIS	C	38:TYR	N	2.21
1	H	91:GLN	C	93:GLY	N	2.14
1	1	141(G):ILE	C	144:PRO	N	2.10
1	M	141(G):ILE	C	144:PRO	N	2.09
1	N	70:TYR	C	72:GLY	N	2.09
1	2	70:TYR	C	72:GLY	N	2.06
1	I	-1:GLY	C	1:GLY	N	2.04
1	W	-1:GLY	C	1:GLY	N	2.04
1	1	-1:GLY	C	1:THR	N	2.02
1	M	-1:GLY	C	1:THR	N	1.94

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	36:HIS	C	38:TYR	N	1.89
1	N	92:ASP	C	94:ASN	N	1.86

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%)	0.31	14 (5%) 30 24	27, 40, 61, 79	0
1	O	250/250 (100%)	0.57	22 (8%) 15 12	30, 45, 71, 82	0
2	B	235/245 (95%)	0.73	25 (10%) 11 9	27, 45, 72, 79	0
2	P	235/245 (95%)	0.73	27 (11%) 9 7	27, 47, 77, 81	0
3	C	241/243 (99%)	1.01	47 (19%) 3 2	29, 53, 92, 111	0
3	Q	241/243 (99%)	1.43	76 (31%) 1 1	33, 58, 102, 121	0
4	D	242/250 (96%)	0.78	28 (11%) 9 7	27, 47, 83, 90	0
4	R	242/250 (96%)	0.88	30 (12%) 8 6	27, 49, 81, 93	0
5	E	233/234 (99%)	0.71	19 (8%) 17 14	33, 47, 77, 86	0
5	S	233/234 (99%)	0.92	39 (16%) 4 3	32, 50, 78, 93	0
6	F	237/248 (95%)	0.48	15 (6%) 26 20	26, 43, 76, 86	0
6	T	237/248 (95%)	0.43	8 (3%) 48 42	26, 43, 67, 84	0
7	G	243/252 (96%)	0.26	13 (5%) 32 26	24, 39, 65, 86	0
7	U	243/252 (96%)	0.16	7 (2%) 53 48	24, 38, 58, 77	0
8	H	222/222 (100%)	0.08	7 (3%) 50 44	25, 34, 49, 74	0
8	V	222/222 (100%)	0.23	8 (3%) 46 40	28, 37, 52, 78	0
9	I	204/205 (99%)	-0.08	4 (1%) 65 60	23, 33, 45, 60	0
9	W	204/205 (99%)	0.06	4 (1%) 65 60	25, 35, 48, 64	0
10	J	198/198 (100%)	0.25	10 (5%) 33 28	28, 36, 52, 111	0
10	X	198/198 (100%)	0.27	11 (5%) 30 24	28, 38, 52, 120	0
11	K	212/212 (100%)	0.04	4 (1%) 66 61	23, 33, 49, 62	0
11	Y	212/212 (100%)	0.09	4 (1%) 66 61	25, 35, 51, 58	0
12	L	222/241 (92%)	0.11	4 (1%) 67 63	24, 35, 53, 60	0
12	Z	222/241 (92%)	0.04	4 (1%) 67 63	24, 34, 51, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	233/266 (87%)	-0.04	4 (1%) 69 64	22, 33, 47, 50	0
13	M	233/266 (87%)	0.08	4 (1%) 69 64	24, 35, 48, 52	0
14	2	196/196 (100%)	-0.05	2 (1%) 79 76	25, 32, 47, 63	0
14	N	196/196 (100%)	-0.02	4 (2%) 65 60	25, 32, 48, 59	0
All	All	6336/6524 (97%)	0.39	444 (7%) 22 18	22, 39, 74, 121	0

All (444) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	-1	MET	9.7
4	D	123(B)	GLU	9.7
13	M	-8	THR	9.4
2	B	217	ALA	9.0
10	J	-1	MET	8.5
3	Q	56	LEU	8.3
5	S	4	PHE	7.6
10	J	192	ALA	7.3
3	Q	55	THR	7.1
6	F	12	ASN	7.0
4	R	123(A)	GLY	6.8
4	R	123(E)	SER	6.8
3	C	7	GLY	6.7
4	R	123(D)	ALA	6.6
3	C	9	ASP	6.6
7	U	240	ASP	6.4
2	B	54	VAL	6.4
6	F	180(F)	GLY	6.3
4	R	123(C)	GLY	6.3
4	D	123(E)	SER	6.3
6	F	184	LEU	6.0
2	P	54	VAL	6.0
4	D	123(A)	GLY	5.9
3	Q	203	THR	5.8
6	T	12	ASN	5.8
1	O	4	MET	5.7
3	C	8	TYR	5.7
4	D	12	VAL	5.6
13	1	-8	THR	5.6
5	S	206	SER	5.5
4	R	126	ARG	5.4
4	D	123(D)	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
3	C	57	LYS	5.4
10	X	192	ALA	5.3
1	O	202	VAL	5.2
2	P	217	ALA	5.2
5	E	203	ASP	5.1
7	G	240	ASP	5.1
3	C	11	ALA	5.0
3	C	208	LYS	5.0
5	E	4	PHE	5.0
4	R	123(B)	GLU	5.0
11	K	208	ASN	4.9
4	D	127	LEU	4.9
3	C	55	THR	4.9
4	R	123(F)	GLY	4.9
7	G	6	ALA	4.9
4	D	10	ARG	4.8
6	T	240	ILE	4.8
3	C	56	LEU	4.8
10	X	191	GLN	4.8
4	R	123(G)	GLU	4.7
3	Q	54	SER	4.7
3	Q	58	LEU	4.7
3	C	207	ALA	4.6
4	R	11	GLY	4.6
2	B	218	ASN	4.6
6	F	201	ALA	4.6
1	O	6	ASP	4.6
3	C	206	GLY	4.6
12	Z	144(J)	ASN	4.6
3	Q	57	LYS	4.6
11	K	210	ILE	4.5
4	R	127	LEU	4.5
1	A	5	THR	4.5
5	E	207(E)	ASN	4.5
4	R	9	ASP	4.5
3	Q	64	PRO	4.4
3	Q	59	GLN	4.4
4	D	123(C)	GLY	4.4
10	J	168	MET	4.4
3	Q	208	LYS	4.4
3	C	209	ASN	4.4
6	T	13	SER	4.4

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Mol	Chain	Res	Type	RSRZ
5	S	203	ASP	4.4
4	R	10	ARG	4.4
5	S	63	TYR	4.4
1	A	4	MET	4.4
2	P	218	ASN	4.3
4	D	123(G)	GLU	4.3
3	Q	207	ALA	4.2
1	O	5	THR	4.2
3	Q	201	VAL	4.1
1	A	217	ASP	4.1
7	G	236	ILE	4.1
3	Q	240	LYS	4.1
2	P	239	THR	4.1
4	D	123	PHE	4.0
2	B	216(B)	GLY	3.9
7	U	218	ASP	3.9
3	Q	198	LEU	3.9
2	B	239	THR	3.9
8	V	223	ASP	3.9
12	Z	144(R)	LYS	3.9
3	Q	236	ILE	3.8
3	Q	185	THR	3.8
1	O	217(O)	ASP	3.8
4	D	9	ASP	3.8
7	U	199	ASP	3.8
3	Q	200	VAL	3.7
6	T	199	LEU	3.7
10	J	193	GLN	3.7
5	S	209	ASN	3.7
3	C	58	LEU	3.7
3	Q	62(A)	ILE	3.7
7	U	6	ALA	3.6
10	J	191	GLN	3.6
6	F	13	SER	3.6
1	A	235	ALA	3.6
3	Q	182	PRO	3.6
2	P	63	THR	3.5
3	Q	222	VAL	3.5
5	E	207(C)	VAL	3.5
5	S	10	GLY	3.5
2	B	64	THR	3.5
3	Q	232	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
7	G	8	TYR	3.5
2	B	62	ASP	3.5
3	C	185	THR	3.5
1	A	200	SER	3.5
3	Q	196	SER	3.5
5	S	55	ALA	3.5
3	Q	7	GLY	3.4
3	Q	184	ALA	3.4
5	E	206	SER	3.4
6	F	206	LYS	3.4
7	G	237	ALA	3.4
8	V	221	ILE	3.4
3	Q	224	LEU	3.4
4	D	123(F)	GLY	3.4
5	S	57	GLU	3.4
5	S	56	ASP	3.4
2	P	216(B)	GLY	3.4
10	X	188	ASP	3.4
4	D	235	LYS	3.4
2	B	55	THR	3.4
2	P	59	LEU	3.4
3	Q	63	THR	3.4
1	O	7	ARG	3.4
3	Q	229	ILE	3.4
4	D	126	ARG	3.4
6	F	204	ASP	3.3
13	M	61	ASP	3.3
2	P	57	THR	3.3
2	P	64	THR	3.3
3	Q	233	VAL	3.3
1	O	235	ALA	3.3
2	B	63	THR	3.3
2	B	127	GLY	3.3
8	V	182	LYS	3.3
3	C	53	ARG	3.3
3	Q	61	THR	3.3
2	B	218(D)	GLY	3.3
5	S	195	GLU	3.3
6	F	240	ILE	3.3
3	Q	8	TYR	3.3
5	E	5	ARG	3.3
3	Q	209	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
8	V	222	CYS	3.2
2	P	13	THR	3.2
4	D	11	GLY	3.2
5	S	5	ARG	3.2
1	A	203	GLU	3.2
4	R	123	PHE	3.2
5	E	207	LEU	3.2
3	Q	238	GLN	3.1
3	C	12	LEU	3.1
3	Q	40	VAL	3.1
3	Q	210	ILE	3.1
5	S	12	THR	3.1
3	Q	231	GLN	3.1
10	X	193	GLN	3.1
3	C	54	SER	3.1
6	T	22	PHE	3.1
11	Y	210	ILE	3.1
1	O	217(P)	LYS	3.0
2	B	57	THR	3.0
5	S	204	GLU	3.0
10	J	190	PHE	3.0
12	L	194	ASP	3.0
3	Q	206	GLY	3.0
12	L	144(K)	LYS	3.0
3	C	203	THR	3.0
4	R	243	ALA	3.0
10	X	49	ALA	3.0
2	B	61	GLN	3.0
8	H	221	ILE	3.0
3	Q	53	ARG	3.0
11	Y	211	GLY	3.0
3	C	233	VAL	3.0
3	Q	223	ALA	3.0
4	D	122	ARG	3.0
2	P	223	ILE	2.9
3	C	201	VAL	2.9
3	Q	211	GLU	2.9
3	Q	237	GLU	2.9
1	O	233	LEU	2.9
3	C	232	TYR	2.9
3	Q	226	SER	2.9
3	Q	44	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	14	ILE	2.9
5	S	208(A)	VAL	2.9
1	A	7	ARG	2.9
6	F	205	ASN	2.9
6	T	203	GLU	2.9
6	F	202	HIS	2.9
2	B	216(A)	LYS	2.9
5	S	32	LYS	2.9
4	D	61	SER	2.9
7	G	184(M)	SER	2.9
3	Q	190	VAL	2.9
7	U	239	GLN	2.9
12	Z	-9	GLN	2.9
4	D	241	GLU	2.9
1	O	55	SER	2.8
3	Q	65	SER	2.8
3	C	229	ILE	2.8
3	Q	186	VAL	2.8
3	Q	217	PRO	2.8
3	C	235	GLN	2.8
4	R	242	ALA	2.8
6	T	206	LYS	2.8
5	S	126	SER	2.8
3	Q	194	VAL	2.8
6	F	203	GLU	2.8
9	W	181	LYS	2.8
14	N	116	GLY	2.8
4	D	13	SER	2.8
2	B	13	THR	2.8
10	X	189	ASP	2.8
3	C	241	GLN	2.7
2	P	218(C)	GLY	2.7
2	P	55	THR	2.7
5	E	204	GLU	2.7
3	C	202	GLN	2.7
2	P	63(A)	SER	2.7
3	Q	66	LYS	2.7
1	O	236	LEU	2.7
4	R	12	VAL	2.7
5	S	198	SER	2.7
4	D	125	GLU	2.7
5	E	192	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
5	S	33	GLN	2.7
4	R	192	LEU	2.6
3	Q	180(D)	GLU	2.6
2	B	22	TYR	2.6
2	P	220	TYR	2.6
8	H	120	ASP	2.6
1	A	217(P)	LYS	2.6
1	O	53	LYS	2.6
3	C	242	GLU	2.6
4	D	239	GLU	2.6
3	Q	225	SER	2.6
5	S	199	GLN	2.6
7	G	7	GLY	2.6
14	2	183	GLY	2.6
3	Q	212	ILE	2.6
8	V	53	GLU	2.6
2	P	61	GLN	2.6
2	P	202	THR	2.6
3	Q	180	TYR	2.6
4	R	238	LYS	2.6
9	I	122(A)	LYS	2.6
5	S	178	ARG	2.6
3	C	211	GLU	2.6
5	E	189	LEU	2.6
2	B	204(A)	SER	2.6
9	W	122(A)	LYS	2.6
1	A	6	ASP	2.5
1	O	203	GLU	2.5
2	P	219(A)	VAL	2.5
3	C	230	ASN	2.5
5	E	33	GLN	2.5
4	D	238	LYS	2.5
2	P	22	TYR	2.5
13	1	61	ASP	2.5
3	C	174	GLU	2.5
6	T	206(A)	GLU	2.5
3	Q	22	PHE	2.5
7	G	179(C)	LYS	2.5
2	P	56	SER	2.5
3	Q	193	THR	2.5
7	G	174	THR	2.5
2	P	218(B)	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
3	Q	218	ASP	2.5
5	S	208(B)	ASP	2.5
10	X	10	ASP	2.5
3	C	240	LYS	2.5
2	P	204(A)	SER	2.5
1	A	234	GLU	2.5
3	C	187	GLU	2.5
3	Q	144(A)	ASP	2.5
5	S	127	TYR	2.5
8	V	145	ASP	2.5
1	O	64	LEU	2.5
3	Q	170	LYS	2.5
7	G	233	LEU	2.5
3	C	226	SER	2.5
4	R	13	SER	2.5
3	C	180(D)	GLU	2.4
3	C	188	GLU	2.4
4	R	205	GLU	2.4
2	B	220	TYR	2.4
3	C	236	ILE	2.4
10	J	189	ASP	2.4
11	Y	145	ASP	2.4
5	S	6	ASN	2.4
13	I	29	ASN	2.4
3	Q	234	THR	2.4
11	K	183	GLY	2.4
3	Q	9	ASP	2.4
1	A	236	LEU	2.4
10	X	187	VAL	2.4
5	S	172	ALA	2.4
9	W	-8	SER	2.4
3	C	210	ILE	2.4
3	Q	50	CYS	2.4
14	N	92	ASP	2.4
12	L	144(P)	LEU	2.4
4	D	242	ALA	2.4
2	B	202	THR	2.4
4	D	244	GLU	2.4
6	F	206(B)	GLU	2.4
9	I	-8	SER	2.4
3	C	52	ARG	2.4
8	V	197	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
4	R	158	TYR	2.4
2	B	234	VAL	2.4
6	F	206(C)	LYS	2.4
3	Q	187	GLU	2.4
5	S	60	SER	2.3
5	S	171	GLY	2.3
8	H	223	ASP	2.3
3	Q	215	VAL	2.3
4	R	235	LYS	2.3
3	Q	239	GLU	2.3
9	I	121	GLU	2.3
10	J	49	ALA	2.3
5	E	12	THR	2.3
2	P	238	ILE	2.3
3	Q	197	LEU	2.3
5	S	51	LEU	2.3
7	G	218	ASP	2.3
11	Y	105(B)	LYS	2.3
7	U	8	TYR	2.3
4	D	231	GLU	2.3
3	C	223	ALA	2.3
1	A	9	SER	2.3
3	Q	243	GLN	2.3
4	R	237	LEU	2.3
5	S	189	LEU	2.3
7	G	235	ALA	2.3
14	N	181	ALA	2.3
2	P	20	ARG	2.3
3	Q	202	GLN	2.3
5	E	199	GLN	2.3
1	O	61	SER	2.3
4	R	239	GLU	2.3
4	R	122	ARG	2.3
4	D	243	ALA	2.2
3	C	63	THR	2.2
3	Q	192	LEU	2.2
5	E	198	SER	2.2
10	X	190	PHE	2.2
8	H	219	VAL	2.2
1	A	8	TYR	2.2
4	R	168	GLY	2.2
4	R	240	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	26	TYR	2.2
5	S	52	LYS	2.2
5	S	65	LYS	2.2
4	D	237	LEU	2.2
10	J	24	ILE	2.2
4	R	244	GLU	2.2
3	C	183	PRO	2.2
3	Q	183	PRO	2.2
2	B	219(E)	VAL	2.2
7	G	129	MET	2.2
1	O	217(N)	THR	2.2
3	C	234	THR	2.2
3	Q	189	CYS	2.2
5	S	201	LEU	2.2
11	K	211	GLY	2.2
13	M	11	GLY	2.2
14	2	187(J)	LEU	2.2
5	S	197	ILE	2.2
1	A	55	SER	2.2
1	O	54	SER	2.2
3	Q	214	VAL	2.1
5	S	54	ASN	2.1
2	P	232	ILE	2.1
5	E	180(F)	ILE	2.1
8	V	218	ILE	2.1
8	H	222	CYS	2.1
9	W	121	GLU	2.1
2	B	63(A)	SER	2.1
8	H	145	ASP	2.1
5	S	49	VAL	2.1
1	O	59	ALA	2.1
6	F	43	ASN	2.1
2	B	59	LEU	2.1
3	C	49	GLY	2.1
3	C	224	LEU	2.1
5	S	233	ILE	2.1
3	Q	52	ARG	2.1
10	J	10	ASP	2.1
2	P	53	LYS	2.1
3	Q	175	PHE	2.1
10	X	183	GLY	2.1
13	1	30	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	202	ARG	2.1
1	O	199	GLU	2.1
9	I	181	LYS	2.1
3	C	16	SER	2.1
3	Q	16	SER	2.1
3	C	243	GLN	2.1
5	S	58	LEU	2.1
5	E	128	GLY	2.1
5	S	174	THR	2.1
3	C	221	ILE	2.1
5	S	9	ASP	2.1
13	M	105(A)	SER	2.1
3	Q	38	VAL	2.0
5	E	7	ASN	2.0
12	Z	144(Q)	LEU	2.0
3	Q	180(C)	LYS	2.0
12	L	144(Q)	LYS	2.0
1	O	8	TYR	2.0
1	O	65	SER	2.0
4	R	57	PRO	2.0
5	S	200	SER	2.0
7	U	129	MET	2.0
3	C	215	VAL	2.0
3	Q	172	VAL	2.0
3	Q	180(B)	ARG	2.0
8	H	197	ARG	2.0
1	O	110	LYS	2.0
2	B	53	LYS	2.0
5	E	129	GLY	2.0
6	F	241	ASN	2.0
2	P	158	THR	2.0
2	B	182	ASP	2.0
4	R	62	ASP	2.0
14	N	105(A)	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

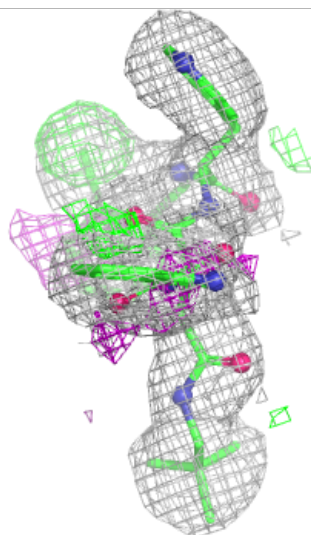
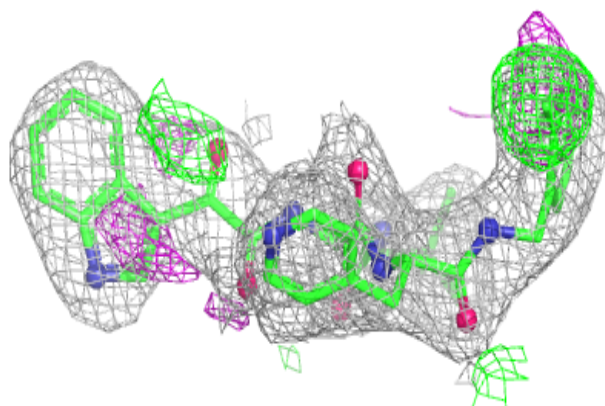
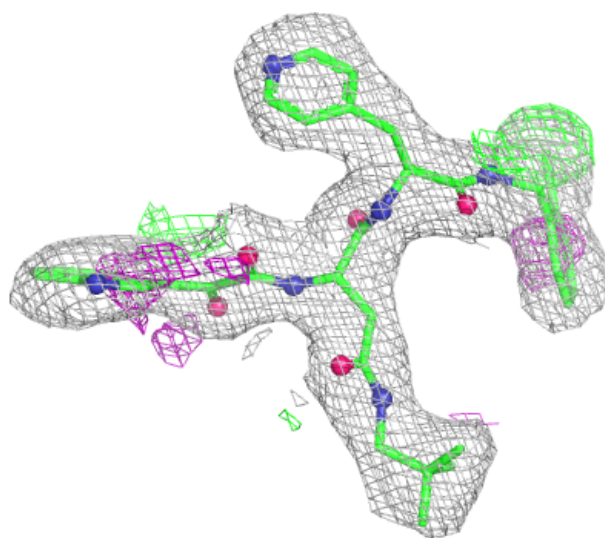
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	I	195	1/1	0.56	0.26	54,54,54,54	0
15	MG	L	195	1/1	0.65	0.18	48,48,48,48	0
15	MG	L	196	1/1	0.78	0.15	50,50,50,50	0
15	MG	F	243	1/1	0.84	0.31	121,121,121,121	0
16	L3T	Y	212	46/46	0.87	0.14	33,37,51,52	0
15	MG	I	196	1/1	0.88	0.11	43,43,43,43	0
16	L3T	K	213	46/46	0.90	0.13	33,36,51,52	0
15	MG	K	212	1/1	0.90	0.08	39,39,39,39	0
15	MG	N	188	1/1	0.93	0.08	36,36,36,36	0
15	MG	F	242	1/1	0.94	0.14	67,67,67,67	0
17	MES	K	214	12/12	0.96	0.13	55,56,57,57	0
17	MES	Y	213	12/12	0.96	0.13	58,59,60,60	0
15	MG	G	241	1/1	0.97	0.05	39,39,39,39	0
15	MG	H	224	1/1	0.97	0.10	44,44,44,44	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

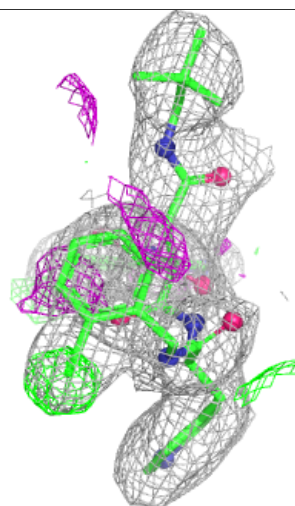
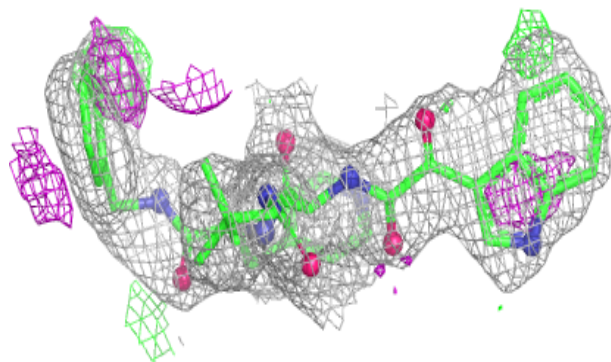
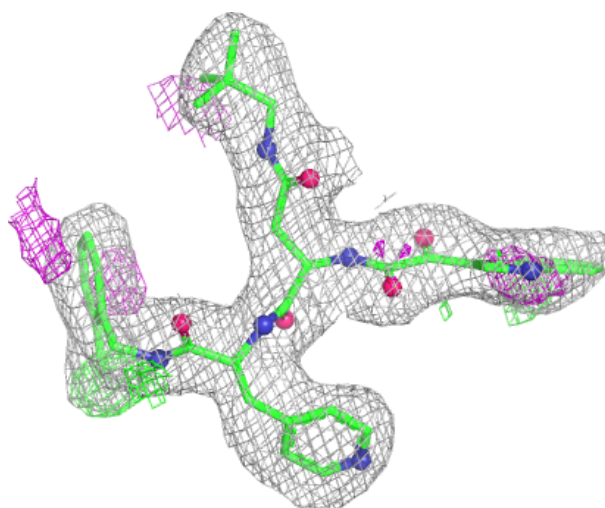
Electron density around L3T Y 212:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around L3T K 213:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.