



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:29 AM UTC

PDB ID : 4EU2 / pdb_00004eu2
Title : Crystal structure of 20s proteasome with novel inhibitor K-7174
Authors : Kikuchi, J.; Shibayama, N.; Yamada, S.; Wada, T.; Nobuyoshi, M.; Izumi, T.; Akutsu, M.; Kano, Y.; Ohki, M.; Sugiyama, K.; Park, S.-Y.; Furukawa, Y.
Deposited on : 2012-04-25
Resolution : 2.51 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

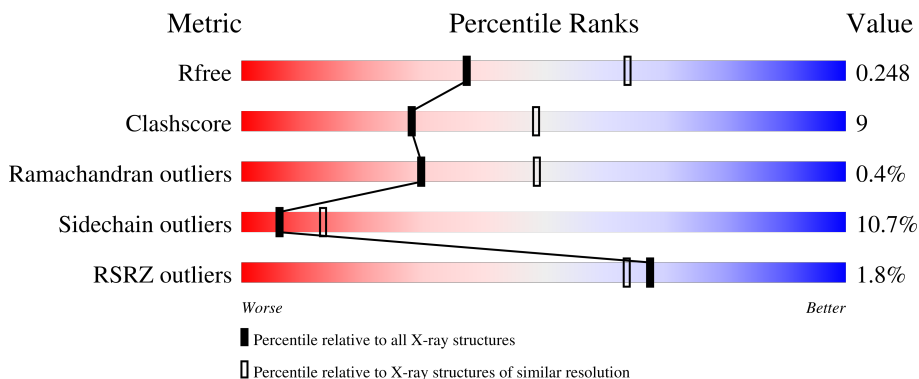
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	241	
1	O	241	
2	B	250	
2	P	250	
3	C	244	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	244	3% 71% 25% 5%
4	D	241	4% 73% 24% .
4	R	241	7% 68% 27% 5%
5	E	242	3% 70% 25% 5%
5	S	242	5% 69% 25% 6%
6	F	233	% 69% 27% .
6	T	233	4% 61% 32% 6%
7	G	244	% 73% 24% .
7	U	244	3% 72% 23% 5%
8	H	196	72% 24% .
8	V	196	77% 21% .
9	I	222	% 79% 21%
9	W	222	% 69% 26% 5%
10	J	204	77% 20% .
10	X	204	% 80% 18% .
11	K	198	% 74% 23% ..
11	Y	198	% 76% 19% 5% .
12	L	212	83% 14% .
12	Z	212	86% 10% .
13	1	222	73% 23% .
13	M	222	76% 23% .
14	2	233	73% 24% .
14	N	233	77% 20% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	WPI	I	301	-	X	-	-
15	WPI	Z	301	-	X	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50701 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 C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	241	Total	C	N	O	S	0	0	0
			1903	1212	319	364	8			
1	O	241	Total	C	N	O	S	0	0	0
			1903	1212	319	364	8			

- Molecule 2 is a protein called Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	249	Total	C	N	O	S	0	0	0
			1906	1213	314	375	4			
2	P	249	Total	C	N	O	S	0	0	0
			1906	1213	314	375	4			

- Molecule 3 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			
3	Q	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			

- Molecule 4 is a protein called Proteasome component PRE6.

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

- Molecule 5 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
5	S	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

- Molecule 6 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	232	Total	C	N	O	S	0	0	0
			1784	1120	311	349	4			
6	T	232	Total	C	N	O	S	0	0	0
			1784	1120	311	349	4			

- Molecule 7 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
7	U	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

- Molecule 8 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
8	V	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 9 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
9	W	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 10 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	X	204	1581	1010	258	305	8	0	0	0

- Molecule 11 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	196	1570	997	266	301	6	0	0	0
11	Y	196	1570	997	266	301	6	0	0	0

- Molecule 12 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	212	1646	1045	282	312	7	0	0	0
12	Z	212	1646	1045	282	312	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	33	ARG	LYS	conflict	UNP P30656
Z	33	ARG	LYS	conflict	UNP P30656

- Molecule 13 is a protein called Proteasome component C5.

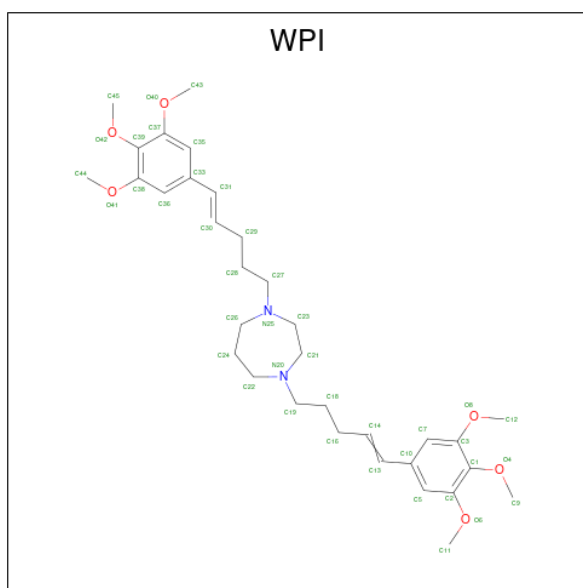
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	222	1757	1115	303	335	4	0	0	0
13	1	222	1757	1115	303	335	4	0	0	0

- Molecule 14 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	233	1824	1154	312	351	7	0	0	0
14	2	233	1824	1154	312	351	7	0	0	0

- Molecule 15 is 1,4-bis[(4E)-5-(3,4,5-trimethoxyphenyl)pent-4-en-1-yl]-1,4-diazepane (CCD

ID: WPI (formula: C₃₃H₄₈N₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
15	H	1	Total	C	N	O	0	0
			41	33	2	6		
15	I	1	Total	C	N	O	0	0
			41	33	2	6		
15	L	1	Total	C	N	O	0	0
			41	33	2	6		
15	V	1	Total	C	N	O	0	0
			41	33	2	6		
15	W	1	Total	C	N	O	0	0
			41	33	2	6		
15	Z	1	Total	C	N	O	0	0
			41	33	2	6		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	47	Total	O	0	0
			47	47		
16	B	27	Total	O	0	0
			27	27		
16	C	34	Total	O	0	0
			34	34		
16	D	35	Total	O	0	0
			35	35		
16	E	30	Total	O	0	0
			30	30		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	F	18	Total O 18 18	0	0
16	G	36	Total O 36 36	0	0
16	H	34	Total O 34 34	0	0
16	I	29	Total O 29 29	0	0
16	J	47	Total O 47 47	0	0
16	K	34	Total O 34 34	0	0
16	L	46	Total O 46 46	0	0
16	M	51	Total O 51 51	0	0
16	N	44	Total O 44 44	0	0
16	O	33	Total O 33 33	0	0
16	P	32	Total O 32 32	0	0
16	Q	33	Total O 33 33	0	0
16	R	18	Total O 18 18	0	0
16	S	23	Total O 23 23	0	0
16	T	19	Total O 19 19	0	0
16	U	38	Total O 38 38	0	0
16	V	47	Total O 47 47	0	0
16	W	36	Total O 36 36	0	0
16	X	36	Total O 36 36	0	0
16	Y	49	Total O 49 49	0	0
16	Z	41	Total O 41 41	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	1	41	Total O 41 41	0	0
16	2	51	Total O 51 51	0	0

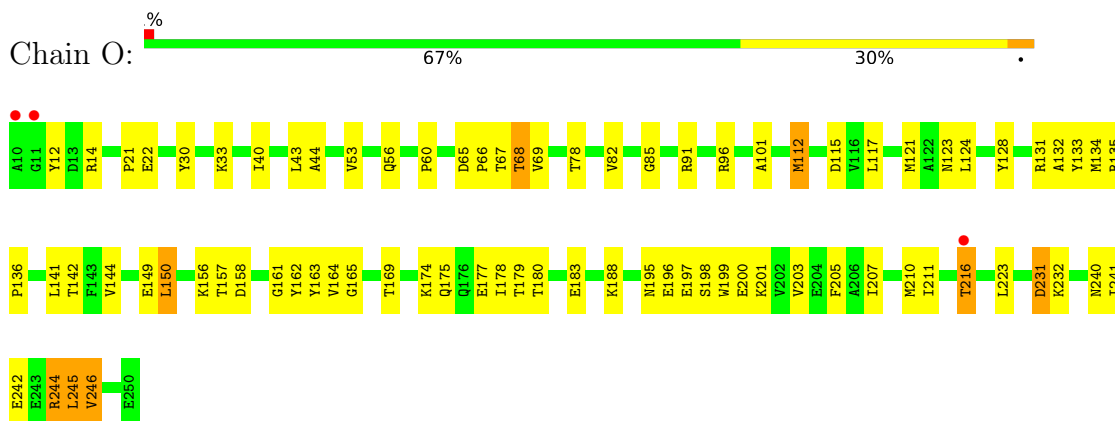
3 Residue-property plots [i](#)

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

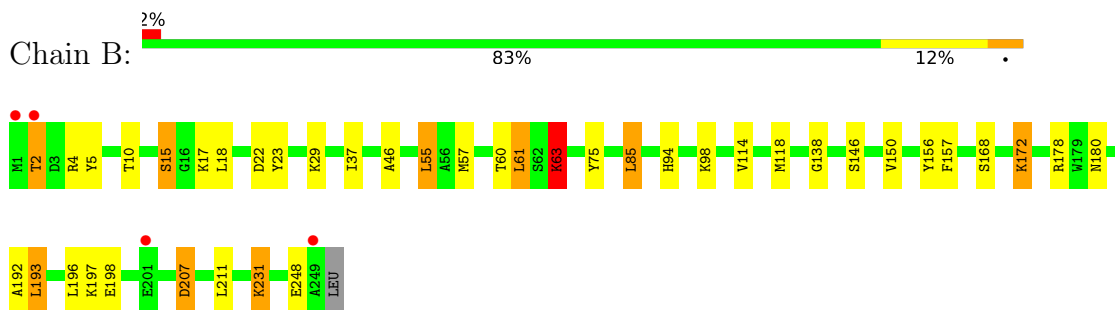
- Molecule 1: Proteasome component C7-alpha



- Molecule 1: Proteasome component C7-alpha



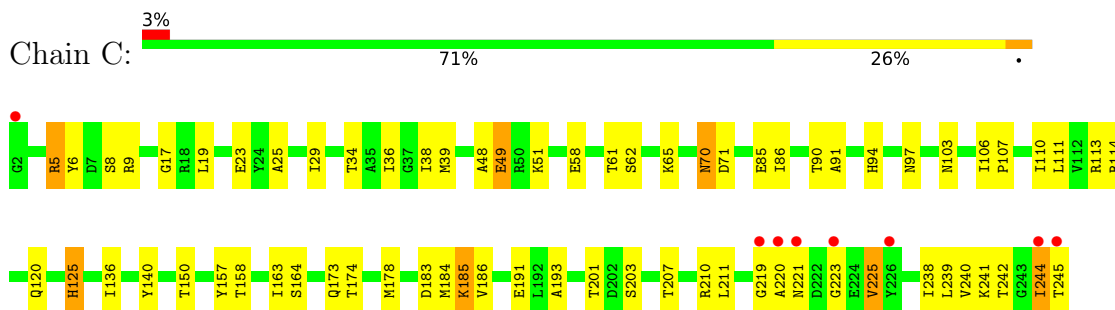
- Molecule 2: Proteasome component Y7



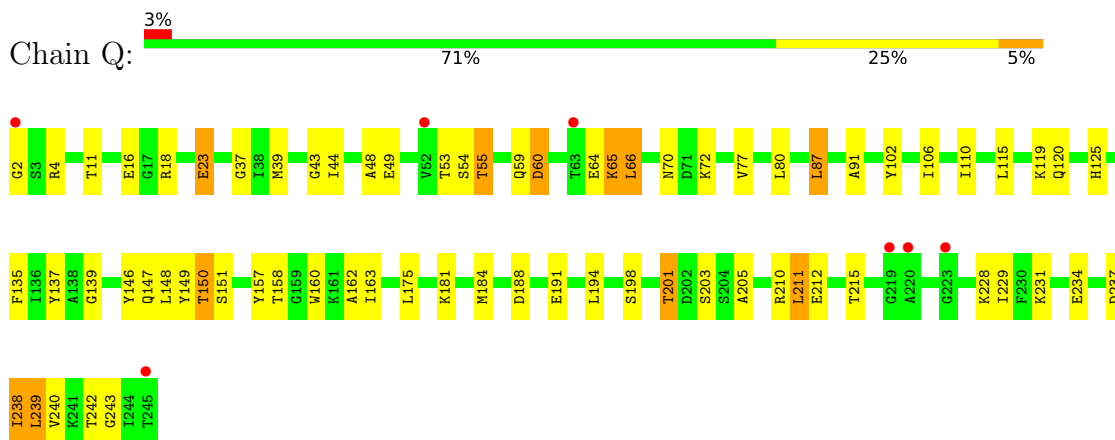
- Molecule 2: Proteasome component Y7



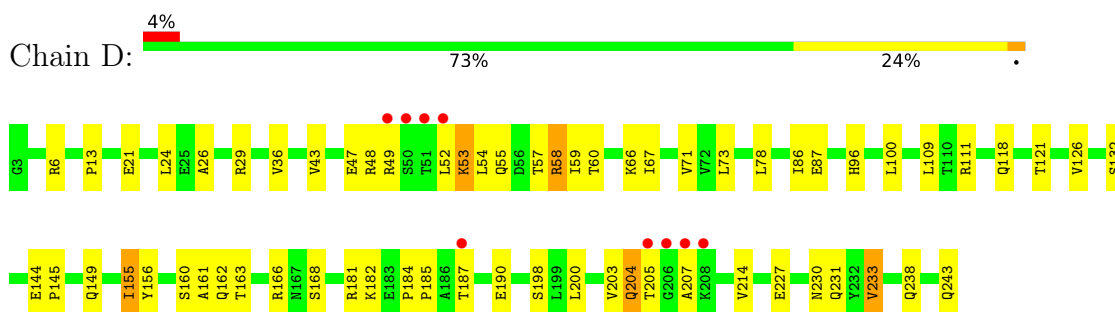
- Molecule 3: Proteasome component Y13



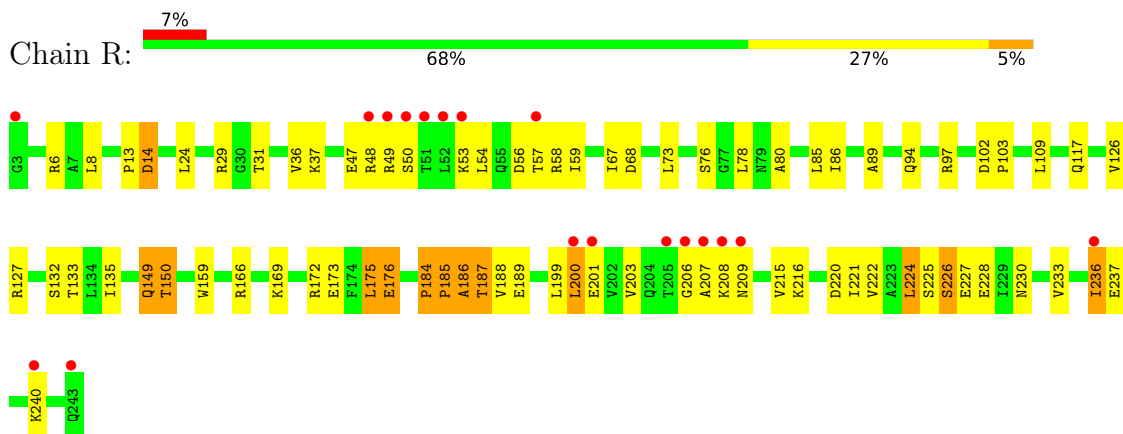
- Molecule 3: Proteasome component Y13



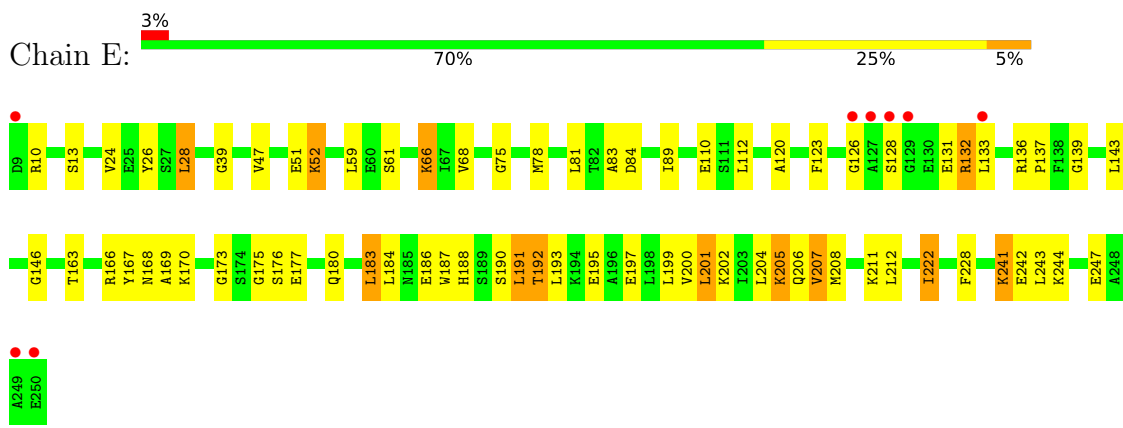
- Molecule 4: Proteasome component PRE6



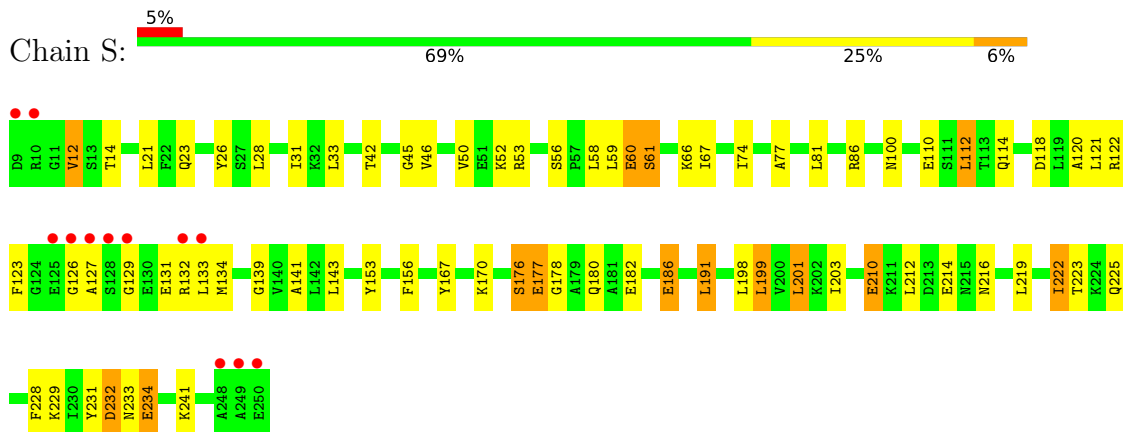
- Molecule 4: Proteasome component PRE6



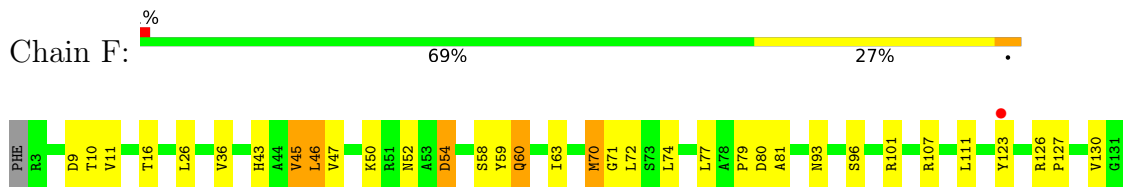
• Molecule 5: Proteasome component PUP2

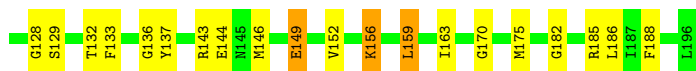


• Molecule 5: Proteasome component PUP2

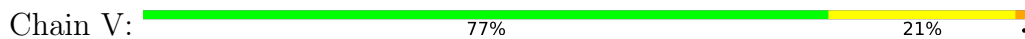


• Molecule 6: Proteasome component PRE5

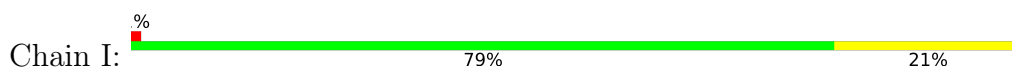




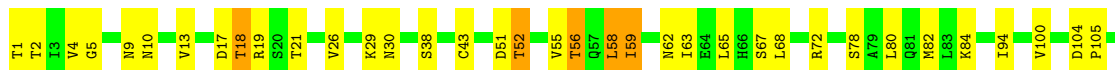
- Molecule 8: Proteasome component PRE3



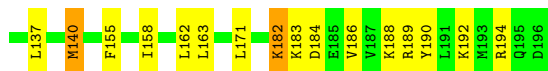
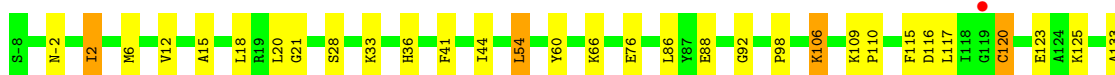
- Molecule 9: Proteasome component PUP1



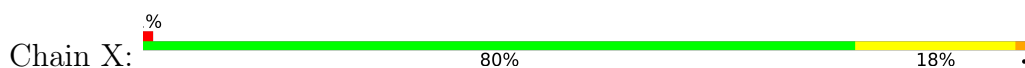
- Molecule 9: Proteasome component PUP1

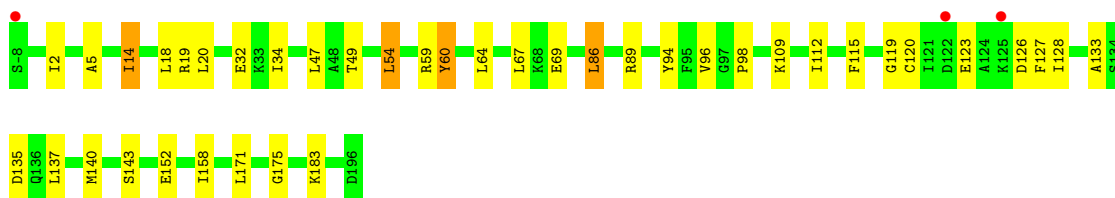


- Molecule 10: Proteasome component PUP3

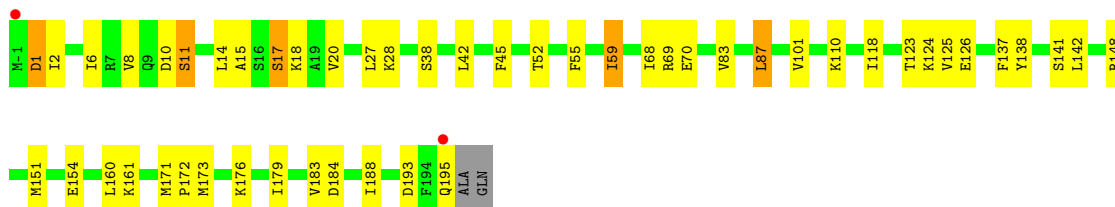


- Molecule 10: Proteasome component PUP3

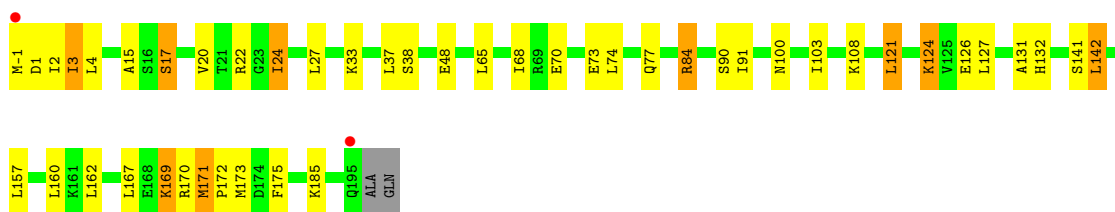
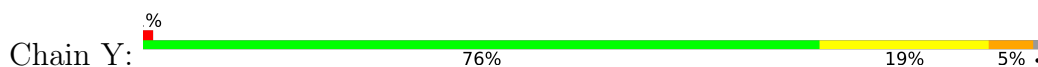




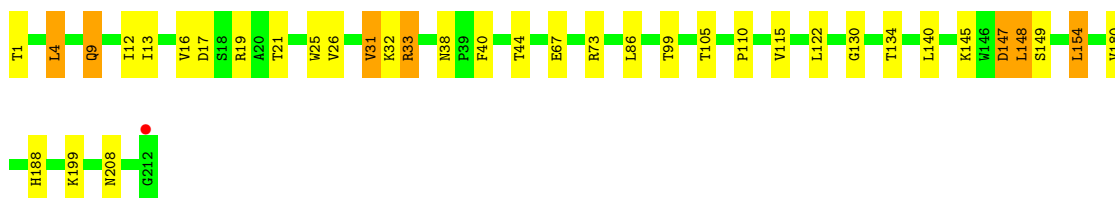
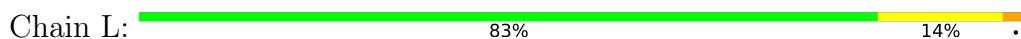
• Molecule 11: Proteasome component C11



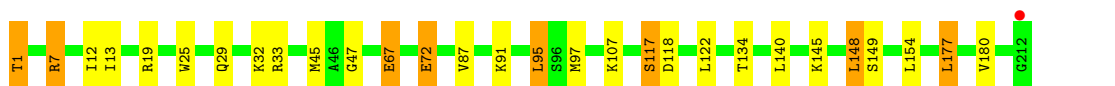
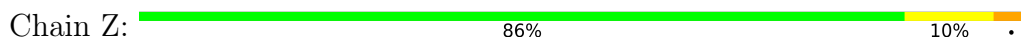
• Molecule 11: Proteasome component C11



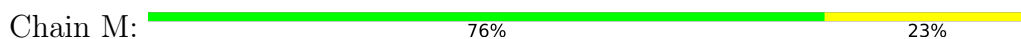
• Molecule 12: Proteasome component PRE2

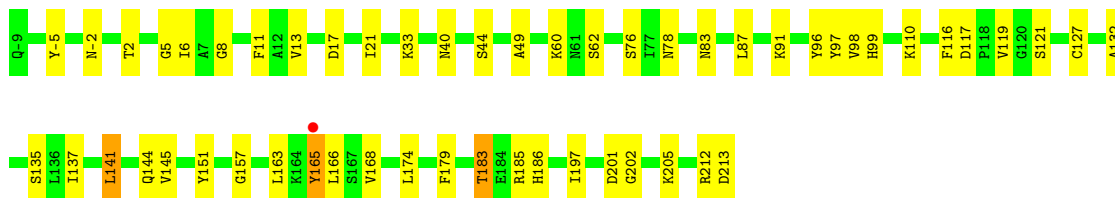


• Molecule 12: Proteasome component PRE2



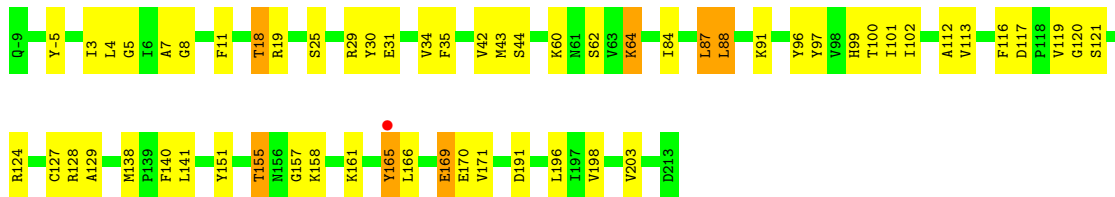
• Molecule 13: Proteasome component C5





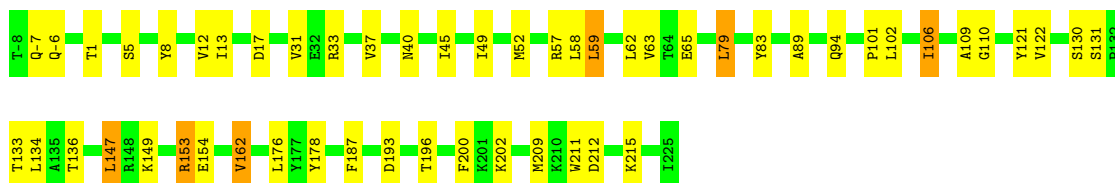
- Molecule 13: Proteasome component C5

Chain 1: 73% 23%



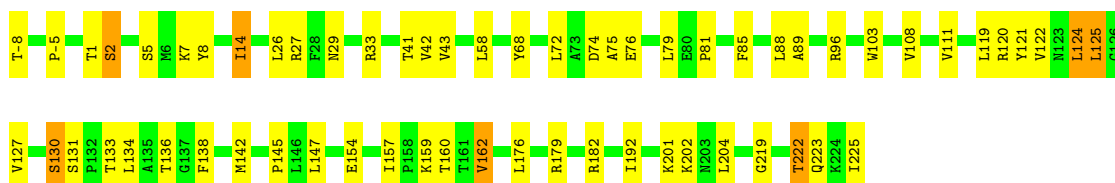
- Molecule 14: Proteasome component PRE4

Chain N: 77% 20%



- Molecule 14: Proteasome component PRE4

Chain 2: 73% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.26Å 301.36Å 143.96Å 90.00° 112.86° 90.00°	Depositor
Resolution (Å)	45.70 – 2.51 45.70 – 2.51	Depositor EDS
% Data completeness (in resolution range)	87.6 (45.70-2.51) 87.6 (45.70-2.51)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.202 , 0.255 0.197 , 0.248	Depositor DCC
R_{free} test set	15842 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtrriage
Anisotropy	0.909	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	50701	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: WPI

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	0.55	0/1941	0.98	7/2629 (0.3%)
1	O	0.57	0/1941	0.89	2/2629 (0.1%)
2	B	0.54	0/1943	0.89	2/2631 (0.1%)
2	P	0.53	0/1943	0.91	1/2631 (0.0%)
3	C	0.53	0/1935	0.87	3/2618 (0.1%)
3	Q	0.53	0/1935	0.89	1/2618 (0.0%)
4	D	0.52	0/1920	0.88	1/2598 (0.0%)
4	R	0.54	0/1920	0.88	2/2598 (0.1%)
5	E	0.54	0/1887	0.86	2/2541 (0.1%)
5	S	0.49	0/1887	0.85	0/2541
6	F	0.49	0/1811	0.85	3/2447 (0.1%)
6	T	0.50	0/1811	0.92	4/2447 (0.2%)
7	G	0.49	0/1937	0.87	2/2614 (0.1%)
7	U	0.50	0/1937	0.91	3/2614 (0.1%)
8	H	0.55	0/1541	0.93	2/2087 (0.1%)
8	V	0.55	0/1541	0.91	0/2087
9	I	0.58	0/1716	0.92	0/2326
9	W	0.54	0/1716	0.90	2/2326 (0.1%)
10	J	0.52	0/1611	0.84	0/2174
10	X	0.55	0/1611	0.89	2/2174 (0.1%)
11	K	0.53	0/1598	0.87	2/2154 (0.1%)
11	Y	0.56	0/1598	0.91	2/2154 (0.1%)
12	L	0.56	0/1683	0.91	2/2277 (0.1%)
12	Z	0.51	0/1683	0.84	0/2277
13	1	0.50	0/1795	0.91	3/2420 (0.1%)
13	M	0.54	0/1795	0.90	2/2420 (0.1%)
14	2	0.57	0/1855	0.88	1/2514 (0.0%)
14	N	0.54	0/1855	0.89	0/2514
All	All	0.53	0/50346	0.89	51/68060 (0.1%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ILE	CB-CA-C	-8.36	105.48	114.35
1	A	87	ILE	N-CA-CB	8.20	115.67	110.50
1	A	158	ASP	CA-C-N	-7.81	111.78	120.45
1	A	158	ASP	C-N-CA	-7.81	111.78	120.45
12	L	38	ASN	CA-C-N	-7.72	111.55	120.12
12	L	38	ASN	C-N-CA	-7.72	111.55	120.12
6	T	148	GLN	CA-C-N	7.21	128.86	119.84
6	T	148	GLN	C-N-CA	7.21	128.86	119.84
8	H	117	GLY	N-CA-C	-7.20	105.12	115.27
4	D	184	PRO	O-C-N	6.97	124.52	121.31
2	B	63	LYS	N-CA-C	-6.97	105.05	113.97
9	W	180	ILE	N-CA-C	6.59	116.74	110.42
3	C	244	ILE	N-CA-C	-6.38	107.08	113.20
3	Q	139	GLY	N-CA-C	6.26	120.24	110.91
7	U	129	ARG	CA-C-N	-6.23	114.23	120.21
7	U	129	ARG	C-N-CA	-6.23	114.23	120.21
6	T	55	GLU	N-CA-C	-6.22	105.65	113.18
11	Y	127	LEU	CA-C-N	6.22	125.96	119.05
11	Y	127	LEU	C-N-CA	6.22	125.96	119.05
11	K	38	SER	CA-C-N	-6.10	113.53	119.87
11	K	38	SER	C-N-CA	-6.10	113.53	119.87
13	M	49	ALA	N-CA-C	6.09	117.92	111.28
14	2	27	ARG	N-CA-C	6.03	117.65	111.14
10	X	59	ARG	N-CA-C	-5.94	104.44	111.03
7	G	11	ASN	N-CA-C	5.88	117.77	111.36
6	T	150	SER	N-CA-C	-5.75	105.76	112.89
7	U	13	VAL	N-CA-C	5.70	116.42	109.30
4	R	184	PRO	O-C-N	5.66	123.81	121.15
5	E	120	ALA	N-CA-C	5.63	118.62	111.69
6	F	148	GLN	CA-C-N	5.62	125.33	119.82
6	F	148	GLN	C-N-CA	5.62	125.33	119.82
2	B	138	GLY	N-CA-C	5.57	119.80	110.56
13	1	161	LYS	CA-C-N	5.44	125.61	119.90
13	1	161	LYS	C-N-CA	5.44	125.61	119.90
1	A	135	ARG	CA-C-N	-5.42	115.00	120.21
1	A	135	ARG	C-N-CA	-5.42	115.00	120.21
7	G	106	ILE	N-CA-C	5.42	114.86	108.96
2	P	68	THR	N-CA-C	-5.30	99.65	108.23
3	C	225	VAL	N-CA-C	5.24	115.12	107.37
5	E	66	LYS	N-CA-C	-5.23	106.85	114.12
8	H	62	HIS	N-CA-C	5.20	116.64	111.07
10	X	119	GLY	N-CA-C	5.16	121.62	114.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	85	GLY	CA-C-N	5.07	124.98	119.76
1	O	85	GLY	C-N-CA	5.07	124.98	119.76
13	1	165	TYR	N-CA-C	5.05	117.98	109.95
3	C	223	GLY	N-CA-C	-5.05	106.48	114.10
4	R	237	GLU	N-CA-C	-5.04	105.67	111.07
1	A	161	GLY	N-CA-C	-5.04	108.11	115.72
6	F	157	TYR	N-CA-C	-5.03	106.32	112.90
13	M	212	ARG	N-CA-C	5.01	118.43	112.72
9	W	21	THR	N-CA-C	5.01	116.57	108.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1903	0	1898	49	0
1	O	1903	0	1898	53	0
2	B	1906	0	1918	25	0
2	P	1906	0	1918	44	0
3	C	1905	0	1901	35	0
3	Q	1905	0	1901	44	0
4	D	1891	0	1900	38	0
4	R	1891	0	1900	45	0
5	E	1862	0	1836	41	0
5	S	1862	0	1836	42	0
6	F	1784	0	1788	40	0
6	T	1784	0	1788	45	0
7	G	1897	0	1886	30	0
7	U	1897	0	1886	46	0
8	H	1512	0	1481	40	0
8	V	1512	0	1481	30	0
9	I	1685	0	1688	24	0
9	W	1685	0	1688	38	0
10	J	1581	0	1574	21	0
10	X	1581	0	1574	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	1570	0	1577	25	0
11	Y	1570	0	1577	27	0
12	L	1646	0	1595	23	0
12	Z	1646	0	1595	19	0
13	1	1757	0	1711	39	0
13	M	1757	0	1711	27	0
14	2	1824	0	1832	36	0
14	N	1824	0	1832	30	0
15	H	41	0	48	5	0
15	I	41	0	48	7	0
15	L	41	0	48	5	0
15	V	41	0	48	11	0
15	W	41	0	48	3	0
15	Z	41	0	48	7	0
16	1	41	0	0	1	0
16	2	51	0	0	2	0
16	A	47	0	0	0	0
16	B	27	0	0	0	0
16	C	34	0	0	0	0
16	D	35	0	0	0	0
16	E	30	0	0	0	0
16	F	18	0	0	0	0
16	G	36	0	0	0	0
16	H	34	0	0	1	0
16	I	29	0	0	0	0
16	J	47	0	0	0	0
16	K	34	0	0	1	0
16	L	46	0	0	0	0
16	M	51	0	0	0	0
16	N	44	0	0	1	0
16	O	33	0	0	1	0
16	P	32	0	0	0	0
16	Q	33	0	0	0	0
16	R	18	0	0	0	0
16	S	23	0	0	1	0
16	T	19	0	0	0	0
16	U	38	0	0	0	0
16	V	47	0	0	0	0
16	W	36	0	0	0	0
16	X	36	0	0	0	0
16	Y	49	0	0	1	0
16	Z	41	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	50701	0	49458	884	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 9.

All (884) 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)
1:O:165:GLY:H	2:P:60:THR:HG21	1.14	1.09
7:U:245:GLU:O	7:U:246:ILE:HG22	1.56	1.04
7:U:246:ILE:HG13	7:U:246:ILE:O	1.60	0.99
8:V:45:ARG:HD2	8:V:52:THR:HG23	1.48	0.94
3:Q:70:ASN:HB3	3:Q:72:LYS:H	1.40	0.87
8:H:40:LYS:HE2	8:H:182:GLY:HA2	1.57	0.86
6:T:50:LYS:HB2	6:T:59:TYR:HB3	1.58	0.85
11:K:171:MET:HE3	11:K:173:MET:HB2	1.60	0.84
4:R:215:VAL:HG12	4:R:221:ILE:HG12	1.61	0.82
9:W:18:THR:HG23	9:W:30:ASN:HA	1.62	0.82
7:G:36:SER:HB3	7:G:49:VAL:HG23	1.61	0.81
7:U:245:GLU:O	7:U:246:ILE:CG2	2.30	0.80
7:U:246:ILE:O	7:U:246:ILE:CG1	2.33	0.77
1:A:54:ILE:HD11	1:A:223:LEU:HD22	1.67	0.77
2:P:68:THR:HG22	2:P:70:ASP:H	1.50	0.76
4:D:121:THR:HG22	5:E:136:ARG:HH21	1.49	0.75
14:2:43:VAL:HG22	14:2:108:VAL:HG22	1.67	0.75
12:Z:91:LYS:HE3	15:Z:301:WPI:H8	1.68	0.75
6:T:33:SER:HB3	6:T:62:LYS:HE3	1.68	0.75
9:I:205:PHE:HB3	9:I:209:THR:HG21	1.67	0.75
8:H:45:ARG:HD2	8:H:52:THR:HG23	1.68	0.75
7:U:245:GLU:C	7:U:246:ILE:CG2	2.59	0.75
8:H:1:THR:HB	8:H:33:LYS:HZ3	1.51	0.74
13:1:198:VAL:HG22	13:1:203:VAL:HG22	1.70	0.74
13:1:155:THR:HG23	13:1:158:LYS:H	1.53	0.73
1:O:165:GLY:N	2:P:60:THR:HG21	1.98	0.73
3:C:125:HIS:HB3	4:D:126:VAL:HG12	1.70	0.73
4:R:47:GLU:OE1	4:R:166:ARG:NH2	2.21	0.73
3:Q:125:HIS:HB3	4:R:126:VAL:HG12	1.72	0.72
9:I:3:ILE:HG13	9:I:99:ILE:HD12	1.72	0.71
3:Q:49:GLU:OE2	3:Q:210:ARG:NH2	2.23	0.71
13:M:165:TYR:HD2	13:M:166:LEU:H	1.38	0.71
13:M:213:ASP:OD1	9:W:19:ARG:NH2	2.23	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:59:GLU:H	2:P:59:GLU:CD	1.99	0.71
4:R:216:LYS:HB2	4:R:220:ASP:HB3	1.72	0.71
7:U:80:LEU:HD12	7:U:132:GLY:HA3	1.71	0.70
14:N:1:THR:O	14:N:33:ARG:NH2	2.25	0.70
9:W:18:THR:HG22	9:W:171:SER:HB2	1.72	0.70
5:S:222:ILE:HG22	5:S:228:PHE:HD1	1.57	0.69
12:L:145:LYS:HB2	12:L:148:LEU:HD13	1.75	0.69
8:H:152:VAL:HA	8:H:175:MET:HE1	1.75	0.69
6:F:198:SER:HA	6:F:201:LEU:HD22	1.74	0.68
7:U:247:ASN:C	7:U:247:ASN:ND2	2.51	0.68
5:S:182:GLU:HB3	5:S:203:ILE:HD13	1.73	0.68
13:1:117:ASP:HB3	13:1:119:VAL:H	1.59	0.68
1:A:220:LYS:HB3	1:A:242:GLU:HG2	1.74	0.68
2:P:64:VAL:HG11	2:P:212:ALA:HB2	1.74	0.68
8:H:128:GLY:HA2	15:H:300:WPI:H48	1.75	0.67
4:R:73:LEU:HD12	4:R:135:ILE:HG12	1.76	0.67
8:H:1:THR:HG23	15:H:300:WPI:H53	1.76	0.67
5:E:180:GLN:NE2	6:F:54:ASP:OD1	2.27	0.67
2:P:186:GLU:OE2	2:P:246:ARG:NH2	2.25	0.67
8:H:103:ASP:HB2	8:H:106:ASN:HB2	1.76	0.67
14:2:124:LEU:HD13	14:2:125:LEU:HD13	1.77	0.67
2:B:94:HIS:HA	2:B:98:LYS:HB3	1.77	0.66
4:D:162:GLN:OE1	4:D:163:THR:N	2.26	0.66
2:P:106:PRO:HG2	2:P:109:LEU:HB2	1.77	0.66
4:D:207:ALA:HB2	4:D:233:VAL:HG21	1.78	0.66
1:A:87:ILE:HD12	1:A:88:PRO:HD3	1.76	0.65
1:A:157:THR:HG22	1:A:163:TYR:HB2	1.77	0.65
11:K:15:ALA:HB2	11:K:160:LEU:HD21	1.77	0.65
4:D:53:LYS:O	4:D:54:LEU:HB2	1.96	0.65
9:I:46:ALA:HB1	15:I:301:WPI:H45	1.79	0.65
12:Z:1:THR:OG1	15:Z:301:WPI:H46	1.97	0.64
2:P:239:THR:HG23	2:P:242:GLU:HB2	1.79	0.64
12:Z:1:THR:HG21	12:Z:33:ARG:CZ	2.27	0.64
8:V:129:SER:HA	15:V:201:WPI:H52	1.78	0.64
9:W:163:ILE:HG23	9:W:170:GLY:HA2	1.78	0.64
10:J:117:LEU:HD23	10:J:117:LEU:H	1.63	0.64
5:S:31:ILE:HD13	5:S:141:ALA:HB2	1.79	0.64
1:A:78:THR:HG22	1:A:231:ASP:HA	1.78	0.64
4:D:200:LEU:HD11	4:D:233:VAL:HG12	1.79	0.64
7:G:169:GLN:CD	7:G:169:GLN:H	2.06	0.64
7:U:94:GLU:HG2	7:U:114:ARG:HB3	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:46:ALA:HA	15:I:301:WPI:H51	1.78	0.64
13:M:179:PHE:O	13:M:183:THR:HG22	1.98	0.64
13:1:117:ASP:HB2	13:1:121:SER:H	1.63	0.63
11:Y:-1:MET:HE3	11:Y:1:ASP:H	1.63	0.63
2:P:68:THR:HB	2:P:71:ILE:HB	1.79	0.63
9:W:62:ASN:HB3	9:W:82:MET:HE1	1.80	0.63
11:K:137:PHE:HB3	12:Z:134:THR:HG21	1.80	0.63
8:H:45:ARG:HH11	8:H:52:THR:CG2	2.12	0.63
6:F:77:LEU:HD12	6:F:79:PRO:HD2	1.81	0.63
13:1:18:THR:HG21	13:1:30:TYR:CD1	2.33	0.63
14:2:111:VAL:HG23	14:2:192:ILE:HG22	1.80	0.63
3:Q:48:ALA:HB1	3:Q:65:LYS:HD3	1.80	0.63
1:A:220:LYS:HD3	1:A:242:GLU:HG3	1.80	0.62
14:N:89:ALA:HA	14:N:122:VAL:HG21	1.81	0.62
8:V:44:CYS:HB2	8:V:98:ILE:HB	1.80	0.62
1:O:101:ALA:HA	1:O:112:MET:HE2	1.82	0.62
4:D:118:GLN:O	4:D:121:THR:HB	1.99	0.62
2:P:213:ILE:HG23	2:P:238:LEU:HD11	1.81	0.62
11:Y:169:LYS:HG3	11:Y:170:ARG:HG2	1.82	0.62
1:A:87:ILE:HG12	7:G:157:TRP:CZ2	2.36	0.61
7:U:246:ILE:O	7:U:247:ASN:CB	2.48	0.61
9:W:199:LYS:NZ	10:X:143:SER:O	2.33	0.61
7:G:94:GLU:HG2	7:G:114:ARG:HB3	1.82	0.61
12:L:21:THR:HG22	12:L:26:VAL:HA	1.83	0.61
9:W:58:LEU:HD23	9:W:59:ILE:HD12	1.82	0.61
10:X:14:ILE:HG23	10:X:34:ILE:HD13	1.81	0.61
8:H:136:GLY:HA2	8:V:161:GLN:HG3	1.81	0.61
12:L:13:ILE:HD12	12:L:154:LEU:HD13	1.83	0.61
2:P:4:ARG:HH22	5:S:126:GLY:HA3	1.65	0.61
10:X:126:ASP:OD1	10:X:127:PHE:N	2.29	0.61
1:A:82:VAL:HG12	1:A:142:THR:HB	1.81	0.61
1:A:204:GLU:OE2	1:A:244:ARG:NH1	2.33	0.61
8:H:13:ILE:HG21	8:H:175:MET:HE2	1.82	0.61
4:R:97:ARG:HD3	4:R:103:PRO:HG3	1.81	0.61
3:Q:234:GLU:O	3:Q:238:ILE:HG22	2.01	0.60
13:1:19:ARG:NE	13:1:191:ASP:OD2	2.32	0.60
8:V:13:ILE:HG12	8:V:177:VAL:HG13	1.83	0.60
8:H:36:ARG:HD2	14:2:225:ILE:HD11	1.82	0.60
3:Q:181:LYS:H	3:Q:184:MET:HE2	1.65	0.60
9:W:4:VAL:HG12	9:W:126:SER:HB3	1.83	0.60
1:O:123:ASN:OD1	2:P:83:ARG:NH1	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:201:WPI:H6	14:2:182:ARG:HG3	1.84	0.60
11:Y:91:ILE:HG12	11:Y:121:LEU:HB2	1.83	0.60
7:G:119:VAL:HG21	7:G:150:LEU:HD21	1.84	0.59
1:O:203:VAL:O	1:O:207:ILE:HG12	2.03	0.59
6:T:156:LEU:HD23	7:U:58:LEU:HA	1.85	0.59
3:Q:184:MET:HG2	3:Q:188:ASP:HB2	1.85	0.59
5:S:52:LYS:NZ	5:S:61:SER:O	2.35	0.59
3:Q:160:TRP:CD2	3:Q:163:ILE:HD13	2.37	0.59
5:E:192:THR:CG2	5:E:195:GLU:H	2.16	0.59
10:X:18:LEU:HD12	10:X:175:GLY:HA3	1.85	0.59
12:L:147:ASP:OD2	12:L:147:ASP:N	2.35	0.59
2:B:114:VAL:HG12	2:B:118:MET:HE2	1.85	0.58
3:C:91:ALA:HB1	3:C:111:LEU:HD11	1.84	0.58
6:F:81:ALA:HB2	6:F:130:VAL:HG21	1.85	0.58
8:H:22:THR:HG22	8:H:27:ALA:HB2	1.84	0.58
8:H:156:LYS:HE3	8:H:188:PHE:CD1	2.37	0.58
14:N:178:TYR:HD2	9:W:139:GLU:HG3	1.68	0.58
2:P:205:ASN:H	2:P:208:THR:HG22	1.68	0.58
4:D:187:THR:HG22	4:D:190:GLU:HB2	1.84	0.58
10:J:12:VAL:HG13	10:J:110:PRO:HB3	1.85	0.58
7:U:37:ILE:HD11	7:U:48:ALA:HB3	1.85	0.58
4:D:121:THR:CG2	5:E:136:ARG:HH21	2.17	0.58
3:Q:60:ASP:OD1	3:Q:60:ASP:N	2.22	0.58
6:F:134:ILE:HB	6:F:145:LEU:HB2	1.85	0.58
8:H:32:ASP:OD2	8:H:185:ARG:NH2	2.36	0.58
8:V:115:LEU:HD13	15:V:201:WPI:H47	1.85	0.58
14:2:89:ALA:HA	14:2:122:VAL:HG21	1.84	0.58
3:Q:2:GLY:HA3	6:T:123:TYR:CE1	2.39	0.58
6:T:43:HIS:HB3	6:T:215:ILE:HD11	1.85	0.58
7:U:247:ASN:C	7:U:247:ASN:HD22	2.12	0.58
11:K:11:SER:HB3	11:K:184:ASP:HB3	1.85	0.57
6:T:63:ILE:HG21	6:T:214:ALA:HB2	1.85	0.57
3:Q:44:ILE:HD11	3:Q:146:TYR:HB3	1.86	0.57
13:1:7:ALA:HB2	13:1:113:VAL:HG23	1.87	0.57
2:P:42:GLY:HA3	2:P:185:LEU:HD13	1.85	0.57
4:R:14:ASP:OD2	4:R:14:ASP:N	2.34	0.57
8:V:59:VAL:HG22	8:V:81:VAL:HG12	1.86	0.57
13:M:165:TYR:HD2	13:M:166:LEU:N	2.01	0.57
1:O:177:GLU:N	1:O:177:GLU:OE1	2.38	0.57
2:P:227:ILE:HG22	2:P:229:THR:HG23	1.86	0.57
3:Q:119:LYS:NZ	3:Q:151:SER:OG	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:81:LEU:HD12	5:S:139:GLY:HA3	1.87	0.57
1:A:70:SER:HA	1:A:224:GLU:OE2	2.05	0.57
9:I:104:ASP:HB2	9:I:105:PRO:HD2	1.87	0.57
4:D:187:THR:HG23	4:D:190:GLU:H	1.70	0.57
9:I:128:GLY:HA2	15:I:301:WPI:H42	1.86	0.57
11:K:59:ILE:HG13	11:K:83:VAL:HG22	1.87	0.57
3:C:70:ASN:OD1	3:C:71:ASP:N	2.37	0.56
7:U:69:VAL:HG22	7:U:92:ARG:HG3	1.87	0.56
13:1:43:MET:HG3	13:1:102:ILE:HG22	1.86	0.56
9:I:128:GLY:O	9:I:131:SER:HB2	2.05	0.56
3:Q:64:GLU:HG3	3:Q:65:LYS:HG2	1.87	0.56
8:V:4:MET:HB3	8:V:126:ILE:HG22	1.87	0.56
15:V:201:WPI:H6	14:2:182:ARG:CD	2.36	0.56
12:Z:118:ASP:OD1	15:Z:301:WPI:H16	2.04	0.56
4:R:48:ARG:NH1	4:R:208:LYS:HE2	2.20	0.56
5:S:127:ALA:HB3	5:S:132:ARG:HD2	1.87	0.56
8:H:1:THR:OG1	15:H:300:WPI:H46	2.06	0.56
11:Y:22:ARG:HG3	11:Y:27:LEU:HD12	1.87	0.56
12:L:130:GLY:HA2	15:L:301:WPI:H42	1.87	0.56
7:U:245:GLU:C	7:U:246:ILE:HG23	2.30	0.56
11:Y:84:ARG:HG3	11:Y:124:LYS:HB3	1.88	0.56
1:A:100:GLU:HG2	1:A:120:ARG:HG2	1.88	0.56
14:N:17:ASP:O	14:N:33:ARG:NH1	2.34	0.56
1:O:131:ARG:HD3	1:O:133:TYR:HE2	1.71	0.56
6:F:72:LEU:HD22	6:F:132:LEU:HD22	1.88	0.56
4:D:203:VAL:HG12	4:D:205:THR:H	1.71	0.56
5:S:167:TYR:CE1	5:S:170:LYS:HD3	2.41	0.56
5:S:176:SER:O	5:S:180:GLN:N	2.24	0.56
5:E:68:VAL:HG21	5:E:89:ILE:HD13	1.88	0.55
13:1:8:GLY:HA3	13:1:11:PHE:CE2	2.41	0.55
4:D:26:ALA:HB1	4:D:78:LEU:HD13	1.88	0.55
10:J:15:ALA:HB1	10:J:162:LEU:HD22	1.88	0.55
2:P:222:LEU:HD13	2:P:232:GLY:HA2	1.89	0.55
5:S:186:GLU:HG2	5:S:199:LEU:HD11	1.86	0.55
12:Z:12:ILE:HB	12:Z:180:VAL:HB	1.89	0.55
13:1:166:LEU:HD23	13:1:170:GLU:HG2	1.88	0.55
5:E:166:ARG:HB3	6:F:58:SER:HB3	1.87	0.55
15:V:201:WPI:H6	14:2:182:ARG:NE	2.21	0.55
10:X:96:VAL:HG23	10:X:98:PRO:HD3	1.89	0.55
14:2:131:SER:HB3	14:2:133:THR:O	2.06	0.55
5:E:192:THR:HG22	5:E:195:GLU:H	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:28:LYS:HD3	12:L:122:LEU:HD22	1.87	0.55
6:F:72:LEU:HB3	6:F:134:ILE:HD13	1.89	0.55
8:H:136:GLY:CA	8:V:161:GLN:HG3	2.37	0.55
4:R:175:LEU:HB3	5:S:58:LEU:HD11	1.88	0.55
6:T:70:MET:HE2	6:T:105:VAL:HG22	1.89	0.55
3:Q:106:ILE:HD11	3:Q:110:ILE:HG22	1.88	0.55
9:W:67:SER:HB2	9:W:72:ARG:O	2.06	0.55
6:T:107:ARG:NH2	14:2:68:TYR:O	2.39	0.55
15:V:201:WPI:H6	14:2:182:ARG:HE	1.70	0.55
10:X:98:PRO:HB2	10:X:115:PHE:CD2	2.42	0.55
11:K:1:ASP:OD1	11:K:1:ASP:N	2.36	0.55
14:N:178:TYR:CD2	9:W:139:GLU:HG3	2.42	0.55
5:S:120:ALA:C	5:S:122:ARG:H	2.15	0.54
5:S:234:GLU:H	5:S:234:GLU:CD	2.15	0.54
10:X:2:ILE:HG21	10:X:133:ALA:HB3	1.87	0.54
13:1:91:LYS:HD3	13:1:96:TYR:CE2	2.42	0.54
8:H:82:PHE:HB3	8:H:113:ILE:HD13	1.89	0.54
5:S:74:ILE:HD13	5:S:112:LEU:HD22	1.88	0.54
1:A:220:LYS:HD3	1:A:242:GLU:CG	2.37	0.54
15:L:301:WPI:H51	15:L:301:WPI:C45	2.37	0.54
6:F:46:LEU:HD22	6:F:135:ILE:HG12	1.90	0.54
1:O:199:TRP:O	1:O:203:VAL:HG13	2.07	0.54
4:R:149:GLN:HG2	4:R:159:TRP:NE1	2.22	0.54
6:T:45:VAL:HG22	6:T:215:ILE:HD13	1.90	0.54
7:U:246:ILE:O	7:U:247:ASN:CG	2.51	0.54
4:D:155:ILE:HD12	5:E:83:ALA:HB2	1.90	0.54
13:M:117:ASP:HB3	13:M:119:VAL:H	1.73	0.54
13:1:127:CYS:SG	13:1:141:LEU:HD23	2.48	0.54
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.90	0.54
4:R:226:SER:O	4:R:230:ASN:N	2.37	0.54
6:T:182:ILE:HD11	6:T:188:GLU:HB3	1.89	0.54
8:V:45:ARG:HH11	8:V:52:THR:CG2	2.20	0.54
12:Z:97:MET:N	12:Z:117:SER:OG	2.39	0.53
11:Y:2:ILE:H	11:Y:17:SER:HB3	1.73	0.53
2:P:160:LYS:HD3	2:P:179:TRP:CZ3	2.44	0.53
6:T:128:TYR:O	6:T:149:PRO:HB3	2.07	0.53
6:T:206:LEU:HD12	6:T:206:LEU:H	1.72	0.53
3:C:9:ARG:HD3	4:D:6:ARG:CZ	2.39	0.53
1:O:179:THR:HG23	2:P:55:LEU:HD12	1.91	0.53
13:M:141:LEU:O	13:M:145:VAL:HB	2.09	0.53
8:H:48:SER:O	8:H:52:THR:HB	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:148:ARG:HB2	11:K:151:MET:HG3	1.90	0.53
11:K:193:ASP:OD1	11:K:193:ASP:N	2.42	0.53
11:Y:15:ALA:HB2	11:Y:160:LEU:HD21	1.91	0.53
11:K:183:VAL:HG22	11:K:188:ILE:HG12	1.91	0.52
13:M:99:HIS:HD2	13:M:116:PHE:O	1.92	0.52
4:R:29:ARG:HB2	4:R:29:ARG:CZ	2.38	0.52
5:S:12:VAL:HG22	5:S:23:GLN:HG3	1.92	0.52
6:F:50:LYS:HB3	6:F:59:TYR:HB3	1.90	0.52
9:I:174:ASP:OD2	9:I:188:ARG:NH1	2.37	0.52
1:O:161:GLY:O	2:P:83:ARG:NH2	2.40	0.52
3:C:25:ALA:O	3:C:29:ILE:HG13	2.09	0.52
4:D:58:ARG:HD3	4:D:59:ILE:HG23	1.91	0.52
2:B:15:SER:OG	2:B:17:LYS:HG2	2.09	0.52
3:C:238:ILE:HA	3:C:241:LYS:HB2	1.92	0.52
16:1:306:HOH:O	14:2:-8:THR:HG23	2.09	0.52
3:C:36:ILE:HD13	3:C:164:SER:HB3	1.92	0.52
7:G:35:THR:HB	7:G:167:GLY:H	1.75	0.52
8:V:115:LEU:CD1	15:V:201:WPI:H47	2.39	0.52
6:F:176:LEU:HA	6:F:179:PHE:CE2	2.45	0.52
13:M:13:VAL:HG12	13:M:197:ILE:HG13	1.91	0.52
4:R:184:PRO:O	4:R:186:ALA:N	2.43	0.52
4:R:207:ALA:HB2	4:R:233:VAL:HG21	1.91	0.52
5:S:77:ALA:HB3	5:S:143:LEU:HB2	1.92	0.52
9:W:172:ASN:HD22	9:W:192:THR:HA	1.75	0.52
10:X:112:ILE:HD12	10:X:128:ILE:HG12	1.91	0.52
13:M:76:SER:OG	13:M:78:ASN:OD1	2.23	0.51
4:R:97:ARG:HH11	4:R:103:PRO:HG3	1.76	0.51
5:S:45:GLY:HA2	5:S:153:TYR:CE1	2.45	0.51
5:S:177:GLU:OE2	5:S:178:GLY:N	2.34	0.51
7:U:94:GLU:HG3	7:U:114:ARG:HH11	1.75	0.51
1:A:105:ARG:HH22	14:2:222:THR:HG23	1.74	0.51
6:F:101:ARG:HG3	14:N:83:TYR:CZ	2.45	0.51
14:N:45:ILE:HD12	14:N:52:MET:HG3	1.92	0.51
1:O:91:ARG:HD2	16:O:317:HOH:O	2.09	0.51
4:R:172:ARG:O	4:R:176:GLU:HG2	2.09	0.51
3:C:245:THR:HG23	3:C:245:THR:OXT	2.11	0.51
12:L:17:ASP:OD2	12:L:33:ARG:NH2	2.44	0.51
13:M:17:ASP:OD1	13:M:33:LYS:NZ	2.43	0.51
4:R:31:THR:HG21	4:R:49:ARG:HG2	1.92	0.51
6:F:63:ILE:HG21	6:F:214:ALA:HB2	1.93	0.51
13:M:137:ILE:HG22	13:M:141:LEU:HD22	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:44:ALA:HB2	1:O:53:VAL:HG12	1.92	0.51
1:O:207:ILE:HD12	1:O:223:LEU:HD13	1.93	0.51
4:R:185:PRO:O	4:R:187:THR:N	2.43	0.51
11:Y:48:GLU:HG2	15:Z:301:WPI:H6	1.92	0.51
1:O:242:GLU:O	1:O:246:VAL:HG12	2.11	0.51
13:1:18:THR:HG22	13:1:31:GLU:H	1.74	0.51
14:N:8:TYR:CE1	14:N:162:VAL:HG22	2.46	0.51
6:T:232:LYS:HE3	6:T:233:TYR:CE2	2.45	0.51
14:2:42:VAL:HG23	14:2:192:ILE:HD11	1.93	0.51
1:A:62:LYS:HE3	7:G:176:GLU:HG2	1.93	0.51
5:E:188:HIS:CE1	5:E:191:LEU:HG	2.46	0.51
12:L:12:ILE:HB	12:L:180:VAL:HB	1.92	0.51
6:T:46:LEU:HD22	6:T:135:ILE:HG12	1.93	0.51
9:W:110:LEU:HG	9:W:125:LEU:HD12	1.92	0.51
9:W:172:ASN:ND2	9:W:192:THR:HG22	2.25	0.51
14:2:1:THR:O	14:2:33:ARG:NH2	2.44	0.51
6:F:156:LEU:HD13	6:F:159:THR:HB	1.93	0.51
3:Q:238:ILE:HG12	3:Q:238:ILE:O	2.10	0.51
8:V:112:THR:HG22	8:V:120:HIS:HB2	1.92	0.51
3:Q:91:ALA:HB2	3:Q:115:LEU:HD22	1.93	0.50
12:Z:19:ARG:HH21	12:Z:29:GLN:HE22	1.57	0.50
13:1:84:ILE:HG22	13:1:88:LEU:HD22	1.94	0.50
3:C:173:GLN:HE21	4:D:52:LEU:HD12	1.76	0.50
3:Q:66:LEU:HD22	3:Q:212:GLU:HB3	1.93	0.50
9:W:1:THR:HB	15:W:301:WPI:H52	1.93	0.50
1:O:112:MET:HE3	1:O:117:LEU:HD13	1.93	0.50
6:T:50:LYS:HB3	6:T:60:GLN:O	2.11	0.50
14:2:121:TYR:HE1	14:2:136:THR:HG22	1.75	0.50
2:B:10:THR:HG22	2:B:18:LEU:HD22	1.94	0.50
3:C:136:ILE:HG12	3:C:150:THR:HG22	1.92	0.50
4:D:96:HIS:CD2	4:D:100:LEU:HD13	2.47	0.50
8:H:67:THR:HA	8:H:71:GLY:O	2.12	0.50
5:E:51:GLU:HG3	5:E:208:MET:HG2	1.94	0.50
3:Q:11:THR:O	4:R:127:ARG:HD3	2.11	0.50
11:Y:108:LYS:HE2	11:Y:185:LYS:O	2.12	0.50
11:Y:185:LYS:HG2	16:Y:217:HOH:O	2.11	0.50
5:E:173:GLY:O	5:E:176:SER:OG	2.29	0.50
1:O:40:ILE:HG23	1:O:56:GLN:HB2	1.92	0.50
1:O:132:ALA:HB2	2:P:9:LEU:HD21	1.94	0.50
1:O:200:GLU:O	1:O:203:VAL:HG22	2.12	0.50
10:X:5:ALA:HB2	10:X:14:ILE:HG13	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:159:THR:OG1	6:T:160:ALA:N	2.43	0.50
8:H:149:GLU:CD	8:H:149:GLU:H	2.20	0.49
7:U:246:ILE:O	7:U:247:ASN:OD1	2.30	0.49
9:W:52:THR:O	9:W:56:THR:HB	2.12	0.49
5:E:52:LYS:NZ	5:E:61:SER:O	2.45	0.49
9:I:148:LYS:HD2	9:I:177:VAL:HG11	1.94	0.49
14:N:200:PHE:HE2	14:N:202:LYS:HG3	1.77	0.49
13:1:3:ILE:HG13	13:1:101:ILE:HD12	1.92	0.49
6:F:11:VAL:O	7:G:129:ARG:HB3	2.12	0.49
13:M:151:TYR:CD1	13:M:157:GLY:HA2	2.47	0.49
6:T:54:ASP:HB3	6:T:56:LEU:H	1.77	0.49
14:2:5:SER:HB3	14:2:14:ILE:HG13	1.93	0.49
1:O:21:PRO:HA	2:P:23:TYR:CD1	2.47	0.49
12:Z:95:LEU:HB2	16:Z:403:HOH:O	2.12	0.49
5:E:146:GLY:HA2	5:E:222:ILE:HG12	1.92	0.49
11:Y:100:ASN:HB3	11:Y:132:HIS:CG	2.47	0.49
13:1:3:ILE:HD12	13:1:44:SER:HB3	1.94	0.49
14:2:119:LEU:O	14:2:130:SER:OG	2.24	0.49
5:E:202:LYS:HE2	5:E:206:GLN:OE1	2.12	0.49
7:G:90:ARG:HG2	7:G:118:TYR:CD2	2.47	0.49
13:M:151:TYR:CG	13:M:157:GLY:HA2	2.48	0.49
1:O:82:VAL:HG13	1:O:142:THR:HB	1.95	0.49
2:P:210:GLU:HG2	2:P:237:LYS:HE2	1.93	0.49
6:T:171:TYR:HB2	6:T:199:GLN:HG3	1.93	0.49
4:D:87:GLU:OE2	11:K:69:ARG:NH1	2.45	0.49
5:E:169:ALA:HB1	5:E:183:LEU:HG	1.93	0.49
14:2:85:PHE:CZ	14:2:120:ARG:HG2	2.47	0.49
3:C:17:GLY:O	4:D:29:ARG:NH2	2.42	0.49
6:F:167:GLY:HA3	6:F:199:GLN:O	2.13	0.49
3:Q:150:THR:O	3:Q:157:TYR:HA	2.13	0.49
3:Q:215:THR:HG22	3:Q:228:LYS:HB3	1.95	0.49
14:2:142:MET:HE1	14:2:179:ARG:HG3	1.94	0.49
9:I:222:ASP:OD2	10:J:66:LYS:NZ	2.45	0.48
14:N:45:ILE:HG12	14:N:106:ILE:HG13	1.95	0.48
1:O:78:THR:HG22	1:O:231:ASP:HA	1.95	0.48
3:Q:18:ARG:HB3	3:Q:23:GLU:OE1	2.13	0.48
8:V:48:SER:HB3	8:V:51:ASP:HB2	1.95	0.48
11:Y:17:SER:HB2	11:Y:175:PHE:HB2	1.95	0.48
2:B:63:LYS:HG3	2:B:75:TYR:CE2	2.48	0.48
1:O:150:LEU:HD22	9:W:72:ARG:NH2	2.27	0.48
5:S:46:VAL:HG23	5:S:153:TYR:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:ILE:HG13	3:C:164:SER:N	2.29	0.48
5:E:193:LEU:O	5:E:197:GLU:HG3	2.12	0.48
1:O:162:TYR:CE1	2:P:80:PRO:HD3	2.48	0.48
10:X:152:GLU:H	10:X:152:GLU:CD	2.20	0.48
3:C:5:ARG:HD2	3:C:6:TYR:CZ	2.48	0.48
11:K:14:LEU:HD12	11:K:42:LEU:HD23	1.96	0.48
5:S:214:GLU:HG3	5:S:233:ASN:HB3	1.96	0.48
6:T:215:ILE:HD12	6:T:216:VAL:H	1.79	0.48
7:U:39:ILE:HD12	7:U:195:ALA:HB2	1.95	0.48
8:V:38:HIS:CE1	8:V:73:PRO:HD2	2.47	0.48
8:V:161:GLN:HE21	8:V:165:TRP:HE1	1.62	0.48
13:1:117:ASP:HB2	13:1:121:SER:N	2.27	0.48
1:A:88:PRO:HG3	7:G:155:SER:N	2.28	0.48
1:A:165:GLY:HA3	2:B:60:THR:HG21	1.96	0.48
2:B:63:LYS:HG3	2:B:75:TYR:HE2	1.78	0.48
5:S:45:GLY:HA2	5:S:153:TYR:CD1	2.48	0.48
7:U:53:ILE:HG13	7:U:211:PHE:HA	1.95	0.48
1:A:156:LYS:O	1:A:163:TYR:HA	2.14	0.48
6:F:213:ILE:HG23	6:F:225:TYR:HB2	1.95	0.48
10:J:76:GLU:OE1	10:J:76:GLU:N	2.37	0.48
12:L:40:PHE:HB3	12:L:73:ARG:HH21	1.79	0.48
3:Q:231:LYS:HB2	3:Q:234:GLU:HG3	1.94	0.48
4:R:89:ALA:HB1	4:R:109:LEU:HD11	1.95	0.48
7:U:68:VAL:HG12	16:2:304:HOH:O	2.13	0.48
1:A:82:VAL:CG1	1:A:142:THR:HB	2.44	0.48
6:F:43:HIS:HB2	6:F:189:LEU:HD23	1.96	0.48
7:G:41:CYS:HB2	7:G:186:LEU:O	2.14	0.48
6:T:45:VAL:HG23	6:T:189:LEU:HD23	1.95	0.48
7:U:246:ILE:O	7:U:247:ASN:HB3	2.13	0.48
8:V:155:ILE:HG22	8:V:175:MET:HE2	1.95	0.48
1:A:77:ARG:HH22	8:H:39:ASP:CG	2.22	0.48
11:K:118:ILE:HA	11:K:123:THR:O	2.14	0.48
6:T:77:LEU:HD12	6:T:79:PRO:HD2	1.95	0.48
9:W:179:GLU:HB3	9:W:182:LYS:HG3	1.95	0.47
1:A:133:TYR:CZ	1:A:134:MET:HE2	2.49	0.47
4:D:47:GLU:OE2	4:D:166:ARG:NH2	2.47	0.47
14:N:12:VAL:HG21	14:N:109:ALA:HB1	1.96	0.47
5:S:232:ASP:OD2	5:S:232:ASP:N	2.44	0.47
12:Z:118:ASP:OD2	15:Z:301:WPI:H21	2.15	0.47
3:C:140:TYR:CD2	3:C:225:VAL:HG21	2.49	0.47
5:E:175:GLY:HA3	5:E:207:VAL:HG11	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:2:ILE:H	11:K:17:SER:HB3	1.78	0.47
3:Q:148:LEU:HB3	3:Q:160:TRP:O	2.14	0.47
9:W:5:GLY:O	9:W:124:TYR:HA	2.13	0.47
1:A:115:ASP:HB3	1:A:155:TYR:CZ	2.49	0.47
6:F:50:LYS:HE2	6:F:212:SER:HB2	1.97	0.47
6:F:52:ASN:ND2	6:F:54:ASP:O	2.48	0.47
7:G:55:SER:OG	7:G:56:LYS:N	2.47	0.47
6:T:151:GLY:O	7:U:82:PRO:HG3	2.14	0.47
1:A:12:TYR:C	1:A:14:ARG:H	2.22	0.47
5:E:168:ASN:HB3	5:E:187:TRP:CZ2	2.50	0.47
9:I:147:THR:HG23	9:I:150:GLU:OE1	2.14	0.47
11:K:45:PHE:HB3	11:K:101:VAL:HG12	1.96	0.47
8:H:129:SER:H	15:H:300:WPI:H47	1.79	0.47
14:N:63:VAL:HG22	14:N:79:LEU:HD23	1.96	0.47
5:S:121:LEU:HA	5:S:123:PHE:CE2	2.50	0.47
6:T:182:ILE:HG12	6:T:182:ILE:O	2.14	0.47
1:A:87:ILE:HA	1:A:90:ALA:HB3	1.96	0.47
12:L:99:THR:HG22	12:L:115:VAL:O	2.14	0.47
1:O:68:THR:HG21	7:U:158:GLY:HA3	1.96	0.47
3:Q:54:SER:OG	3:Q:55:THR:N	2.48	0.47
3:Q:239:LEU:HD12	3:Q:239:LEU:HA	1.77	0.47
4:R:159:TRP:CZ2	5:S:59:LEU:HD12	2.49	0.47
7:G:188:ALA:O	7:G:192:VAL:HG12	2.15	0.47
9:I:128:GLY:C	15:I:301:WPI:H42	2.40	0.47
1:O:141:LEU:O	1:O:156:LYS:HA	2.14	0.47
9:W:26:VAL:HG11	9:W:29:LYS:HG2	1.97	0.47
6:F:107:ARG:O	6:F:111:LEU:HG	2.14	0.47
14:N:17:ASP:OD1	14:N:33:ARG:NH1	2.47	0.47
1:A:68:THR:HG21	7:G:158:GLY:H	1.80	0.47
6:F:132:LEU:HD12	6:F:147:PHE:CD2	2.50	0.47
8:H:137:TYR:CE1	8:V:140:LYS:HG3	2.50	0.47
9:W:152:ILE:HD11	9:W:177:VAL:HG21	1.97	0.47
9:W:172:ASN:ND2	9:W:192:THR:HA	2.29	0.47
10:X:60:TYR:C	10:X:60:TYR:CD2	2.93	0.47
11:Y:167:LEU:O	11:Y:171:MET:HB2	2.15	0.47
14:2:7:LYS:HD2	14:2:157:ILE:HD13	1.96	0.47
5:E:75:GLY:HA3	5:E:228:PHE:CE1	2.50	0.46
8:H:51:ASP:O	8:H:55:ILE:HG13	2.15	0.46
4:R:53:LYS:O	4:R:54:LEU:HB2	2.14	0.46
5:S:219:LEU:HB3	5:S:231:TYR:CD2	2.51	0.46
7:U:194:GLN:O	7:U:198:ILE:HG13	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:34:VAL:HG12	13:1:196:LEU:HD22	1.97	0.46
5:E:132:ARG:HB3	5:E:133:LEU:H	1.54	0.46
6:T:36:VAL:HG22	6:T:160:ALA:HB2	1.96	0.46
11:Y:171:MET:HB3	11:Y:171:MET:HE3	1.56	0.46
15:L:301:WPI:H51	15:L:301:WPI:O42	2.15	0.46
7:U:169:GLN:CD	7:U:169:GLN:H	2.24	0.46
3:C:150:THR:O	3:C:157:TYR:HA	2.14	0.46
5:E:205:LYS:NZ	5:E:247:GLU:OE1	2.48	0.46
10:X:47:LEU:HG	10:X:49:THR:HG22	1.97	0.46
8:H:55:ILE:HD11	8:H:93:LEU:HD13	1.98	0.46
11:K:118:ILE:HG12	11:K:124:LYS:HB2	1.98	0.46
12:L:9:GLN:NE2	12:L:148:LEU:O	2.44	0.46
3:Q:102:TYR:CE1	11:Y:74:LEU:HD21	2.50	0.46
8:V:48:SER:O	8:V:52:THR:HB	2.16	0.46
11:Y:1:ASP:CG	11:Y:33:LYS:HE2	2.40	0.46
3:C:94:HIS:CD2	3:C:114:ARG:HG2	2.51	0.46
3:C:106:ILE:HD11	3:C:110:ILE:HG22	1.97	0.46
5:E:81:LEU:HD12	5:E:139:GLY:HA3	1.98	0.46
6:F:54:ASP:OD2	6:F:54:ASP:N	2.48	0.46
8:H:48:SER:HB3	8:H:51:ASP:HB2	1.95	0.46
8:H:156:LYS:HE3	8:H:188:PHE:CE1	2.50	0.46
1:O:203:VAL:HG21	1:O:244:ARG:HD3	1.97	0.46
2:P:175:LEU:HD22	2:P:195:THR:HG21	1.98	0.46
4:R:169:LYS:HB2	4:R:169:LYS:HE3	1.70	0.46
14:2:142:MET:O	14:2:145:PRO:HD2	2.16	0.46
3:C:163:ILE:HG13	3:C:164:SER:H	1.80	0.46
8:H:132:THR:O	8:V:133:PHE:HA	2.16	0.46
10:J:-2:ASN:HA	10:J:21:GLY:O	2.15	0.46
2:B:60:THR:C	2:B:61:LEU:HD22	2.41	0.46
13:M:185:ARG:HH21	9:W:29:LYS:HE2	1.81	0.46
14:N:37:VAL:HG21	14:N:59:LEU:HG	1.98	0.46
2:P:109:LEU:HD12	2:P:109:LEU:HA	1.73	0.46
4:R:67:ILE:HG21	4:R:109:LEU:HD21	1.97	0.46
5:S:191:LEU:HD21	5:S:199:LEU:HD22	1.97	0.46
3:C:240:VAL:HA	3:C:245:THR:HA	1.98	0.46
10:J:2:ILE:HG21	10:J:133:ALA:HB3	1.99	0.46
10:J:115:PHE:HA	10:J:120:CYS:O	2.15	0.46
12:L:1:THR:HB	15:L:301:WPI:C36	2.46	0.46
14:N:193:ASP:HB3	14:N:196:THR:OG1	2.16	0.46
7:U:187:SER:HB2	7:U:190:GLU:HB2	1.97	0.46
1:A:34:ALA:O	1:A:37:GLN:HG2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:LEU:HD12	2:B:85:LEU:HA	1.79	0.45
6:F:179:PHE:HA	6:F:182:ILE:HG13	1.97	0.45
10:J:140:MET:HE3	13:1:140:PHE:HA	1.98	0.45
9:W:9:ASN:OD1	9:W:10:ASN:N	2.50	0.45
10:X:98:PRO:HB2	10:X:115:PHE:HD2	1.80	0.45
2:B:193:LEU:HD12	2:B:193:LEU:HA	1.78	0.45
2:B:207:ASP:OD1	2:B:207:ASP:N	2.50	0.45
1:O:69:VAL:HA	7:U:157:TRP:CZ3	2.52	0.45
12:Z:47:GLY:HA2	15:Z:301:WPI:H40	1.98	0.45
3:C:113:ARG:NH2	11:K:70:GLU:OE2	2.49	0.45
3:C:191:GLU:HG2	3:C:242:THR:HG22	1.97	0.45
4:D:53:LYS:HE2	4:D:54:LEU:HD12	1.98	0.45
5:E:205:LYS:HG3	5:E:212:LEU:HB3	1.98	0.45
3:Q:147:GLN:HG2	4:R:59:ILE:HG21	1.96	0.45
4:R:159:TRP:CH2	5:S:56:SER:HB3	2.51	0.45
6:T:16:THR:HB	6:T:18:ARG:HG3	1.98	0.45
15:V:201:WPI:H6	14:2:182:ARG:CG	2.45	0.45
10:X:19:ARG:HD3	10:X:171:LEU:O	2.16	0.45
2:B:5:TYR:OH	7:G:126:ASN:ND2	2.42	0.45
9:I:137:VAL:HG21	9:I:161:ALA:HB2	1.98	0.45
12:L:25:TRP:CH2	13:M:135:SER:HA	2.51	0.45
12:L:154:LEU:HD21	12:L:188:HIS:CG	2.52	0.45
3:Q:201:THR:HG22	3:Q:203:SER:HB3	1.96	0.45
4:R:37:LYS:NZ	5:S:60:GLU:OE2	2.50	0.45
4:D:36:VAL:HG12	4:D:161:ALA:HB1	1.97	0.45
9:I:2:THR:OG1	9:I:130:GLY:HA3	2.16	0.45
2:P:24:ALA:O	2:P:28:VAL:HG23	2.17	0.45
11:Y:38:SER:HB3	11:Y:73:GLU:HG3	1.99	0.45
2:B:37:ILE:HD12	2:B:192:ALA:HB2	1.98	0.45
6:F:36:VAL:HG22	6:F:160:ALA:HB2	1.97	0.45
1:O:117:LEU:O	1:O:121:MET:HG2	2.17	0.45
5:S:210:GLU:HB3	5:S:216:ASN:ND2	2.32	0.45
3:C:38:ILE:HD12	3:C:193:ALA:HB2	1.98	0.45
1:O:14:ARG:HD3	1:O:14:ARG:HA	1.74	0.45
2:P:196:LEU:HD13	2:P:209:ILE:HD12	1.98	0.45
7:U:51:LYS:HE2	7:U:51:LYS:HB3	1.62	0.45
8:V:129:SER:HA	15:V:201:WPI:C45	2.45	0.45
9:W:135:MET:O	9:W:139:GLU:HB2	2.16	0.45
5:E:39:GLY:HA2	5:E:47:VAL:O	2.17	0.45
8:H:129:SER:H	15:H:300:WPI:C43	2.29	0.45
15:W:301:WPI:H37	15:W:301:WPI:H32	1.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:8:TYR:CZ	14:2:162:VAL:HG13	2.52	0.45
4:D:73:LEU:HD22	4:D:86:ILE:HG12	1.99	0.45
7:G:48:ALA:HA	7:G:214:GLU:O	2.17	0.45
4:R:133:THR:O	4:R:149:GLN:HA	2.17	0.45
1:A:214:LEU:HB3	1:A:216:THR:HG22	1.99	0.45
2:B:150:VAL:HG23	2:B:156:TYR:HB3	1.99	0.45
4:D:55:GLN:NE2	4:D:60:THR:HG21	2.32	0.45
9:I:173:VAL:HB	9:I:191:LEU:HB2	1.99	0.45
1:O:240:ASN:O	1:O:244:ARG:HG2	2.16	0.45
10:J:188:LYS:HE2	10:J:190:TYR:CE2	2.52	0.44
1:O:231:ASP:O	1:O:232:LYS:HB2	2.17	0.44
3:Q:120:GLN:HG3	4:R:80:ALA:HB1	1.99	0.44
6:T:46:LEU:HB2	6:T:214:ALA:HB3	1.99	0.44
15:Z:301:WPI:H33	15:Z:301:WPI:H37	1.52	0.44
5:E:241:LYS:O	5:E:244:LYS:HG2	2.17	0.44
7:G:94:GLU:HG3	7:G:114:ARG:HH11	1.83	0.44
1:O:135:ARG:HG3	1:O:136:PRO:O	2.17	0.44
5:S:86:ARG:HA	5:S:86:ARG:HD3	1.75	0.44
3:C:239:LEU:HD23	3:C:239:LEU:HA	1.88	0.44
8:H:182:GLY:HA3	16:H:403:HOH:O	2.17	0.44
14:N:211:TRP:CH2	8:V:171:GLY:HA2	2.52	0.44
2:P:165:GLY:O	2:P:168:SER:HB3	2.17	0.44
3:Q:137:TYR:HB2	3:Q:149:TYR:HB2	1.99	0.44
10:X:89:ARG:HG3	10:X:94:TYR:CE2	2.52	0.44
12:Z:7:ARG:HB3	12:Z:12:ILE:HG12	1.99	0.44
3:C:107:PRO:HD2	3:C:110:ILE:HD12	1.98	0.44
4:D:163:THR:HG23	4:D:168:SER:HB2	1.98	0.44
8:H:133:PHE:HA	8:V:132:THR:O	2.17	0.44
9:I:1:THR:OG1	15:I:301:WPI:H50	2.16	0.44
11:K:18:LYS:HG2	11:K:179:ILE:HG13	1.99	0.44
14:N:153:ARG:NH2	16:N:320:HOH:O	2.50	0.44
13:M:132:ALA:HB1	13:M:186:HIS:CE1	2.52	0.44
1:O:131:ARG:HD3	1:O:133:TYR:CE2	2.52	0.44
7:U:110:ALA:O	7:U:114:ARG:HG2	2.18	0.44
13:1:29:ARG:NH1	13:1:191:ASP:OD1	2.44	0.44
10:J:182:LYS:HB3	10:J:182:LYS:HE2	1.72	0.44
12:L:19:ARG:O	12:L:33:ARG:NH2	2.49	0.44
12:L:31:VAL:HG12	12:L:33:ARG:HG2	1.98	0.44
1:O:135:ARG:HB3	7:U:12:SER:OG	2.17	0.44
4:R:236:ILE:O	4:R:240:LYS:HB2	2.18	0.44
6:T:146:GLU:O	6:T:153:VAL:HA	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:62:ASN:CB	9:W:82:MET:HE1	2.47	0.44
1:A:81:MET:HE3	1:A:83:VAL:CG2	2.48	0.44
2:B:17:LYS:HE3	2:B:22:ASP:OD2	2.17	0.44
3:C:19:LEU:O	3:C:23:GLU:HG2	2.18	0.44
6:F:176:LEU:HD13	7:G:57:LEU:HD23	2.00	0.44
9:I:128:GLY:CA	15:I:301:WPI:H42	2.47	0.44
11:K:171:MET:HA	11:K:172:PRO:HD3	1.89	0.44
1:O:12:TYR:C	1:O:14:ARG:H	2.26	0.44
4:R:175:LEU:HD12	4:R:175:LEU:HA	1.80	0.44
11:Y:3:ILE:HD13	11:Y:3:ILE:HA	1.73	0.44
12:Z:25:TRP:HH2	13:1:138:MET:HB2	1.83	0.44
2:B:196:LEU:HA	2:B:196:LEU:HD12	1.77	0.44
7:G:56:LYS:HA	7:G:56:LYS:HD3	1.63	0.44
9:W:51:ASP:HB3	9:W:94:ILE:HG23	2.00	0.44
11:Y:142:LEU:HG	11:Y:162:LEU:HD23	1.99	0.44
12:Z:145:LYS:HB2	12:Z:148:LEU:HD13	2.00	0.44
1:A:127:ILE:HD13	1:A:131:ARG:HD2	2.00	0.44
5:E:123:PHE:CE2	5:E:137:PRO:HG3	2.53	0.44
13:M:205:LYS:HB2	13:M:205:LYS:HE3	1.60	0.44
14:N:17:ASP:HA	14:N:187:PHE:CB	2.48	0.44
14:N:131:SER:HB3	14:N:133:THR:O	2.18	0.44
2:P:106:PRO:HA	2:P:140:ASP:HB3	2.00	0.44
3:Q:77:VAL:HG22	3:Q:135:PHE:CE1	2.53	0.44
1:A:105:ARG:HH2	14:2:222:THR:CG2	2.31	0.43
6:F:70:MET:HE2	6:F:70:MET:HB3	1.84	0.43
8:H:59:VAL:HG22	8:H:81:VAL:HG12	2.00	0.43
12:L:44:THR:O	12:L:99:THR:OG1	2.30	0.43
14:N:-7:GLN:NE2	14:N:101:PRO:O	2.51	0.43
1:O:205:PHE:C	1:O:205:PHE:CD2	2.96	0.43
4:R:200:LEU:HA	4:R:203:VAL:HG12	1.98	0.43
6:T:13:PHE:HB2	7:U:22:GLN:OE1	2.18	0.43
7:U:201:LEU:O	7:U:204:GLU:HG2	2.18	0.43
8:V:175:MET:HE3	8:V:188:PHE:CE2	2.53	0.43
12:Z:67:GLU:HG3	12:Z:72:GLU:O	2.18	0.43
6:F:185:ASN:ND2	6:F:188:GLU:HB2	2.32	0.43
10:J:33:LYS:HB3	10:J:44:ILE:O	2.18	0.43
13:M:40:ASN:OD1	13:M:202:GLY:HA2	2.18	0.43
1:O:128:TYR:CE1	1:O:134:MET:HE2	2.53	0.43
8:V:190:PRO:C	8:V:192:GLU:H	2.26	0.43
6:F:80:ASP:OD1	6:F:126:ARG:NH1	2.49	0.43
10:J:54:LEU:HD12	10:J:54:LEU:HA	1.73	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:194:VAL:O	6:T:197:ILE:HG22	2.18	0.43
7:U:87:LEU:HD11	7:U:119:VAL:HG22	1.99	0.43
8:V:107:LYS:HB2	8:V:107:LYS:HE3	1.83	0.43
1:A:115:ASP:OD2	1:A:115:ASP:N	2.52	0.43
6:F:187:ASP:OD2	6:F:187:ASP:N	2.51	0.43
7:G:246:ILE:HG13	7:G:247:ASN:OD1	2.19	0.43
2:P:149:GLN:O	2:P:156:TYR:HA	2.19	0.43
2:P:196:LEU:HD23	2:P:196:LEU:HA	1.82	0.43
4:R:13:PRO:HA	5:S:26:TYR:CD1	2.54	0.43
4:R:94:GLN:HG3	11:Y:65:LEU:HB2	2.00	0.43
9:W:129:SER:HB3	15:W:301:WPI:C44	2.49	0.43
9:W:162:GLY:O	9:W:166:ASP:HB3	2.19	0.43
4:D:238:GLN:H	4:D:238:GLN:HG2	1.70	0.43
7:G:208:GLU:HG2	7:G:209:LYS:HG2	2.00	0.43
8:H:4:MET:SD	8:H:159:LEU:HD13	2.58	0.43
10:J:36:HIS:HB3	10:J:41:PHE:CD1	2.53	0.43
11:K:184:ASP:HB2	16:K:205:HOH:O	2.18	0.43
12:L:4:LEU:HD13	12:L:140:LEU:HD11	2.00	0.43
13:M:185:ARG:NH2	9:W:29:LYS:HE2	2.33	0.43
14:N:133:THR:HG21	14:N:147:LEU:HB3	2.01	0.43
3:Q:87:LEU:HD12	3:Q:87:LEU:HA	1.72	0.43
6:T:15:PRO:HA	7:U:25:TYR:CG	2.53	0.43
3:C:49:GLU:OE2	3:C:210:ARG:NH2	2.51	0.43
4:D:67:ILE:HG21	4:D:109:LEU:HD21	2.01	0.43
5:E:13:SER:HB3	6:F:126:ARG:HG2	2.00	0.43
5:S:53:ARG:HA	16:S:303:HOH:O	2.19	0.43
9:W:138:LEU:HD12	9:W:138:LEU:HA	1.89	0.43
5:E:84:ASP:CG	5:E:136:ARG:HH22	2.27	0.43
6:F:191:LYS:HA	6:F:194:VAL:HG12	2.01	0.43
14:N:62:LEU:HD12	14:N:62:LEU:HA	1.72	0.43
2:P:203:GLU:O	2:P:208:THR:HG21	2.19	0.43
3:Q:43:GLY:HA2	3:Q:146:TYR:CE1	2.53	0.43
6:T:130:VAL:O	6:T:149:PRO:HG3	2.19	0.43
1:A:12:TYR:C	1:A:14:ARG:N	2.77	0.43
1:A:240:ASN:O	1:A:244:ARG:HG2	2.18	0.43
2:B:46:ALA:HB1	2:B:196:LEU:HD22	2.01	0.43
4:D:13:PRO:HA	5:E:26:TYR:CD1	2.53	0.43
6:F:227:GLY:O	6:F:230:VAL:HG12	2.19	0.43
2:P:193:LEU:HD12	2:P:193:LEU:HA	1.86	0.43
3:Q:181:LYS:O	3:Q:184:MET:HB2	2.19	0.43
4:R:73:LEU:HD22	4:R:86:ILE:HG12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:131:GLU:HB3	5:S:133:LEU:HG	2.00	0.43
11:Y:4:LEU:HD23	11:Y:131:ALA:HB2	2.00	0.43
13:1:-5:TYR:CD1	13:1:97:TYR:HB2	2.54	0.43
14:2:119:LEU:HG	14:2:134:LEU:HD12	2.00	0.43
3:Q:242:THR:HG22	3:Q:243:GLY:H	1.84	0.43
12:Z:13:ILE:HD12	12:Z:154:LEU:HD23	1.99	0.43
13:1:88:LEU:HD23	13:1:120:GLY:HA2	2.01	0.43
1:A:198:SER:OG	1:A:200:GLU:HG2	2.18	0.43
5:E:167:TYR:CZ	5:E:170:LYS:HD3	2.54	0.43
6:F:126:ARG:HD2	6:F:127:PRO:O	2.19	0.43
6:F:201:LEU:HD21	6:F:206:LEU:HG	2.01	0.43
7:G:165:GLY:O	7:G:168:ARG:HB3	2.19	0.43
2:P:40:THR:HG23	2:P:183:LEU:O	2.19	0.43
3:Q:120:GLN:CG	4:R:80:ALA:HB1	2.49	0.43
6:T:46:LEU:HG	6:T:73:SER:HB3	1.99	0.43
11:Y:171:MET:HA	11:Y:172:PRO:HD3	1.88	0.43
14:2:142:MET:C	14:2:145:PRO:HD2	2.44	0.43
1:A:69:VAL:HA	7:G:157:TRP:CZ3	2.53	0.42
4:R:48:ARG:HB3	4:R:209:ASN:HA	2.01	0.42
4:R:117:GLN:OE1	4:R:150:THR:HG23	2.19	0.42
10:X:54:LEU:HA	10:X:54:LEU:HD12	1.62	0.42
4:D:55:GLN:HE21	4:D:60:THR:HG21	1.84	0.42
7:G:15:SER:OG	7:G:17:ASP:OD2	2.28	0.42
7:G:53:ILE:HG13	7:G:211:PHE:HA	2.00	0.42
9:I:110:LEU:HG	9:I:125:LEU:HD12	2.01	0.42
10:J:106:LYS:HE3	10:J:106:LYS:HB3	1.88	0.42
14:N:121:TYR:HB2	14:N:134:LEU:HD13	2.01	0.42
1:O:174:LYS:O	1:O:178:ILE:HG13	2.19	0.42
1:O:188:LYS:HB3	1:O:188:LYS:HE2	1.78	0.42
1:O:211:ILE:HG23	1:O:216:THR:O	2.19	0.42
7:U:78:SER:HB2	7:U:164:THR:HG23	2.01	0.42
8:V:112:THR:CG2	8:V:120:HIS:HB2	2.49	0.42
11:Y:20:VAL:HG11	12:Z:122:LEU:HD11	2.01	0.42
13:1:100:THR:HB	13:1:116:PHE:HB2	2.00	0.42
1:A:72:ILE:HG13	1:A:224:GLU:OE1	2.20	0.42
2:B:57:MET:HE3	2:B:60:THR:HG21	2.01	0.42
5:E:175:GLY:HA3	5:E:207:VAL:CG1	2.49	0.42
1:O:158:ASP:OD2	1:O:162:TYR:HB2	2.20	0.42
3:Q:211:LEU:HD12	3:Q:211:LEU:HA	1.89	0.42
4:R:73:LEU:HD12	4:R:135:ILE:CG1	2.47	0.42
6:T:71:GLY:HA3	6:T:222:PHE:CZ	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:91:LYS:HD3	13:1:96:TYR:CZ	2.54	0.42
13:1:116:PHE:HA	13:1:121:SER:O	2.19	0.42
3:C:241:LYS:HB3	3:C:241:LYS:HE2	1.79	0.42
8:H:107:LYS:HB3	8:H:108:GLY:H	1.65	0.42
11:K:20:VAL:HG11	12:L:122:LEU:HD11	2.01	0.42
14:N:40:ASN:O	14:N:110:GLY:HA3	2.19	0.42
6:T:46:LEU:HD12	6:T:46:LEU:HA	1.85	0.42
8:V:175:MET:HB2	8:V:186:LEU:HB2	2.02	0.42
1:A:123:ASN:O	1:A:127:ILE:HG23	2.19	0.42
3:C:173:GLN:HE21	4:D:52:LEU:CD1	2.32	0.42
3:C:219:GLY:C	3:C:221:ASN:H	2.28	0.42
4:D:230:ASN:O	4:D:233:VAL:HG23	2.20	0.42
5:E:78:MET:HE1	5:E:89:ILE:HD11	2.01	0.42
13:M:83:ASN:C	13:M:83:ASN:HD22	2.26	0.42
3:Q:39:MET:HG3	3:Q:44:ILE:HD13	2.01	0.42
6:T:207:THR:HG22	6:T:208:VAL:H	1.85	0.42
10:X:49:THR:O	11:Y:84:ARG:NH2	2.52	0.42
13:1:4:LEU:HD13	13:1:129:ALA:HB2	2.01	0.42
13:1:35:PHE:O	13:1:42:VAL:HA	2.19	0.42
3:C:183:ASP:OD2	3:C:183:ASP:N	2.52	0.42
4:D:181:ARG:NH2	5:E:59:LEU:O	2.52	0.42
15:I:301:WPI:H12	15:I:301:WPI:H19	1.56	0.42
14:N:209:MET:HE2	14:N:211:TRP:HE1	1.84	0.42
14:2:-5:PRO:HD3	14:2:103:TRP:CE2	2.54	0.42
14:2:1:THR:OG1	14:2:2:SER:N	2.51	0.42
3:C:185:LYS:HE2	3:C:185:LYS:HB3	1.81	0.42
5:E:24:VAL:O	5:E:28:LEU:HD22	2.20	0.42
13:M:-2:ASN:HA	13:M:21:ILE:O	2.20	0.42
1:O:241:ILE:HG22	1:O:245:LEU:HD22	2.01	0.42
2:P:37:ILE:HD12	2:P:188:ALA:O	2.20	0.42
3:Q:2:GLY:HA3	6:T:123:TYR:CZ	2.54	0.42
6:T:93:ASN:HD22	6:T:93:ASN:HA	1.66	0.42
11:Y:84:ARG:HG3	11:Y:124:LYS:CB	2.49	0.42
13:1:5:GLY:O	13:1:127:CYS:HA	2.19	0.42
14:2:41:THR:OG1	14:2:81:PRO:HG3	2.20	0.42
4:D:144:GLU:HA	4:D:145:PRO:HD2	1.95	0.42
6:F:71:GLY:HA3	6:F:222:PHE:CE1	2.55	0.42
9:I:213:LEU:HD21	10:J:192:LYS:HG3	2.01	0.42
14:N:212:ASP:OD1	14:N:215:LYS:HE3	2.20	0.42
2:P:205:ASN:H	2:P:208:THR:CG2	2.33	0.42
3:Q:242:THR:HG22	3:Q:243:GLY:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:86:HIS:CD2	7:U:86:HIS:C	2.97	0.42
14:2:201:LYS:HB3	14:2:204:LEU:HD11	2.01	0.42
1:A:85:GLY:HA3	1:A:139:VAL:HG12	2.02	0.42
1:A:87:ILE:H	1:A:87:ILE:HG13	1.54	0.42
1:A:232:LYS:HA	1:A:232:LYS:HD2	1.84	0.42
5:E:168:ASN:HB3	5:E:187:TRP:CE2	2.55	0.42
7:G:181:HIS:C	7:G:183:PRO:HD3	2.45	0.42
8:H:175:MET:HB2	8:H:186:LEU:HB2	2.02	0.42
9:I:63:ILE:HD13	9:I:63:ILE:HA	1.88	0.42
1:O:65:ASP:HA	1:O:66:PRO:HD3	1.86	0.42
5:S:210:GLU:HB3	5:S:216:ASN:HD21	1.84	0.42
5:S:222:ILE:O	5:S:222:ILE:HG13	2.18	0.42
14:2:202:LYS:HB3	14:2:202:LYS:HE3	1.88	0.42
5:E:201:LEU:HD12	5:E:201:LEU:HA	1.90	0.42
9:I:8:PHE:HB3	9:I:151:ALA:HB2	2.02	0.42
2:P:222:LEU:HD12	2:P:222:LEU:HA	1.86	0.42
5:S:67:ILE:HG22	5:S:228:PHE:HZ	1.84	0.42
9:W:2:THR:OG1	9:W:130:GLY:HA3	2.20	0.42
9:W:201:LYS:HB3	9:W:203:TYR:CZ	2.55	0.42
2:B:61:LEU:HD13	2:B:61:LEU:HA	1.80	0.41
2:B:231:LYS:HE3	2:B:231:LYS:HB2	1.85	0.41
3:C:201:THR:C	3:C:203:SER:H	2.28	0.41
5:E:186:GLU:HB3	5:E:199:LEU:HD11	2.01	0.41
11:K:138:TYR:OH	11:Y:24:ILE:HG12	2.20	0.41
13:M:91:LYS:HD3	13:M:96:TYR:CE2	2.55	0.41
2:P:82:TYR:O	2:P:86:VAL:HG23	2.20	0.41
3:Q:39:MET:HE1	4:R:56:ASP:OD2	2.20	0.41
7:U:55:SER:OG	7:U:56:LYS:N	2.53	0.41
9:W:173:VAL:HB	9:W:191:LEU:HB2	2.01	0.41
1:A:133:TYR:CE2	1:A:134:MET:HE2	2.55	0.41
1:A:144:VAL:HG12	1:A:154:ILE:HG12	2.02	0.41
1:A:167:LYS:HG2	2:B:55:LEU:O	2.20	0.41
1:A:236:LEU:HB3	1:A:240:ASN:HB2	2.01	0.41
9:I:218:VAL:HB	10:J:186:VAL:HG12	2.01	0.41
13:M:-5:TYR:CE1	13:M:97:TYR:HB2	2.55	0.41
6:T:93:ASN:ND2	13:1:64:LYS:HE3	2.35	0.41
7:U:37:ILE:HG22	7:U:163:ALA:HB2	2.01	0.41
4:D:43:VAL:HG22	4:D:214:VAL:HG22	2.02	0.41
6:F:45:VAL:CG1	6:F:189:LEU:HG	2.50	0.41
14:N:31:VAL:HG11	14:N:49:ILE:HD13	2.01	0.41
1:O:164:VAL:HG12	1:O:165:GLY:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:137:ALA:O	2:P:214:ILE:HG13	2.21	0.41
7:U:37:ILE:HG22	7:U:163:ALA:CB	2.50	0.41
13:1:117:ASP:HB3	13:1:119:VAL:N	2.32	0.41
6:F:46:LEU:HD13	6:F:135:ILE:HG23	2.03	0.41
7:G:78:SER:OG	7:G:164:THR:HG23	2.20	0.41
1:O:30:TYR:O	1:O:33:LYS:HB3	2.20	0.41
2:P:119:GLN:HG3	2:P:120:GLU:N	2.32	0.41
4:R:29:ARG:HB2	4:R:29:ARG:NH1	2.35	0.41
8:V:83:LYS:HG2	8:V:117:GLY:O	2.19	0.41
11:K:176:LYS:NZ	11:Y:169:LYS:HA	2.35	0.41
12:L:17:ASP:O	12:L:33:ARG:HG3	2.21	0.41
3:Q:37:GLY:O	3:Q:162:ALA:HA	2.21	0.41
4:R:68:ASP:OD1	4:R:97:ARG:NH2	2.53	0.41
2:B:55:LEU:HD12	2:B:55:LEU:HA	1.77	0.41
3:C:58:GLU:O	3:C:62:SER:HB2	2.20	0.41
10:J:86:LEU:HD11	10:J:98:PRO:HG2	2.02	0.41
11:K:55:PHE:CZ	11:K:87:LEU:HD13	2.55	0.41
12:L:12:ILE:HG13	12:L:110:PRO:HB3	2.02	0.41
14:N:5:SER:HB2	14:N:13:ILE:O	2.19	0.41
6:T:211:LEU:HB3	6:T:230:VAL:HG21	2.02	0.41
7:U:27:VAL:O	7:U:30:VAL:HB	2.20	0.41
7:U:173:ALA:O	7:U:176:GLU:HB2	2.20	0.41
8:V:129:SER:CA	15:V:201:WPI:H52	2.47	0.41
9:W:104:ASP:HB2	9:W:105:PRO:HD2	2.01	0.41
13:1:151:TYR:CG	13:1:157:GLY:HA2	2.56	0.41
13:M:96:TYR:HB3	13:M:98:VAL:HG22	2.03	0.41
1:O:179:THR:O	1:O:183:GLU:HG3	2.21	0.41
5:S:114:GLN:NE2	5:S:118:ASP:OD1	2.54	0.41
6:T:12:THR:HG23	7:U:22:GLN:HE22	1.84	0.41
6:T:157:TYR:OH	7:U:60:PRO:HD2	2.20	0.41
7:U:169:GLN:H	7:U:169:GLN:NE2	2.18	0.41
12:Z:177:LEU:HD12	12:Z:177:LEU:HA	1.87	0.41
14:2:122:VAL:HA	14:2:127:VAL:O	2.21	0.41
2:B:2:THR:O	2:B:4:ARG:HD3	2.20	0.41
8:H:24:ALA:HB3	14:2:138:PHE:HE2	1.86	0.41
3:Q:184:MET:HG2	3:Q:188:ASP:CB	2.50	0.41
5:S:167:TYR:CG	5:S:170:LYS:HB2	2.55	0.41
6:T:19:LEU:O	6:T:23:GLU:HG3	2.20	0.41
6:T:39:ARG:NH1	6:T:40:SER:O	2.54	0.41
13:1:169:GLU:CD	13:1:169:GLU:H	2.29	0.41
1:A:189:SER:HB3	1:A:191:ILE:HG12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:111:ARG:HE	4:D:111:ARG:HB3	1.61	0.41
8:H:3:ILE:HD12	8:H:98:ILE:HD12	2.03	0.41
10:J:155:PHE:CE1	10:J:189:ARG:HD2	2.56	0.41
13:M:6:ILE:HG13	13:M:127:CYS:HB2	2.03	0.41
14:N:-6:GLN:O	14:N:-6:GLN:HG3	2.21	0.41
14:N:121:TYR:HE1	14:N:136:THR:HG22	1.85	0.41
8:V:14:LEU:O	8:V:175:MET:HA	2.20	0.41
9:W:138:LEU:HD13	9:W:158:ALA:HB2	2.02	0.41
9:W:206:PRO:O	9:W:209:THR:OG1	2.36	0.41
14:2:219:GLY:HA3	14:2:223:GLN:HB3	2.03	0.41
1:A:148:GLU:HB3	1:A:230:LYS:NZ	2.36	0.41
2:B:23:TYR:N	2:B:23:TYR:CD1	2.88	0.41
2:B:168:SER:O	2:B:172:LYS:HB2	2.21	0.41
8:H:45:ARG:HB3	8:H:52:THR:CG2	2.51	0.41
10:J:28:SER:HB2	11:K:125:VAL:HG21	2.03	0.41
12:L:16:VAL:HG21	12:L:33:ARG:HB2	2.03	0.41
13:M:5:GLY:HA2	13:M:13:VAL:O	2.21	0.41
1:O:245:LEU:HD12	1:O:245:LEU:HA	1.82	0.41
2:P:97:TYR:CE1	2:P:109:LEU:HD23	2.56	0.41
3:Q:160:TRP:CE3	3:Q:163:ILE:HD13	2.56	0.41
5:S:201:LEU:HD12	5:S:212:LEU:HD21	2.03	0.41
7:U:17:ASP:OD1	7:U:19:ARG:HD3	2.20	0.41
13:1:43:MET:HE3	13:1:84:ILE:HD13	2.02	0.41
14:2:160:THR:HA	16:2:330:HOH:O	2.20	0.41
1:A:83:VAL:HG11	1:A:90:ALA:CB	2.51	0.40
5:E:78:MET:HE2	5:E:78:MET:HB3	1.93	0.40
6:F:156:LEU:HD23	7:G:58:LEU:HA	2.01	0.40
7:G:106:ILE:HA	7:G:107:PRO:HD3	1.94	0.40
13:M:8:GLY:HA3	13:M:11:PHE:CZ	2.56	0.40
7:U:193:LYS:HE3	7:U:193:LYS:HB2	1.81	0.40
9:W:78:SER:O	9:W:82:MET:HG3	2.21	0.40
13:1:99:HIS:HE1	13:1:128:ARG:HD2	1.87	0.40
1:A:40:ILE:HD13	1:A:40:ILE:HA	1.87	0.40
1:A:77:ARG:HD2	1:A:77:ARG:HA	1.97	0.40
4:D:149:GLN:O	4:D:156:TYR:HA	2.21	0.40
4:D:203:VAL:O	4:D:204:GLN:HG2	2.20	0.40
5:E:243:LEU:O	5:E:247:GLU:HB2	2.21	0.40
9:I:46:ALA:O	9:I:97:TYR:HB2	2.21	0.40
6:T:221:PRO:O	6:T:223:THR:OG1	2.38	0.40
10:X:86:LEU:HD12	10:X:86:LEU:HA	1.88	0.40
12:Z:33:ARG:O	12:Z:45:MET:N	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:87:LEU:HD12	13:1:87:LEU:HA	1.83	0.40
1:A:78:THR:CG2	1:A:231:ASP:HA	2.50	0.40
3:C:97:ASN:OD1	10:J:60:TYR:HE1	2.05	0.40
4:D:48:ARG:HG2	4:D:49:ARG:H	1.86	0.40
5:E:163:THR:HG23	6:F:60:GLN:NE2	2.36	0.40
7:G:68:VAL:HB	7:G:227:HIS:HD1	1.87	0.40
9:I:172:ASN:OD1	9:I:192:THR:HG22	2.20	0.40
12:L:73:ARG:CZ	12:L:105:THR:HG22	2.52	0.40
1:O:53:VAL:HG13	1:O:144:VAL:HG11	2.02	0.40
1:O:178:ILE:HG13	1:O:178:ILE:H	1.69	0.40
2:P:217:GLU:O	2:P:219:PRO:HD3	2.21	0.40
13:1:99:HIS:HD2	13:1:116:PHE:O	2.03	0.40
13:1:112:ALA:HB2	13:1:124:ARG:NH2	2.37	0.40
1:O:12:TYR:C	1:O:14:ARG:N	2.79	0.40
1:O:82:VAL:CG1	1:O:142:THR:HB	2.52	0.40
1:O:196:GLU:HG2	1:O:201:LYS:HB2	2.03	0.40
4:R:224:LEU:HB3	4:R:228:GLU:OE2	2.22	0.40
4:R:236:ILE:H	4:R:236:ILE:HG12	1.72	0.40
5:S:14:THR:HG21	6:T:8:GLY:O	2.20	0.40
15:V:201:WPI:H8	15:V:201:WPI:H1	1.75	0.40
3:C:48:ALA:HB1	3:C:65:LYS:HE3	2.03	0.40
5:E:126:GLY:C	5:E:128:SER:H	2.30	0.40
8:H:143:ARG:NH2	8:H:146:MET:HE3	2.37	0.40
15:L:301:WPI:H51	15:L:301:WPI:H54	2.03	0.40
1:O:124:LEU:HD23	1:O:124:LEU:HA	1.81	0.40
2:P:130:PHE:O	2:P:152:PRO:HB3	2.21	0.40
2:P:215:GLY:O	2:P:234:ARG:NH1	2.53	0.40
4:R:24:LEU:HD23	4:R:24:LEU:HA	1.96	0.40
5:S:50:VAL:HG21	5:S:66:LYS:HB2	2.02	0.40
5:S:143:LEU:HA	5:S:156:PHE:O	2.22	0.40
13:1:-5:TYR:CE1	13:1:97:TYR:HB2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/241 (99%)	229 (96%)	9 (4%)	1 (0%)	30	49
1	O	239/241 (99%)	230 (96%)	7 (3%)	2 (1%)	16	31
2	B	247/250 (99%)	230 (93%)	17 (7%)	0	100	100
2	P	247/250 (99%)	236 (96%)	9 (4%)	2 (1%)	16	31
3	C	242/244 (99%)	232 (96%)	8 (3%)	2 (1%)	16	31
3	Q	242/244 (99%)	231 (96%)	9 (4%)	2 (1%)	16	31
4	D	239/241 (99%)	224 (94%)	13 (5%)	2 (1%)	16	31
4	R	239/241 (99%)	225 (94%)	11 (5%)	3 (1%)	9	18
5	E	240/242 (99%)	228 (95%)	10 (4%)	2 (1%)	16	31
5	S	240/242 (99%)	222 (92%)	16 (7%)	2 (1%)	16	31
6	F	230/233 (99%)	217 (94%)	13 (6%)	0	100	100
6	T	230/233 (99%)	219 (95%)	10 (4%)	1 (0%)	30	49
7	G	242/244 (99%)	234 (97%)	8 (3%)	0	100	100
7	U	242/244 (99%)	229 (95%)	11 (4%)	2 (1%)	16	31
8	H	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
8	V	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
9	I	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
9	W	220/222 (99%)	215 (98%)	4 (2%)	1 (0%)	24	43
10	J	202/204 (99%)	193 (96%)	8 (4%)	1 (0%)	24	43
10	X	202/204 (99%)	195 (96%)	7 (4%)	0	100	100
11	K	194/198 (98%)	185 (95%)	8 (4%)	1 (0%)	24	43
11	Y	194/198 (98%)	185 (95%)	9 (5%)	0	100	100
12	L	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
12	Z	210/212 (99%)	200 (95%)	10 (5%)	0	100	100
13	1	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
13	M	220/222 (99%)	208 (94%)	12 (6%)	0	100	100
14	2	231/233 (99%)	218 (94%)	12 (5%)	1 (0%)	30	49
14	N	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
All	All	6300/6364 (99%)	6002 (95%)	273 (4%)	25 (0%)	30	49

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	131	GLU
5	E	132	ARG
7	U	246	ILE
4	R	185	PRO
4	R	186	ALA
9	W	171	SER
4	D	185	PRO
4	D	204	GLN
11	K	8	VAL
1	O	60	PRO
1	A	195	ASN
3	C	70	ASN
3	C	220	ALA
2	P	52	SER
2	P	166	LYS
3	Q	4	ARG
5	S	134	MET
10	J	92	GLY
3	Q	205	ALA
7	U	34	THR
14	2	75	ALA
1	O	195	ASN
4	R	206	GLY
5	S	129	GLY
6	T	149	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 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	205/205 (100%)	189 (92%)	16 (8%)	11 24
1	O	205/205 (100%)	183 (89%)	22 (11%)	6 13
2	B	208/209 (100%)	189 (91%)	19 (9%)	9 19
2	P	208/209 (100%)	177 (85%)	31 (15%)	3 6
3	C	203/203 (100%)	181 (89%)	22 (11%)	6 13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	203/203 (100%)	180 (89%)	23 (11%)	5	12
4	D	213/213 (100%)	197 (92%)	16 (8%)	12	26
4	R	213/213 (100%)	184 (86%)	29 (14%)	3	8
5	E	198/198 (100%)	176 (89%)	22 (11%)	6	12
5	S	198/198 (100%)	173 (87%)	25 (13%)	4	9
6	F	191/192 (100%)	167 (87%)	24 (13%)	4	9
6	T	191/192 (100%)	153 (80%)	38 (20%)	1	2
7	G	201/201 (100%)	176 (88%)	25 (12%)	4	9
7	U	201/201 (100%)	171 (85%)	30 (15%)	3	6
8	H	162/162 (100%)	151 (93%)	11 (7%)	14	31
8	V	162/162 (100%)	146 (90%)	16 (10%)	7	16
9	I	181/181 (100%)	168 (93%)	13 (7%)	13	28
9	W	181/181 (100%)	155 (86%)	26 (14%)	3	6
10	J	172/172 (100%)	151 (88%)	21 (12%)	5	10
10	X	172/172 (100%)	155 (90%)	17 (10%)	7	16
11	K	174/175 (99%)	157 (90%)	17 (10%)	7	16
11	Y	174/175 (99%)	155 (89%)	19 (11%)	6	13
12	L	169/169 (100%)	155 (92%)	14 (8%)	10	22
12	Z	169/169 (100%)	156 (92%)	13 (8%)	12	25
13	1	185/185 (100%)	174 (94%)	11 (6%)	18	37
13	M	185/185 (100%)	170 (92%)	15 (8%)	11	23
14	2	199/199 (100%)	179 (90%)	20 (10%)	7	15
14	N	199/199 (100%)	184 (92%)	15 (8%)	12	26
All	All	5322/5328 (100%)	4752 (89%)	570 (11%)	6	13

All (570) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	54	ILE
1	A	72	ILE
1	A	87	ILE
1	A	125	SER
1	A	126	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	127	ILE
1	A	163	TYR
1	A	164	VAL
1	A	177	GLU
1	A	187	LYS
1	A	196	GLU
1	A	200	GLU
1	A	231	ASP
1	A	242	GLU
1	A	244	ARG
2	B	2	THR
2	B	15	SER
2	B	29	LYS
2	B	55	LEU
2	B	61	LEU
2	B	63	LYS
2	B	85	LEU
2	B	146	SER
2	B	157	PHE
2	B	172	LYS
2	B	178	ARG
2	B	180	ASN
2	B	193	LEU
2	B	197	LYS
2	B	198	GLU
2	B	207	ASP
2	B	211	LEU
2	B	231	LYS
2	B	248	GLU
3	C	5	ARG
3	C	8	SER
3	C	34	THR
3	C	39	MET
3	C	49	GLU
3	C	51	LYS
3	C	61	THR
3	C	85	GLU
3	C	86	ILE
3	C	90	THR
3	C	103	ASN
3	C	120	GLN
3	C	125	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	158	THR
3	C	174	THR
3	C	178	MET
3	C	184	MET
3	C	185	LYS
3	C	186	VAL
3	C	207	THR
3	C	211	LEU
3	C	244	ILE
4	D	21	GLU
4	D	24	LEU
4	D	53	LYS
4	D	57	THR
4	D	58	ARG
4	D	66	LYS
4	D	71	VAL
4	D	132	SER
4	D	155	ILE
4	D	160	SER
4	D	182	LYS
4	D	198	SER
4	D	227	GLU
4	D	231	GLN
4	D	233	VAL
4	D	243	GLN
5	E	10	ARG
5	E	28	LEU
5	E	52	LYS
5	E	66	LYS
5	E	110	GLU
5	E	112	LEU
5	E	143	LEU
5	E	177	GLU
5	E	183	LEU
5	E	184	LEU
5	E	190	SER
5	E	191	LEU
5	E	192	THR
5	E	200	VAL
5	E	201	LEU
5	E	204	LEU
5	E	205	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	207	VAL
5	E	211	LYS
5	E	222	ILE
5	E	241	LYS
5	E	242	GLU
6	F	9	ASP
6	F	10	THR
6	F	16	THR
6	F	26	LEU
6	F	45	VAL
6	F	46	LEU
6	F	47	VAL
6	F	54	ASP
6	F	60	GLN
6	F	70	MET
6	F	74	LEU
6	F	93	ASN
6	F	96	SER
6	F	123	TYR
6	F	140	SER
6	F	164	ARG
6	F	172	LEU
6	F	181	LYS
6	F	197	ILE
6	F	201	LEU
6	F	208	VAL
6	F	213	ILE
6	F	230	VAL
6	F	234	ILE
7	G	10	SER
7	G	17	ASP
7	G	56	LYS
7	G	61	GLN
7	G	62	LYS
7	G	80	LEU
7	G	97	SER
7	G	100	LYS
7	G	104	THR
7	G	160	LYS
7	G	168	ARG
7	G	170	SER
7	G	176	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	178	LEU
7	G	186	LEU
7	G	190	GLU
7	G	192	VAL
7	G	204	GLU
7	G	217	TRP
7	G	220	LEU
7	G	226	LEU
7	G	228	LYS
7	G	237	GLU
7	G	239	ILE
7	G	244	LYS
8	H	1	THR
8	H	9	LYS
8	H	22	THR
8	H	52	THR
8	H	85	LEU
8	H	88	GLU
8	H	107	LYS
8	H	144	GLU
8	H	149	GLU
8	H	156	LYS
8	H	159	LEU
9	I	13	VAL
9	I	22	GLN
9	I	38	SER
9	I	43	CYS
9	I	55	VAL
9	I	77	VAL
9	I	78	SER
9	I	87	LEU
9	I	113	ILE
9	I	144	GLN
9	I	167	LEU
9	I	180	ILE
9	I	217	ILE
10	J	2	ILE
10	J	6	MET
10	J	18	LEU
10	J	20	LEU
10	J	54	LEU
10	J	88	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	106	LYS
10	J	109	LYS
10	J	116	ASP
10	J	120	CYS
10	J	123	GLU
10	J	125	LYS
10	J	137	LEU
10	J	140	MET
10	J	158	ILE
10	J	163	LEU
10	J	171	LEU
10	J	182	LYS
10	J	183	LYS
10	J	184	ASP
10	J	194	ARG
11	K	1	ASP
11	K	6	ILE
11	K	10	ASP
11	K	11	SER
11	K	17	SER
11	K	27	LEU
11	K	52	THR
11	K	59	ILE
11	K	68	ILE
11	K	87	LEU
11	K	110	LYS
11	K	126	GLU
11	K	141	SER
11	K	142	LEU
11	K	154	GLU
11	K	161	LYS
11	K	195	GLN
12	L	4	LEU
12	L	9	GLN
12	L	31	VAL
12	L	32	LYS
12	L	33	ARG
12	L	67	GLU
12	L	86	LEU
12	L	134	THR
12	L	147	ASP
12	L	148	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	149	SER
12	L	154	LEU
12	L	199	LYS
12	L	208	ASN
13	M	2	THR
13	M	44	SER
13	M	60	LYS
13	M	62	SER
13	M	87	LEU
13	M	110	LYS
13	M	121	SER
13	M	141	LEU
13	M	144	GLN
13	M	163	LEU
13	M	165	TYR
13	M	168	VAL
13	M	174	LEU
13	M	183	THR
13	M	201	ASP
14	N	57	ARG
14	N	58	LEU
14	N	59	LEU
14	N	65	GLU
14	N	79	LEU
14	N	94	GLN
14	N	102	LEU
14	N	106	ILE
14	N	130	SER
14	N	147	LEU
14	N	149	LYS
14	N	153	ARG
14	N	154	GLU
14	N	162	VAL
14	N	176	LEU
1	O	22	GLU
1	O	43	LEU
1	O	67	THR
1	O	68	THR
1	O	96	ARG
1	O	112	MET
1	O	115	ASP
1	O	149	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	150	LEU
1	O	157	THR
1	O	163	TYR
1	O	169	THR
1	O	175	GLN
1	O	180	THR
1	O	197	GLU
1	O	198	SER
1	O	210	MET
1	O	216	THR
1	O	231	ASP
1	O	244	ARG
1	O	245	LEU
1	O	246	VAL
2	P	9	LEU
2	P	11	THR
2	P	25	LEU
2	P	29	LYS
2	P	58	SER
2	P	59	GLU
2	P	68	THR
2	P	85	LEU
2	P	92	VAL
2	P	95	THR
2	P	107	THR
2	P	108	LYS
2	P	119	GLN
2	P	122	THR
2	P	132	VAL
2	P	157	PHE
2	P	169	VAL
2	P	172	LYS
2	P	175	LEU
2	P	176	GLU
2	P	184	GLU
2	P	193	LEU
2	P	194	LEU
2	P	198	GLU
2	P	211	LEU
2	P	229	THR
2	P	239	THR
2	P	241	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	242	GLU
2	P	246	ARG
2	P	248	GLU
3	Q	16	GLU
3	Q	23	GLU
3	Q	53	THR
3	Q	55	THR
3	Q	59	GLN
3	Q	60	ASP
3	Q	65	LYS
3	Q	66	LEU
3	Q	80	LEU
3	Q	87	LEU
3	Q	150	THR
3	Q	158	THR
3	Q	175	LEU
3	Q	191	GLU
3	Q	194	LEU
3	Q	198	SER
3	Q	201	THR
3	Q	211	LEU
3	Q	229	ILE
3	Q	237	ASP
3	Q	238	ILE
3	Q	239	LEU
3	Q	240	VAL
4	R	6	ARG
4	R	8	LEU
4	R	14	ASP
4	R	36	VAL
4	R	50	SER
4	R	57	THR
4	R	58	ARG
4	R	76	SER
4	R	78	LEU
4	R	85	LEU
4	R	102	ASP
4	R	132	SER
4	R	149	GLN
4	R	150	THR
4	R	173	GLU
4	R	175	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	R	176	GLU
4	R	187	THR
4	R	188	VAL
4	R	189	GLU
4	R	199	LEU
4	R	200	LEU
4	R	201	GLU
4	R	222	VAL
4	R	224	LEU
4	R	225	SER
4	R	226	SER
4	R	227	GLU
4	R	236	ILE
5	S	12	VAL
5	S	21	LEU
5	S	28	LEU
5	S	33	LEU
5	S	42	THR
5	S	60	GLU
5	S	61	SER
5	S	100	ASN
5	S	110	GLU
5	S	112	LEU
5	S	176	SER
5	S	177	GLU
5	S	186	GLU
5	S	191	LEU
5	S	198	LEU
5	S	199	LEU
5	S	201	LEU
5	S	210	GLU
5	S	222	ILE
5	S	223	THR
5	S	225	GLN
5	S	229	LYS
5	S	232	ASP
5	S	234	GLU
5	S	241	LYS
6	T	3	ARG
6	T	4	ASN
6	T	11	VAL
6	T	16	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	T	26	LEU
6	T	38	LEU
6	T	46	LEU
6	T	50	LYS
6	T	56	LEU
6	T	57	SER
6	T	61	LYS
6	T	63	ILE
6	T	74	LEU
6	T	84	LEU
6	T	86	ASN
6	T	93	ASN
6	T	97	LEU
6	T	107	ARG
6	T	111	LEU
6	T	112	LEU
6	T	156	LEU
6	T	164	ARG
6	T	170	THR
6	T	172	LEU
6	T	175	THR
6	T	178	THR
6	T	180	ILE
6	T	182	ILE
6	T	191	LYS
6	T	197	ILE
6	T	205	SER
6	T	206	LEU
6	T	207	THR
6	T	212	SER
6	T	219	ASP
6	T	220	THR
6	T	223	THR
6	T	230	VAL
7	U	10	SER
7	U	34	THR
7	U	42	ASN
7	U	52	LEU
7	U	55	SER
7	U	57	LEU
7	U	58	LEU
7	U	62	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	69	VAL
7	U	87	LEU
7	U	97	SER
7	U	115	LEU
7	U	127	SER
7	U	129	ARG
7	U	133	VAL
7	U	134	SER
7	U	142	LYS
7	U	151	GLU
7	U	164	THR
7	U	169	GLN
7	U	172	LYS
7	U	178	LEU
7	U	194	GLN
7	U	207	LYS
7	U	208	GLU
7	U	210	ASP
7	U	244	LYS
7	U	245	GLU
7	U	246	ILE
7	U	247	ASN
8	V	10	ASP
8	V	40	LYS
8	V	52	THR
8	V	63	LEU
8	V	83	LYS
8	V	85	LEU
8	V	103	ASP
8	V	106	ASN
8	V	143	ARG
8	V	149	GLU
8	V	161	GLN
8	V	168	SER
8	V	177	VAL
8	V	178	LEU
8	V	179	THR
8	V	196	LEU
9	W	13	VAL
9	W	17	ASP
9	W	18	THR
9	W	38	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	W	43	CYS
9	W	52	THR
9	W	55	VAL
9	W	56	THR
9	W	58	LEU
9	W	59	ILE
9	W	63	ILE
9	W	65	LEU
9	W	68	LEU
9	W	80	LEU
9	W	84	LYS
9	W	100	VAL
9	W	113	ILE
9	W	138	LEU
9	W	139	GLU
9	W	177	VAL
9	W	180	ILE
9	W	182	LYS
9	W	192	THR
9	W	200	GLN
9	W	214	LYS
9	W	218	VAL
10	X	14	ILE
10	X	20	LEU
10	X	32	GLU
10	X	54	LEU
10	X	60	TYR
10	X	64	LEU
10	X	67	LEU
10	X	69	GLU
10	X	86	LEU
10	X	109	LYS
10	X	120	CYS
10	X	123	GLU
10	X	135	ASP
10	X	137	LEU
10	X	140	MET
10	X	158	ILE
10	X	183	LYS
11	Y	3	ILE
11	Y	17	SER
11	Y	24	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	Y	37	LEU
11	Y	68	ILE
11	Y	70	GLU
11	Y	77	GLN
11	Y	84	ARG
11	Y	90	SER
11	Y	103	ILE
11	Y	121	LEU
11	Y	124	LYS
11	Y	126	GLU
11	Y	141	SER
11	Y	142	LEU
11	Y	157	LEU
11	Y	169	LYS
11	Y	171	MET
11	Y	173	MET
12	Z	1	THR
12	Z	7	ARG
12	Z	32	LYS
12	Z	67	GLU
12	Z	72	GLU
12	Z	87	VAL
12	Z	95	LEU
12	Z	107	LYS
12	Z	117	SER
12	Z	140	LEU
12	Z	148	LEU
12	Z	149	SER
12	Z	177	LEU
13	1	18	THR
13	1	25	SER
13	1	60	LYS
13	1	62	SER
13	1	64	LYS
13	1	87	LEU
13	1	88	LEU
13	1	155	THR
13	1	165	TYR
13	1	169	GLU
13	1	171	VAL
14	2	2	SER
14	2	14	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	2	26	LEU
14	2	29	ASN
14	2	58	LEU
14	2	72	LEU
14	2	74	ASP
14	2	76	GLU
14	2	79	LEU
14	2	88	LEU
14	2	96	ARG
14	2	124	LEU
14	2	125	LEU
14	2	130	SER
14	2	147	LEU
14	2	154	GLU
14	2	159	LYS
14	2	162	VAL
14	2	176	LEU
14	2	222	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	126	GLN
1	A	209	HIS
3	C	94	HIS
3	C	125	HIS
3	C	147	GLN
3	C	173	GLN
4	D	40	ASN
4	D	118	GLN
4	D	122	GLN
4	D	230	ASN
5	E	100	ASN
5	E	114	GLN
5	E	206	GLN
6	F	31	GLN
6	F	119	ASN
6	F	185	ASN
6	F	199	GLN
7	G	169	GLN
7	G	181	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	182	HIS
8	H	69	GLN
9	I	116	HIS
10	J	164	ASN
11	K	117	GLN
11	K	132	HIS
12	L	66	HIS
12	L	133	GLN
12	L	191	HIS
13	M	-7	ASN
13	M	27	ASN
13	M	83	ASN
13	M	86	HIS
13	M	188	GLN
14	N	203	ASN
1	O	240	ASN
3	Q	59	GLN
3	Q	173	GLN
5	S	147	HIS
5	S	157	HIS
5	S	216	ASN
6	T	199	GLN
7	U	67	GLN
7	U	146	HIS
7	U	236	GLN
8	V	28	ASN
8	V	161	GLN
9	W	35	HIS
9	W	116	HIS
9	W	165	ASN
9	W	172	ASN
10	X	148	ASN
10	X	160	GLN
10	X	195	GLN
11	Y	36	GLN
11	Y	145	HIS
12	Z	62	GLN
12	Z	66	HIS
12	Z	190	ASN
13	1	46	ASN
13	1	86	HIS
13	1	99	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	1	149	ASN
14	2	10	ASN
14	2	141	HIS
14	2	186	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	WPI	Z	301	-	43,43,43	2.16	12 (27%)	51,55,55	3.06	26 (50%)
15	WPI	W	301	-	43,43,43	2.08	9 (20%)	51,55,55	2.61	19 (37%)
15	WPI	H	300	-	43,43,43	2.13	11 (25%)	51,55,55	3.12	25 (49%)
15	WPI	V	201	-	43,43,43	2.10	9 (20%)	51,55,55	3.04	22 (43%)
15	WPI	L	301	-	43,43,43	2.20	13 (30%)	51,55,55	2.75	23 (45%)
15	WPI	I	301	-	43,43,43	2.08	12 (27%)	51,55,55	2.96	27 (52%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	WPI	Z	301	-	-	18/28/39/39	0/3/3/3
15	WPI	W	301	-	-	20/28/39/39	0/3/3/3
15	WPI	H	300	-	-	18/28/39/39	0/3/3/3
15	WPI	V	201	-	-	12/28/39/39	0/3/3/3
15	WPI	L	301	-	-	17/28/39/39	0/3/3/3
15	WPI	I	301	-	-	18/28/39/39	0/3/3/3

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	301	WPI	C31-C30	7.10	1.53	1.31
15	V	201	WPI	C31-C30	7.09	1.53	1.31
15	W	301	WPI	C31-C30	7.08	1.53	1.31
15	Z	301	WPI	C13-C14	7.00	1.53	1.31
15	Z	301	WPI	C31-C30	6.98	1.53	1.31
15	L	301	WPI	C13-C14	6.97	1.53	1.31
15	V	201	WPI	C13-C14	6.91	1.52	1.31
15	H	300	WPI	C31-C30	6.83	1.52	1.31
15	H	300	WPI	C13-C14	6.81	1.52	1.31
15	L	301	WPI	C31-C30	6.79	1.52	1.31
15	W	301	WPI	C13-C14	6.73	1.52	1.31
15	I	301	WPI	C13-C14	6.60	1.51	1.31
15	L	301	WPI	C36-C38	3.48	1.44	1.38
15	H	300	WPI	C36-C38	3.42	1.44	1.38
15	L	301	WPI	C10-C13	3.38	1.57	1.47
15	Z	301	WPI	C36-C38	3.36	1.44	1.38
15	Z	301	WPI	C10-C13	3.33	1.57	1.47
15	W	301	WPI	C33-C31	3.25	1.56	1.47
15	V	201	WPI	C7-C3	3.15	1.44	1.38
15	W	301	WPI	C35-C37	3.10	1.44	1.38
15	H	300	WPI	C10-C13	3.08	1.56	1.47
15	Z	301	WPI	C33-C31	3.06	1.56	1.47
15	V	201	WPI	C23-C21	-3.01	1.40	1.51
15	H	300	WPI	C33-C31	3.01	1.56	1.47
15	W	301	WPI	C10-C13	3.01	1.56	1.47
15	L	301	WPI	C35-C37	2.98	1.43	1.38
15	I	301	WPI	C33-C31	2.92	1.55	1.47
15	L	301	WPI	O42-C39	2.91	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	201	WPI	C10-C13	2.90	1.55	1.47
15	H	300	WPI	C23-C21	-2.90	1.40	1.51
15	Z	301	WPI	C23-C21	-2.88	1.40	1.51
15	L	301	WPI	C23-C21	-2.87	1.40	1.51
15	I	301	WPI	C10-C13	2.86	1.55	1.47
15	L	301	WPI	C33-C31	2.84	1.55	1.47
15	V	201	WPI	C33-C31	2.84	1.55	1.47
15	W	301	WPI	C23-C21	-2.81	1.41	1.51
15	I	301	WPI	C36-C38	2.80	1.43	1.38
15	Z	301	WPI	C7-C3	2.76	1.43	1.38
15	W	301	WPI	C36-C38	2.74	1.43	1.38
15	Z	301	WPI	O42-C39	2.73	1.43	1.38
15	H	300	WPI	C7-C3	2.69	1.43	1.38
15	I	301	WPI	C23-C21	-2.69	1.41	1.51
15	L	301	WPI	C5-C2	2.68	1.43	1.38
15	V	201	WPI	O4-C1	2.68	1.43	1.38
15	H	300	WPI	O42-C39	2.67	1.43	1.38
15	L	301	WPI	C7-C3	2.67	1.43	1.38
15	I	301	WPI	O41-C38	2.45	1.41	1.37
15	H	300	WPI	O6-C2	2.45	1.41	1.37
15	Z	301	WPI	C5-C2	2.43	1.43	1.38
15	I	301	WPI	C5-C2	2.41	1.42	1.38
15	W	301	WPI	C5-C2	2.41	1.42	1.38
15	W	301	WPI	C7-C3	2.39	1.42	1.38
15	I	301	WPI	C7-C3	2.39	1.42	1.38
15	V	201	WPI	C3-C1	2.33	1.45	1.41
15	H	300	WPI	C5-C2	2.27	1.42	1.38
15	L	301	WPI	O6-C2	2.27	1.40	1.37
15	Z	301	WPI	O41-C38	2.25	1.40	1.37
15	I	301	WPI	C35-C37	2.22	1.42	1.38
15	I	301	WPI	O42-C39	2.20	1.42	1.38
15	Z	301	WPI	O6-C2	2.11	1.40	1.37
15	L	301	WPI	O41-C38	2.11	1.40	1.37
15	V	201	WPI	O8-C3	2.08	1.40	1.37
15	Z	301	WPI	O40-C43	-2.07	1.37	1.42
15	I	301	WPI	O6-C2	2.05	1.40	1.37
15	L	301	WPI	C37-C39	2.01	1.45	1.41
15	H	300	WPI	O40-C43	-2.01	1.37	1.42

All (142) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	300	WPI	C29-C30-C31	-7.67	108.47	125.48
15	V	201	WPI	C10-C13-C14	-7.59	108.40	126.99
15	I	301	WPI	C16-C14-C13	-7.39	109.09	125.48
15	H	300	WPI	C22-N20-C21	7.31	132.84	113.22
15	Z	301	WPI	C33-C31-C30	-7.19	109.39	126.99
15	W	301	WPI	C16-C14-C13	-7.00	109.95	125.48
15	W	301	WPI	C26-N25-C23	6.91	131.77	113.22
15	V	201	WPI	C16-C14-C13	-6.88	110.22	125.48
15	H	300	WPI	C10-C13-C14	-6.65	110.69	126.99
15	V	201	WPI	C26-N25-C23	6.60	130.94	113.22
15	I	301	WPI	C10-C13-C14	-6.53	111.01	126.99
15	Z	301	WPI	C16-C14-C13	-6.52	111.03	125.48
15	V	201	WPI	O6-C2-C1	6.50	126.28	115.14
15	Z	301	WPI	C22-N20-C21	6.47	130.59	113.22
15	H	300	WPI	C16-C14-C13	-6.46	111.16	125.48
15	Z	301	WPI	C26-N25-C23	6.37	130.31	113.22
15	L	301	WPI	C33-C31-C30	-6.35	111.43	126.99
15	L	301	WPI	C26-N25-C23	6.28	130.09	113.22
15	I	301	WPI	C22-N20-C21	6.24	129.97	113.22
15	W	301	WPI	C22-N20-C21	6.23	129.96	113.22
15	I	301	WPI	C29-C30-C31	-6.21	111.72	125.48
15	V	201	WPI	C22-N20-C21	6.20	129.86	113.22
15	I	301	WPI	C26-N25-C23	6.17	129.79	113.22
15	W	301	WPI	C10-C13-C14	-6.11	112.02	126.99
15	L	301	WPI	C16-C14-C13	-6.10	111.96	125.48
15	I	301	WPI	C33-C31-C30	-5.98	112.34	126.99
15	V	201	WPI	O6-C2-C5	-5.98	113.78	124.08
15	Z	301	WPI	O40-C37-C35	-5.92	113.88	124.08
15	L	301	WPI	C29-C30-C31	-5.91	112.38	125.48
15	H	300	WPI	C33-C31-C30	-5.82	112.73	126.99
15	W	301	WPI	C29-C30-C31	-5.63	113.01	125.48
15	V	201	WPI	C33-C31-C30	-5.62	113.23	126.99
15	H	300	WPI	C26-N25-C23	5.60	128.25	113.22
15	W	301	WPI	C33-C31-C30	-5.46	113.62	126.99
15	Z	301	WPI	C10-C13-C14	-5.46	113.63	126.99
15	I	301	WPI	C44-O41-C38	5.40	125.43	117.51
15	Z	301	WPI	C29-C30-C31	-5.36	113.59	125.48
15	L	301	WPI	C22-N20-C21	5.34	127.55	113.22
15	L	301	WPI	C10-C13-C14	-5.33	113.94	126.99
15	V	201	WPI	C29-C30-C31	-5.32	113.69	125.48
15	H	300	WPI	C12-O8-C3	4.94	124.76	117.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Z	301	WPI	C44-O41-C38	4.77	124.52	117.51
15	H	300	WPI	O8-C3-C1	4.71	123.22	115.14
15	L	301	WPI	C44-O41-C38	4.63	124.30	117.51
15	V	201	WPI	C12-O8-C3	4.23	123.72	117.51
15	Z	301	WPI	O40-C37-C39	4.09	122.14	115.14
15	Z	301	WPI	O41-C38-C39	4.05	122.08	115.14
15	V	201	WPI	O8-C3-C1	3.97	121.94	115.14
15	V	201	WPI	O41-C38-C39	3.96	121.92	115.14
15	H	300	WPI	O6-C2-C1	3.82	121.68	115.14
15	I	301	WPI	O6-C2-C1	3.70	121.49	115.14
15	L	301	WPI	O8-C3-C1	3.63	121.36	115.14
15	I	301	WPI	O41-C38-C39	3.63	121.35	115.14
15	I	301	WPI	O8-C3-C1	3.61	121.32	115.14
15	Z	301	WPI	C18-C19-N20	3.46	123.67	113.93
15	H	300	WPI	O40-C37-C35	-3.46	118.13	124.08
15	Z	301	WPI	C35-C37-C39	3.36	123.96	120.22
15	I	301	WPI	C28-C27-N25	3.31	123.25	113.93
15	H	300	WPI	O8-C3-C7	-3.28	118.43	124.08
15	L	301	WPI	O41-C38-C39	3.21	120.63	115.14
15	Z	301	WPI	C24-C22-N20	3.16	121.32	115.35
15	L	301	WPI	C27-C28-C29	3.16	124.67	112.78
15	H	300	WPI	C45-O42-C39	3.13	123.25	114.74
15	H	300	WPI	O41-C38-C39	3.13	120.49	115.14
15	H	300	WPI	C28-C27-N25	3.12	122.72	113.93
15	H	300	WPI	C24-C26-N25	-3.07	109.54	115.35
15	L	301	WPI	C12-O8-C3	3.07	122.02	117.51
15	Z	301	WPI	C45-O42-C39	3.07	123.07	114.74
15	W	301	WPI	C28-C27-N25	3.04	122.49	113.93
15	V	201	WPI	C44-O41-C38	3.04	121.98	117.51
15	W	301	WPI	O6-C2-C1	3.02	120.32	115.14
15	H	300	WPI	C43-O40-C37	-3.01	113.09	117.51
15	Z	301	WPI	C38-C39-C37	-3.01	116.63	119.56
15	V	201	WPI	C9-O4-C1	3.01	122.91	114.74
15	L	301	WPI	O6-C2-C1	3.01	120.30	115.14
15	L	301	WPI	C33-C36-C38	2.98	124.16	120.15
15	Z	301	WPI	O6-C2-C1	2.96	120.22	115.14
15	H	300	WPI	C44-O41-C38	2.90	121.77	117.51
15	I	301	WPI	O40-C37-C35	-2.90	119.08	124.08
15	H	300	WPI	C35-C37-C39	2.90	123.45	120.22
15	L	301	WPI	O40-C37-C35	-2.86	119.16	124.08
15	I	301	WPI	O40-C37-C39	2.85	120.03	115.14
15	W	301	WPI	O8-C3-C1	2.84	120.01	115.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Z	301	WPI	O8-C3-C1	2.79	119.91	115.14
15	L	301	WPI	O8-C3-C7	-2.78	119.29	124.08
15	I	301	WPI	O8-C3-C7	-2.77	119.31	124.08
15	H	300	WPI	O6-C2-C5	-2.76	119.32	124.08
15	H	300	WPI	C11-O6-C2	2.74	121.53	117.51
15	Z	301	WPI	C33-C36-C38	2.74	123.84	120.15
15	L	301	WPI	C11-O6-C2	2.73	121.51	117.51
15	H	300	WPI	C38-C39-C37	-2.72	116.91	119.56
15	I	301	WPI	C18-C19-N20	2.70	121.53	113.93
15	I	301	WPI	C33-C36-C38	2.69	123.78	120.15
15	I	301	WPI	O6-C2-C5	-2.68	119.46	124.08
15	L	301	WPI	C18-C19-N20	2.66	121.41	113.93
15	W	301	WPI	O41-C38-C39	2.65	119.67	115.14
15	I	301	WPI	C9-O4-C1	2.64	121.91	114.74
15	V	201	WPI	O40-C37-C39	2.63	119.65	115.14
15	V	201	WPI	O40-C37-C35	-2.61	119.58	124.08
15	V	201	WPI	C28-C27-N25	2.60	121.24	113.93
15	Z	301	WPI	C24-C26-N25	-2.56	110.50	115.35
15	Z	301	WPI	C12-O8-C3	2.55	121.25	117.51
15	V	201	WPI	O41-C38-C36	-2.55	119.69	124.08
15	L	301	WPI	C38-C39-C37	-2.54	117.09	119.56
15	W	301	WPI	C9-O4-C1	2.53	121.60	114.74
15	V	201	WPI	O8-C3-C7	-2.52	119.74	124.08
15	I	301	WPI	C43-O40-C37	2.51	121.20	117.51
15	W	301	WPI	C21-C23-N25	2.51	124.77	116.77
15	I	301	WPI	C19-C18-C16	2.48	122.14	112.78
15	H	300	WPI	C27-C28-C29	2.45	122.03	112.78
15	Z	301	WPI	C43-O40-C37	-2.44	113.93	117.51
15	L	301	WPI	C9-O4-C1	2.43	121.34	114.74
15	V	201	WPI	C18-C19-N20	2.42	120.75	113.93
15	H	300	WPI	C33-C36-C38	2.41	123.40	120.15
15	Z	301	WPI	C11-O6-C2	2.41	121.04	117.51
15	W	301	WPI	C27-C28-C29	2.40	121.83	112.78
15	Z	301	WPI	C19-C18-C16	2.39	121.80	112.78
15	L	301	WPI	C19-C18-C16	2.36	121.67	112.78
15	W	301	WPI	O41-C38-C36	-2.35	120.02	124.08
15	V	201	WPI	C24-C26-N25	-2.33	110.95	115.35
15	I	301	WPI	C27-C28-C29	2.30	121.46	112.78
15	L	301	WPI	C45-O42-C39	2.30	120.99	114.74
15	I	301	WPI	C24-C22-N20	2.28	119.66	115.35
15	Z	301	WPI	C36-C38-C39	-2.28	117.69	120.22
15	Z	301	WPI	O41-C38-C36	-2.24	120.22	124.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	300	WPI	C23-C21-N20	2.23	123.88	116.77
15	W	301	WPI	C19-C18-C16	2.22	121.13	112.78
15	I	301	WPI	C11-O6-C2	2.18	120.72	117.51
15	W	301	WPI	C38-C39-C37	-2.18	117.44	119.56
15	W	301	WPI	O8-C3-C7	-2.16	120.35	124.08
15	H	300	WPI	C24-C22-N20	2.16	119.43	115.35
15	I	301	WPI	C23-C21-N20	2.11	123.48	116.77
15	W	301	WPI	C11-O6-C2	2.10	120.59	117.51
15	I	301	WPI	C12-O8-C3	2.09	120.57	117.51
15	Z	301	WPI	C9-O4-C1	2.08	120.38	114.74
15	I	301	WPI	C21-C23-N25	2.08	123.39	116.77
15	I	301	WPI	C36-C38-C39	-2.07	117.92	120.22
15	L	301	WPI	O40-C37-C39	2.06	118.67	115.14
15	W	301	WPI	O6-C2-C5	-2.06	120.53	124.08
15	V	201	WPI	C19-C18-C16	2.03	120.42	112.78
15	V	201	WPI	C27-C28-C29	2.02	120.41	112.78
15	L	301	WPI	O6-C2-C5	-2.01	120.61	124.08

There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	H	300	WPI	C10-C13-C14-C16
15	H	300	WPI	C14-C16-C18-C19
15	H	300	WPI	C18-C19-N20-C22
15	H	300	WPI	C28-C27-N25-C26
15	I	301	WPI	C14-C16-C18-C19
15	I	301	WPI	C18-C19-N20-C22
15	I	301	WPI	C27-C28-C29-C30
15	L	301	WPI	C10-C13-C14-C16
15	L	301	WPI	C18-C19-N20-C21
15	L	301	WPI	C28-C27-N25-C26
15	L	301	WPI	C29-C30-C31-C33
15	V	201	WPI	C18-C19-N20-C22
15	V	201	WPI	C28-C27-N25-C23
15	V	201	WPI	C29-C30-C31-C33
15	W	301	WPI	C10-C13-C14-C16
15	W	301	WPI	C18-C19-N20-C22
15	W	301	WPI	C28-C27-N25-C26
15	W	301	WPI	C29-C30-C31-C33
15	Z	301	WPI	C14-C16-C18-C19
15	Z	301	WPI	C18-C19-N20-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	Z	301	WPI	C28-C27-N25-C26
15	Z	301	WPI	C29-C30-C31-C33
15	L	301	WPI	C36-C38-O41-C44
15	L	301	WPI	C39-C38-O41-C44
15	I	301	WPI	C1-C2-O6-C11
15	H	300	WPI	C39-C38-O41-C44
15	V	201	WPI	C39-C38-O41-C44
15	Z	301	WPI	C39-C37-O40-C43
15	I	301	WPI	C39-C37-O40-C43
15	I	301	WPI	C7-C10-C13-C14
15	I	301	WPI	C30-C31-C33-C35
15	W	301	WPI	C30-C31-C33-C36
15	H	300	WPI	C1-C2-O6-C11
15	H	300	WPI	C30-C31-C33-C36
15	I	301	WPI	C1-C3-O8-C12
15	Z	301	WPI	C7-C10-C13-C14
15	W	301	WPI	C7-C10-C13-C14
15	W	301	WPI	C30-C31-C33-C35
15	I	301	WPI	C39-C38-O41-C44
15	H	300	WPI	C30-C31-C33-C35
15	I	301	WPI	C30-C31-C33-C36
15	V	201	WPI	C30-C31-C33-C35
15	W	301	WPI	C5-C10-C13-C14
15	Z	301	WPI	C5-C10-C13-C14
15	I	301	WPI	C5-C10-C13-C14
15	Z	301	WPI	C35-C37-O40-C43
15	L	301	WPI	C16-C18-C19-N20
15	I	301	WPI	C35-C37-O40-C43
15	H	300	WPI	C16-C18-C19-N20
15	Z	301	WPI	C16-C18-C19-N20
15	V	201	WPI	C30-C31-C33-C36
15	I	301	WPI	C5-C2-O6-C11
15	L	301	WPI	N25-C27-C28-C29
15	H	300	WPI	C36-C38-O41-C44
15	V	201	WPI	C36-C38-O41-C44
15	W	301	WPI	C36-C38-O41-C44
15	I	301	WPI	C36-C38-O41-C44
15	I	301	WPI	C7-C3-O8-C12
15	W	301	WPI	C7-C3-O8-C12
15	Z	301	WPI	C36-C38-O41-C44
15	H	300	WPI	C5-C2-O6-C11
15	H	300	WPI	C7-C3-O8-C12

Continued on next page...

Continued from previous page...

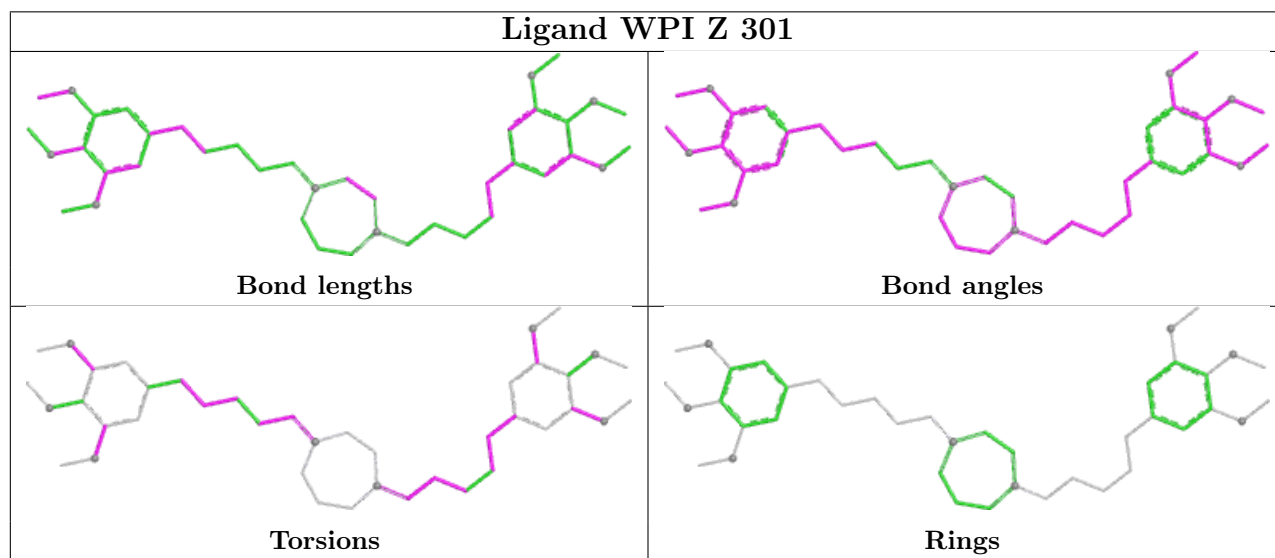
Mol	Chain	Res	Type	Atoms
15	L	301	WPI	C35-C37-O40-C43
15	L	301	WPI	C7-C3-O8-C12
15	W	301	WPI	C16-C18-C19-N20
15	H	300	WPI	C35-C37-O40-C43
15	Z	301	WPI	C7-C3-O8-C12
15	W	301	WPI	C5-C2-O6-C11
15	L	301	WPI	C5-C2-O6-C11
15	Z	301	WPI	C5-C2-O6-C11
15	W	301	WPI	C35-C37-O40-C43
15	Z	301	WPI	C39-C38-O41-C44
15	H	300	WPI	C1-C3-O8-C12
15	W	301	WPI	C39-C38-O41-C44
15	W	301	WPI	C1-C3-O8-C12
15	Z	301	WPI	C1-C3-O8-C12
15	L	301	WPI	C1-C3-O8-C12
15	L	301	WPI	C39-C37-O40-C43
15	Z	301	WPI	N25-C27-C28-C29
15	Z	301	WPI	C10-C13-C14-C16
15	H	300	WPI	N25-C27-C28-C29
15	L	301	WPI	C30-C31-C33-C36
15	L	301	WPI	C1-C2-O6-C11
15	H	300	WPI	C39-C37-O40-C43
15	W	301	WPI	C1-C2-O6-C11
15	W	301	WPI	C39-C37-O40-C43
15	Z	301	WPI	C1-C2-O6-C11
15	L	301	WPI	C30-C31-C33-C35
15	V	201	WPI	C1-C2-O6-C11
15	W	301	WPI	N25-C27-C28-C29
15	V	201	WPI	C7-C10-C13-C14
15	V	201	WPI	C5-C10-C13-C14
15	I	301	WPI	C28-C27-N25-C26
15	I	301	WPI	C29-C30-C31-C33
15	L	301	WPI	C13-C14-C16-C18
15	V	201	WPI	C5-C2-O6-C11
15	W	301	WPI	C13-C14-C16-C18
15	Z	301	WPI	C28-C29-C30-C31
15	V	201	WPI	C16-C18-C19-N20
15	I	301	WPI	C28-C27-N25-C23
15	W	301	WPI	C18-C19-N20-C21
15	H	300	WPI	C5-C10-C13-C14
15	H	300	WPI	C7-C10-C13-C14

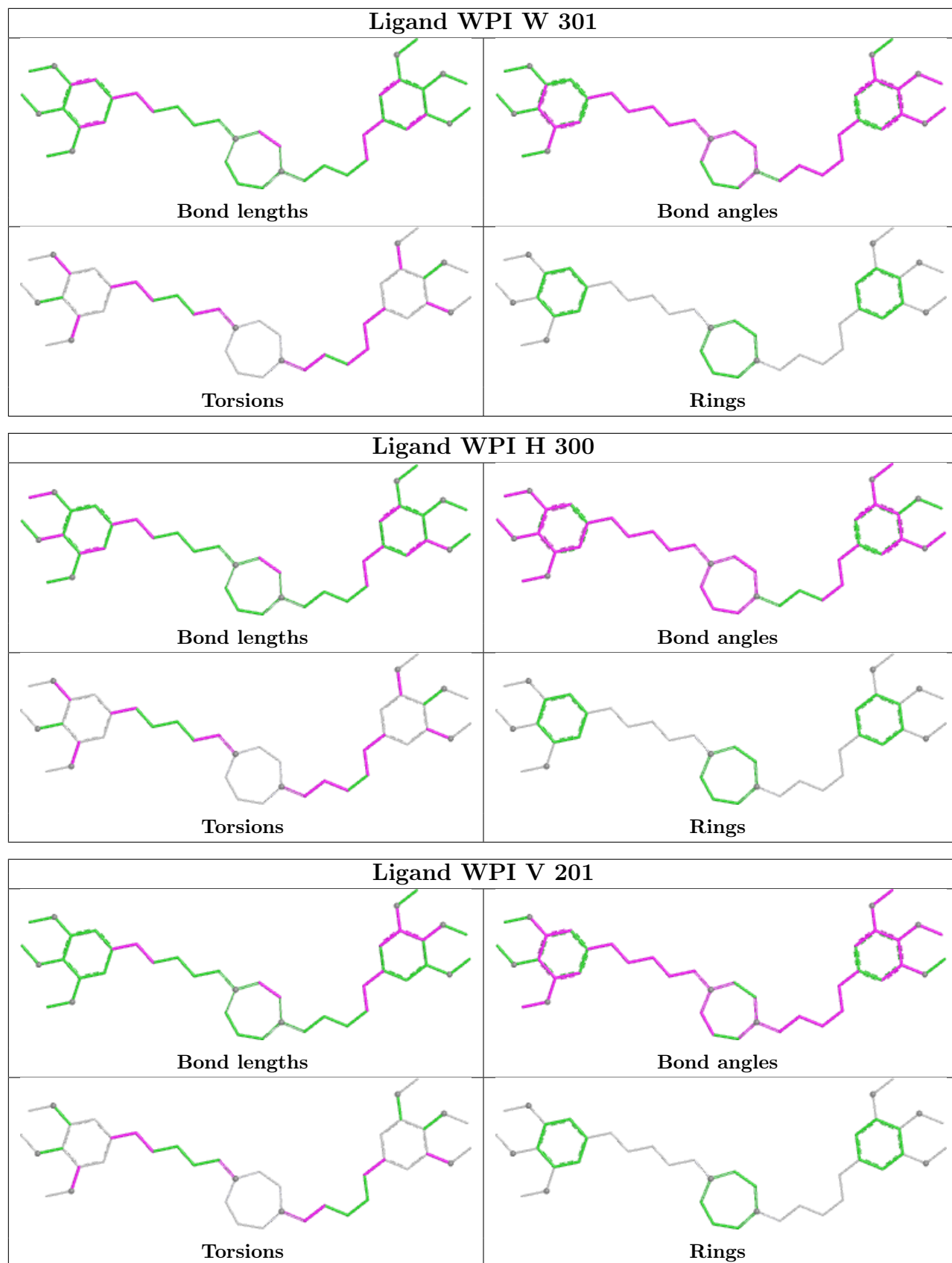
There are no ring outliers.

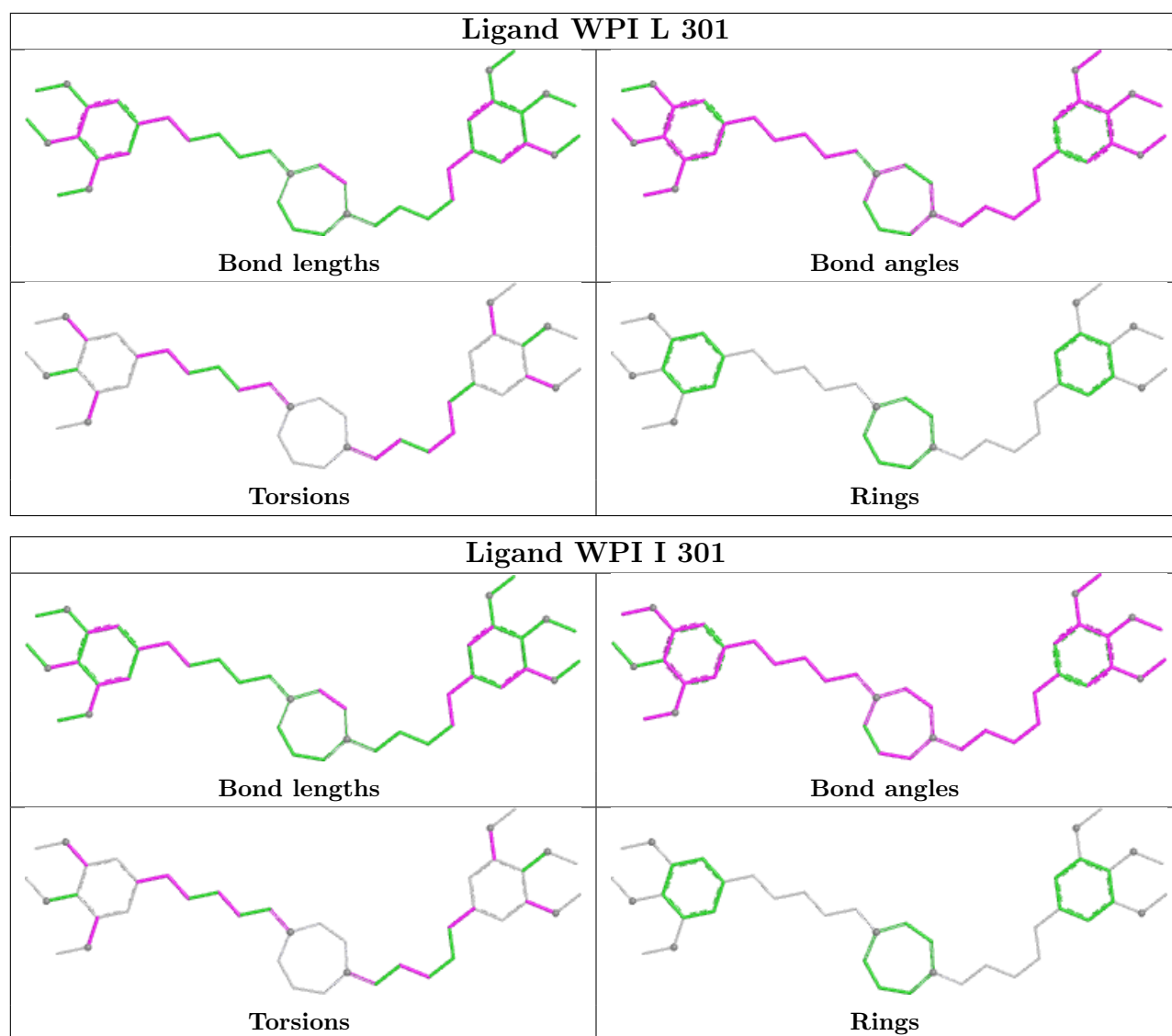
6 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Z	301	WPI	7	0
15	W	301	WPI	3	0
15	H	300	WPI	5	0
15	V	201	WPI	11	0
15	L	301	WPI	5	0
15	I	301	WPI	7	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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	241/241 (100%)	-0.23	3 (1%) 76 73	18, 32, 60, 80	0
1	O	241/241 (100%)	-0.14	3 (1%) 76 73	20, 36, 61, 88	0
2	B	249/250 (99%)	-0.22	4 (1%) 70 67	21, 34, 63, 85	0
2	P	249/250 (99%)	-0.05	6 (2%) 59 55	21, 39, 69, 84	0
3	C	244/244 (100%)	-0.05	8 (3%) 49 45	19, 37, 72, 128	0
3	Q	244/244 (100%)	-0.00	7 (2%) 53 49	18, 37, 71, 110	0
4	D	241/241 (100%)	0.04	9 (3%) 45 40	19, 39, 86, 96	0
4	R	241/241 (100%)	0.36	18 (7%) 20 18	22, 45, 93, 116	0
5	E	242/242 (100%)	0.04	8 (3%) 49 45	20, 40, 69, 122	0
5	S	242/242 (100%)	0.20	12 (4%) 34 30	24, 44, 78, 139	0
6	F	232/233 (99%)	0.14	2 (0%) 81 78	25, 45, 70, 99	0
6	T	232/233 (99%)	0.40	9 (3%) 43 38	25, 47, 75, 96	0
7	G	244/244 (100%)	-0.01	3 (1%) 76 73	22, 40, 71, 85	0
7	U	244/244 (100%)	0.11	7 (2%) 53 49	22, 40, 72, 83	0
8	H	196/196 (100%)	-0.43	0 100 100	19, 27, 46, 64	0
8	V	196/196 (100%)	-0.48	0 100 100	19, 28, 48, 63	0
9	I	222/222 (100%)	-0.31	3 (1%) 73 70	18, 31, 52, 105	0
9	W	222/222 (100%)	-0.31	2 (0%) 81 78	21, 33, 51, 100	0
10	J	204/204 (100%)	-0.43	1 (0%) 87 85	16, 31, 51, 71	0
10	X	204/204 (100%)	-0.42	3 (1%) 72 68	17, 30, 52, 73	0
11	K	196/198 (98%)	-0.45	2 (1%) 79 76	18, 31, 48, 83	0
11	Y	196/198 (98%)	-0.42	2 (1%) 79 76	17, 31, 48, 85	0
12	L	212/212 (100%)	-0.47	1 (0%) 87 85	18, 28, 44, 64	0
12	Z	212/212 (100%)	-0.40	1 (0%) 87 85	20, 31, 50, 69	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	222/222 (100%)	-0.31	1 (0%) 87 85	18, 32, 58, 74	0
13	M	222/222 (100%)	-0.39	1 (0%) 87 85	18, 31, 52, 71	0
14	2	233/233 (100%)	-0.43	0 100 100	18, 29, 44, 59	0
14	N	233/233 (100%)	-0.44	0 100 100	17, 30, 48, 58	0
All	All	6356/6364 (99%)	-0.17	116 (1%) 67 64	16, 34, 68, 139	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	51	THR	7.1
4	R	52	LEU	6.2
5	E	127	ALA	6.1
5	E	133	LEU	5.0
7	U	247	ASN	4.9
4	D	52	LEU	4.7
5	S	9	ASP	4.6
7	U	246	ILE	4.5
4	R	205	THR	4.4
3	Q	52	VAL	4.4
2	P	1	MET	4.3
5	S	127	ALA	4.3
5	S	128	SER	4.2
5	E	126	GLY	4.0
9	W	222	ASP	4.0
5	S	126	GLY	3.9
3	C	245	THR	3.9
4	D	51	THR	3.9
3	Q	220	ALA	3.8
2	B	1	MET	3.8
4	D	206	GLY	3.7
5	S	129	GLY	3.7
3	C	220	ALA	3.7
1	A	10	ALA	3.6
1	O	10	ALA	3.5
12	L	212	GLY	3.5
4	R	53	LYS	3.5
4	R	236	ILE	3.5
2	B	201	GLU	3.4
7	G	4	GLY	3.4
3	Q	245	THR	3.3
3	Q	2	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	F	234	ILE	3.3
6	T	234	ILE	3.3
11	K	-1	MET	3.3
11	K	195	GLN	3.3
4	R	49	ARG	3.3
4	D	50	SER	3.2
5	S	133	LEU	3.2
4	D	207	ALA	3.2
4	R	50	SER	3.2
6	T	123	TYR	3.1
4	D	205	THR	3.1
5	S	132	ARG	3.1
5	E	250	GLU	3.1
3	Q	223	GLY	3.1
2	P	2	THR	3.1
13	1	165	TYR	3.0
3	C	2	GLY	3.0
5	E	128	SER	2.9
3	C	219	GLY	2.9
5	E	9	ASP	2.8
6	F	123	TYR	2.8
4	R	48	ARG	2.8
4	R	206	GLY	2.8
2	B	2	THR	2.8
10	X	-8	SER	2.8
4	D	208	LYS	2.8
5	E	129	GLY	2.7
4	R	200	LEU	2.7
5	E	249	ALA	2.7
1	A	12	TYR	2.7
10	J	119	GLY	2.7
13	M	165	TYR	2.7
7	U	54	THR	2.7
11	Y	195	GLN	2.7
1	O	11	GLY	2.6
11	Y	-1	MET	2.6
3	C	221	ASN	2.6
2	P	52	SER	2.6
2	P	61	LEU	2.5
9	W	221	CYS	2.5
4	R	207	ALA	2.5
4	R	201	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	220	ILE	2.4
3	Q	219	GLY	2.4
5	S	10	ARG	2.4
5	S	248	ALA	2.4
9	I	222	ASP	2.4
2	P	249	ALA	2.4
3	C	244	ILE	2.3
4	D	49	ARG	2.3
4	R	243	GLN	2.3
7	U	181	HIS	2.3
9	I	221	CYS	2.3
6	T	182	ILE	2.3
7	U	4	GLY	2.3
4	R	208	LYS	2.3
10	X	125	LYS	2.3
4	R	209	ASN	2.3
2	B	249	ALA	2.2
4	D	187	THR	2.2
4	R	240	LYS	2.2
6	T	191	LYS	2.2
5	S	250	GLU	2.2
3	Q	63	THR	2.2
7	U	204	GLU	2.2
2	P	4	ARG	2.1
5	S	249	ALA	2.1
1	O	216	THR	2.1
6	T	213	ILE	2.1
1	A	162	TYR	2.1
3	C	226	TYR	2.1
7	G	5	THR	2.1
6	T	208	VAL	2.1
6	T	3	ARG	2.1
5	S	125	GLU	2.1
6	T	55	GLU	2.1
7	U	56	LYS	2.1
3	C	223	GLY	2.0
4	R	3	GLY	2.0
12	Z	212	GLY	2.0
4	R	57	THR	2.0
10	X	122	ASP	2.0
6	T	207	THR	2.0
7	G	60	PRO	2.0

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

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](#)

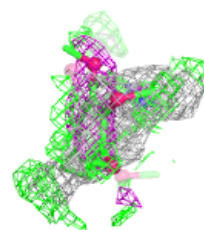
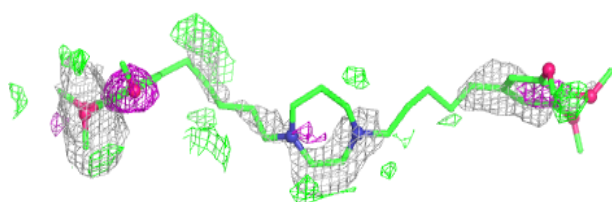
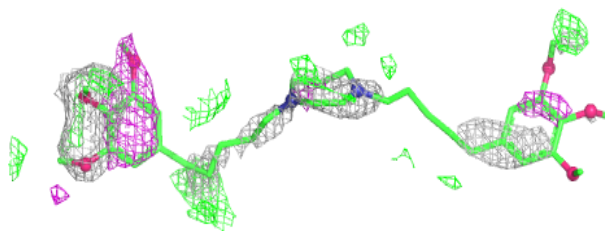
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	WPI	W	301	41/41	0.61	0.37	46,99,128,133	0
15	WPI	I	301	41/41	0.63	0.37	46,94,124,133	0
15	WPI	H	300	41/41	0.64	0.35	40,78,102,107	0
15	WPI	L	301	41/41	0.66	0.33	38,67,111,118	0
15	WPI	Z	301	41/41	0.67	0.31	36,76,123,131	0
15	WPI	V	201	41/41	0.69	0.27	38,67,81,90	0

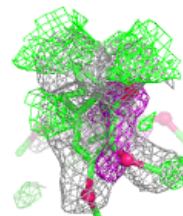
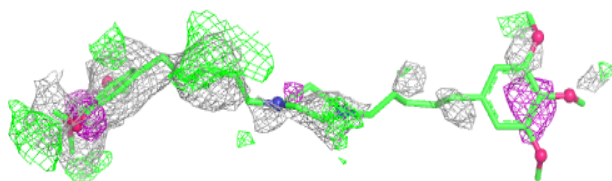
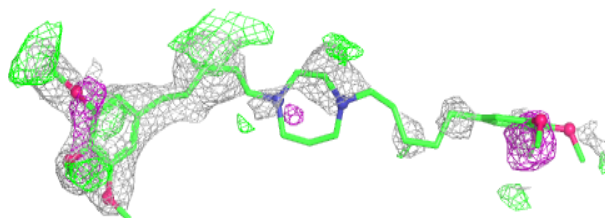
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around WPI W 301:

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

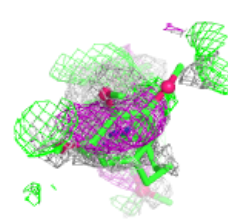
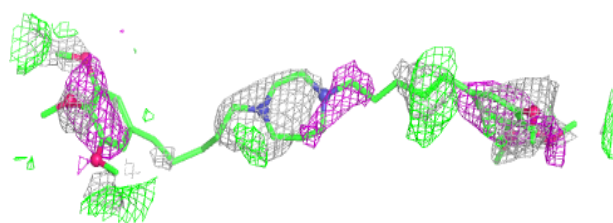
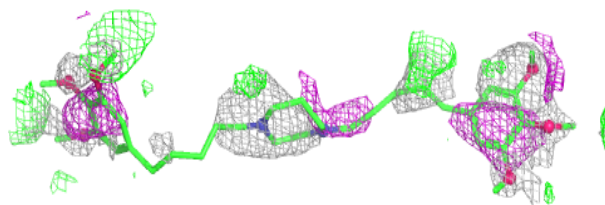
**Electron density around WPI I 301:**

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

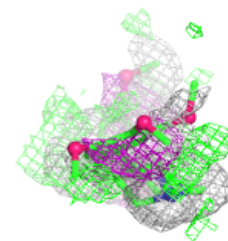
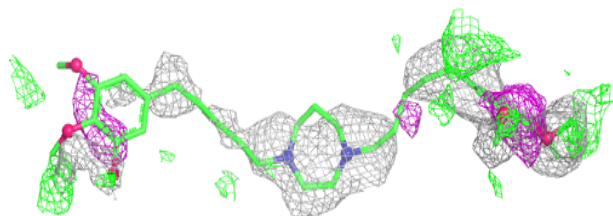
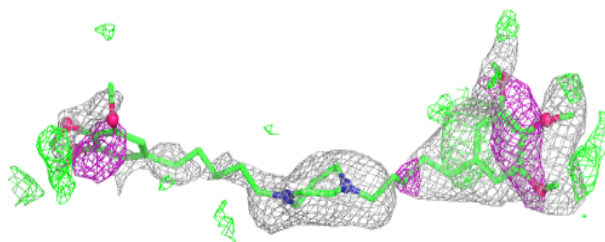


Electron density around WPI H 300:

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

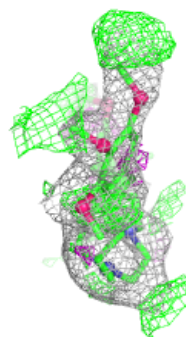
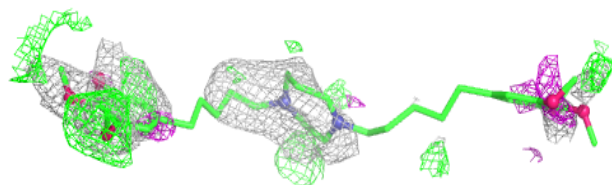
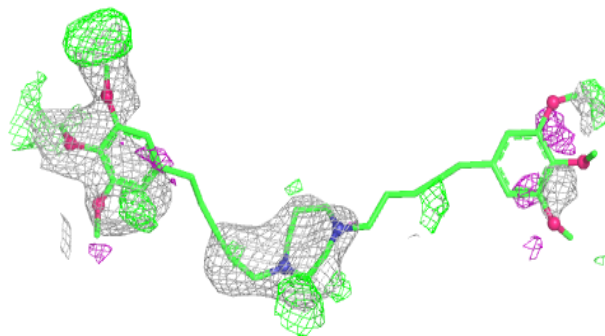
**Electron density around WPI L 301:**

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

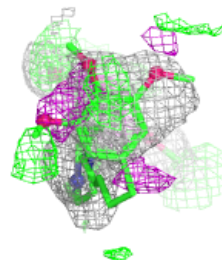
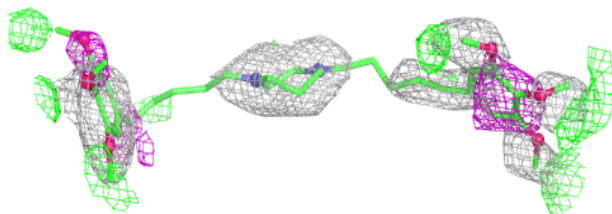
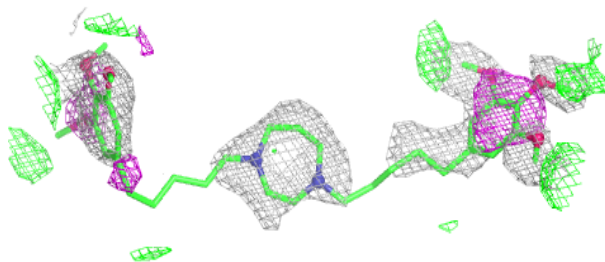


Electron density around WPI Z 301:

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

**Electron density around WPI V 201:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.