



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:53 am BST

PDB ID : 2GPL
Title : TMC-95 based biphenyl-ether macrocycles: specific proteasome inhibitors
Authors : Groll, M.; Goetz, M.; Kaiser, M.; Weyher, E.; Moroder, M.
Deposited on : 2006-04-18
Resolution : 2.81 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

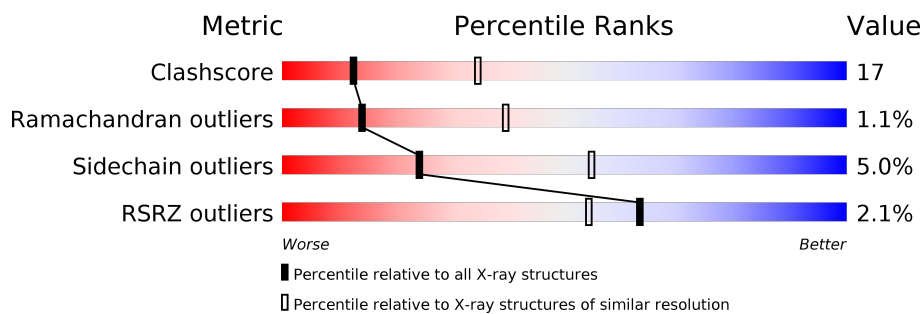
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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))
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>0%</div> <div>78%</div> <div>20%</div> <div>•</div> </div>
1	O	250	<div> <div>2%</div> <div>76%</div> <div>22%</div> <div>•</div> </div>
2	B	244	<div> <div>4%</div> <div>63%</div> <div>31%</div> <div>6%</div> </div>
2	P	244	<div> <div>6%</div> <div>63%</div> <div>31%</div> <div>6%</div> </div>
3	C	241	<div> <div>4%</div> <div>60%</div> <div>36%</div> <div>•</div> </div>
3	Q	241	<div> <div>5%</div> <div>61%</div> <div>35%</div> <div>•</div> </div>
4	D	242	<div> <div>3%</div> <div>76%</div> <div>21%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
4	R	242	 5% 71% 26% .
5	E	233	 2% 60% 34% 6%
5	S	233	 7% 59% 35% 6%
6	F	244	 2% 65% 31% .
6	T	244	 2% 65% 31% .
7	G	243	 % 65% 32% .
7	U	243	 % 65% 32% .
8	H	222	 % 71% 27% .
8	V	222	 % 73% 25% .
9	I	204	 % 74% 25% .
9	W	204	 % 71% 28% .
10	J	198	 2% 68% 30% .
10	X	198	 3% 67% 31% .
11	K	212	 % 74% 24% .
11	Y	212	 % 75% 23% .
12	L	222	 % 68% 29% .
12	Z	222	 % 70% 27% .
13	1	233	 % 70% 27% .
13	M	233	 % 70% 27% .
14	2	196	 % 72% 26% .
14	N	196	 % 71% 26% .

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50714 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

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

- Molecule 3 is a protein called Proteasome component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

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

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
6	T	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

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

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

- Molecule 8 is a protein called Proteasome component PUP1.

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

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

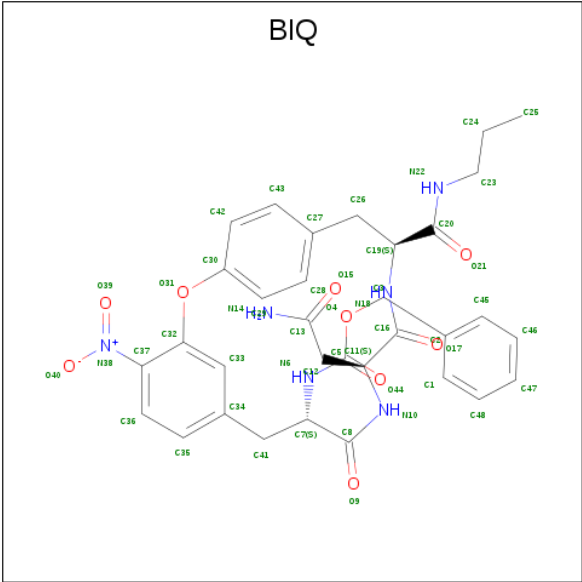
- Molecule 13 is a protein called Proteasome component PRE4.

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

- Molecule 14 is a protein called Proteasome component PRE3.

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

- Molecule 15 is BENZYL [12-(2-AMINO-2-OXOETHYL)-4-NITRO-10,13-DIOXO-15-[(P ROPYLAMINO)CARBONYL]-2-OXA-11,14-DIAZATRICYCLO[15 .2.2.1 3,7]DOCOS A-1(19),3(22),4,6,17,20-HEXAEN-9-YL]CARBAMATE (three-letter code: BIQ) (formula: C₃₃H₃₆N₆O₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	7	0
			48	33	6	9		
15	V	1	Total	C	N	O	6	0
			48	33	6	9		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	43	Total	O	0	0
			43	43		
16	B	27	Total	O	0	0
			27	27		
16	C	32	Total	O	0	0
			32	32		
16	D	30	Total	O	0	0
			30	30		
16	E	14	Total	O	0	0
			14	14		
16	F	38	Total	O	0	0
			38	38		
16	G	51	Total	O	0	0
			51	51		
16	H	37	Total	O	0	0
			37	37		
16	I	48	Total	O	0	0
			48	48		
16	J	44	Total	O	0	0
			44	44		

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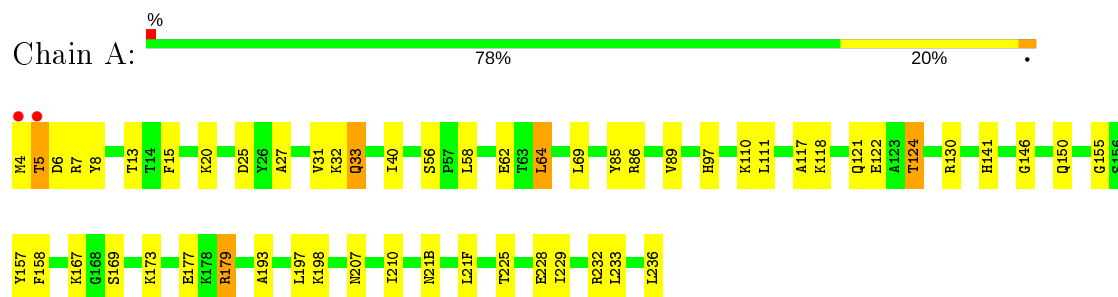
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	K	36	Total 36	O 36	0	0
16	L	49	Total 49	O 49	0	0
16	M	60	Total 60	O 60	0	0
16	N	48	Total 48	O 48	0	0
16	O	27	Total 27	O 27	0	0
16	P	24	Total 24	O 24	0	0
16	Q	22	Total 22	O 22	0	0
16	R	25	Total 25	O 25	0	0
16	S	16	Total 16	O 16	0	0
16	T	36	Total 36	O 36	0	0
16	U	47	Total 47	O 47	0	0
16	V	39	Total 39	O 39	0	0
16	W	44	Total 44	O 44	0	0
16	X	38	Total 38	O 38	0	0
16	Y	42	Total 42	O 42	0	0
16	Z	45	Total 45	O 45	0	0
16	1	59	Total 59	O 59	0	0
16	2	49	Total 49	O 49	0	0

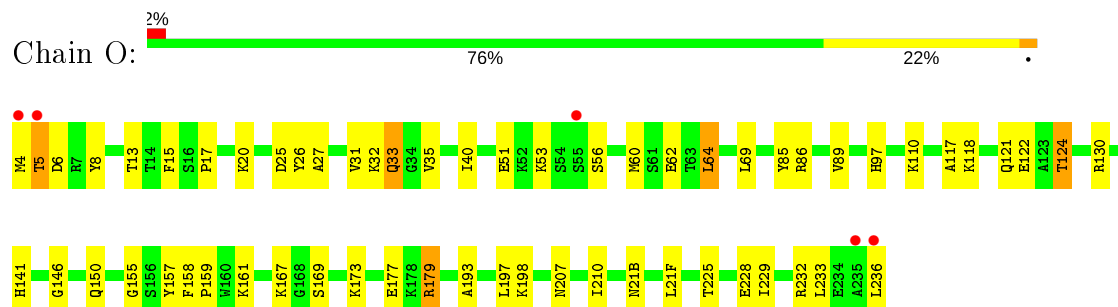
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

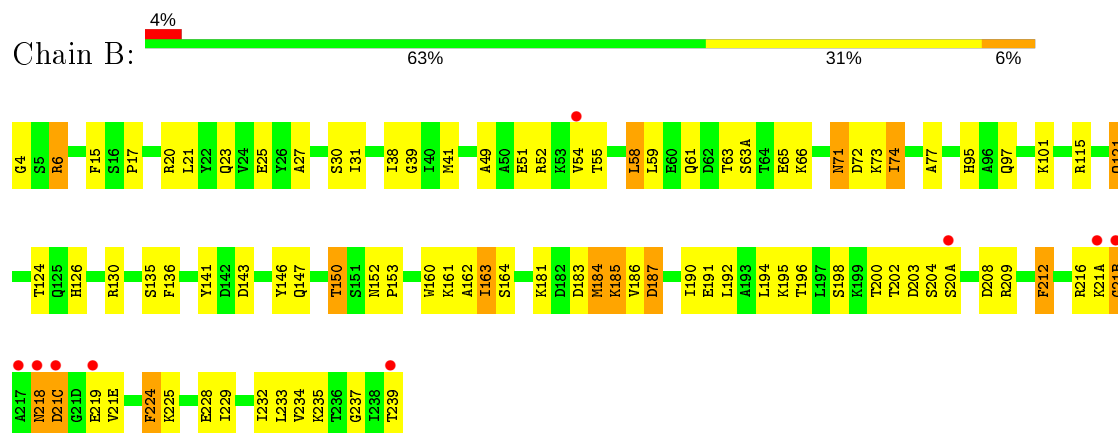
- Molecule 1: Proteasome component Y7



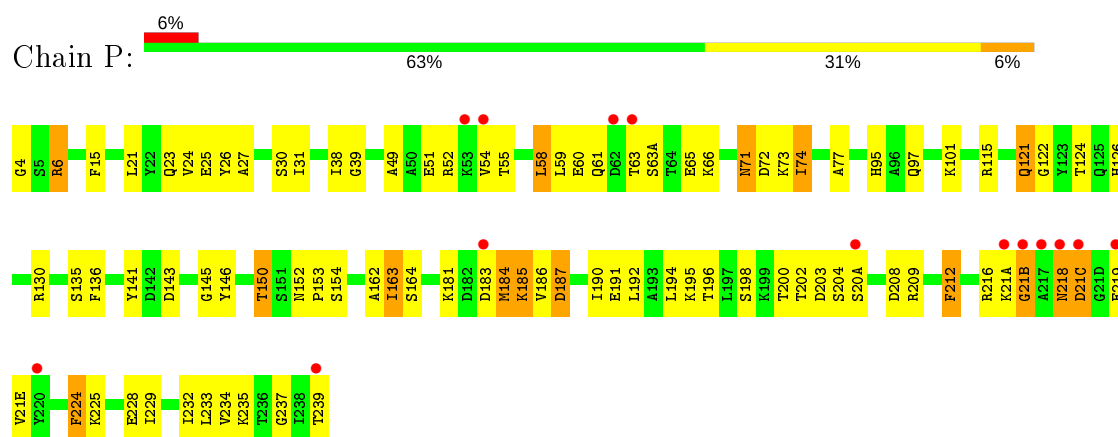
- Molecule 1: Proteasome component Y7



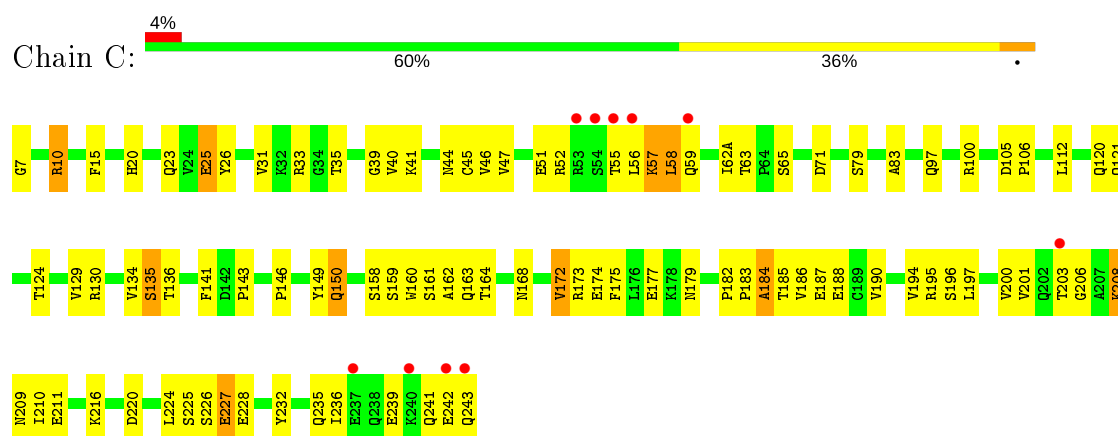
- Molecule 2: Proteasome component Y13



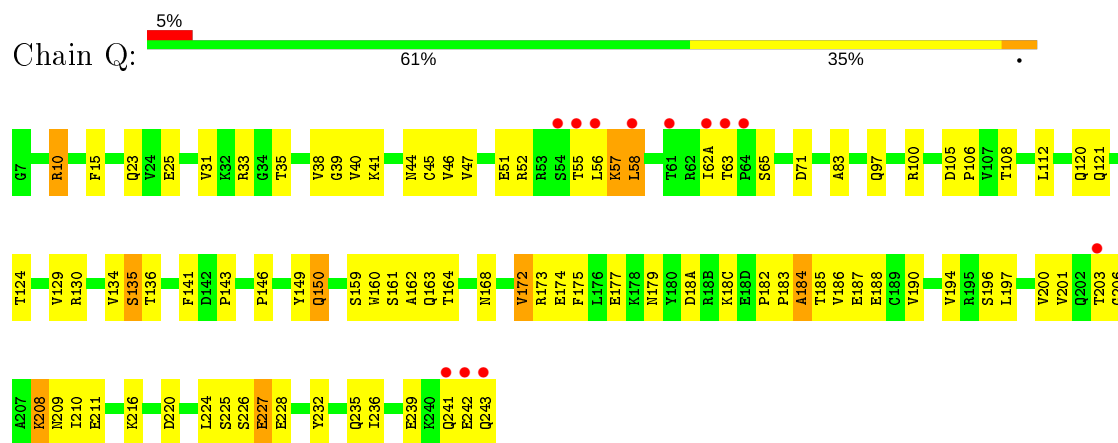
- Molecule 2: Proteasome component Y13



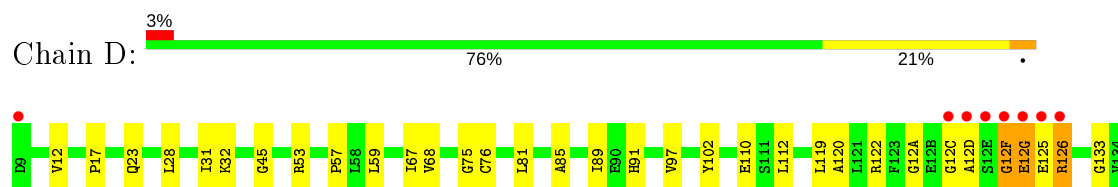
• Molecule 3: Proteasome component PRE6

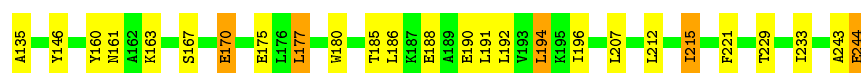


• Molecule 3: Proteasome component PRE6

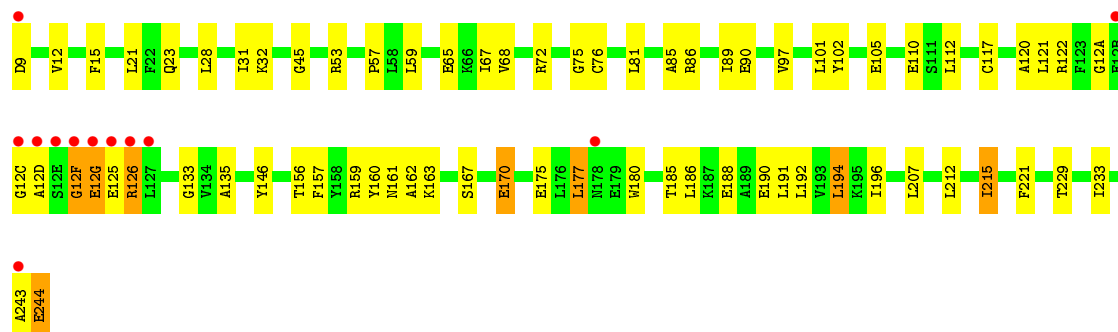


• Molecule 4: Proteasome component PUP2

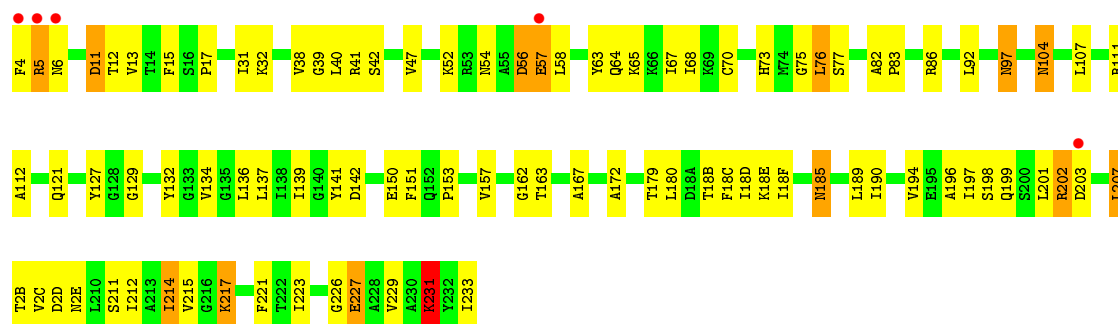




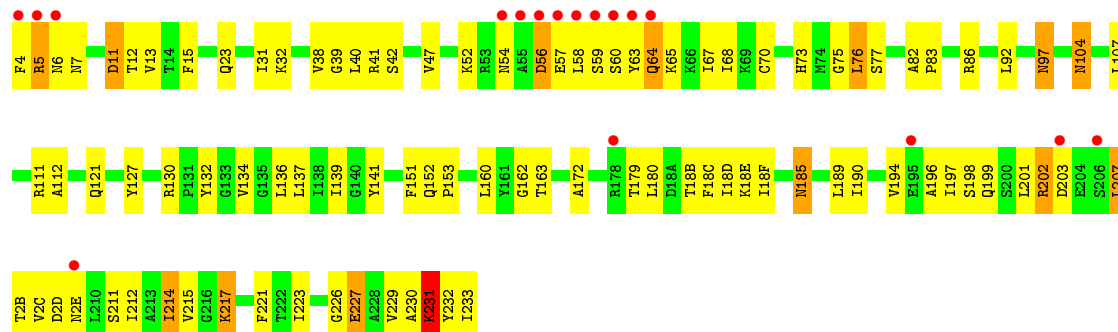
• Molecule 4: Proteasome component PUP2



• Molecule 5: Proteasome component PRE5

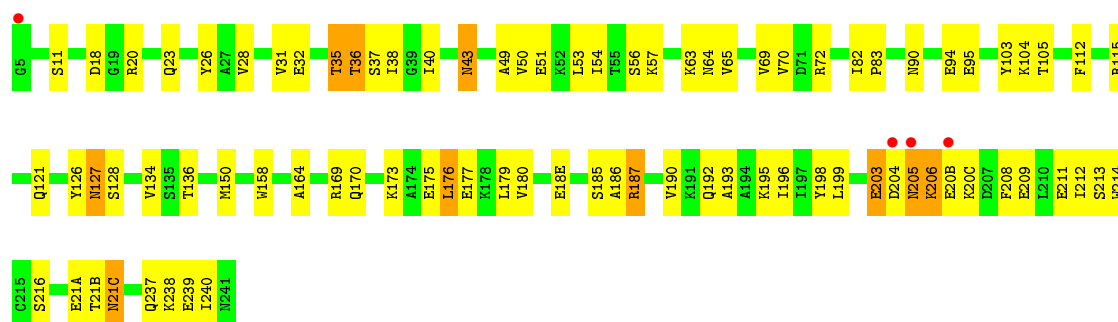


• Molecule 5: Proteasome component PRE5

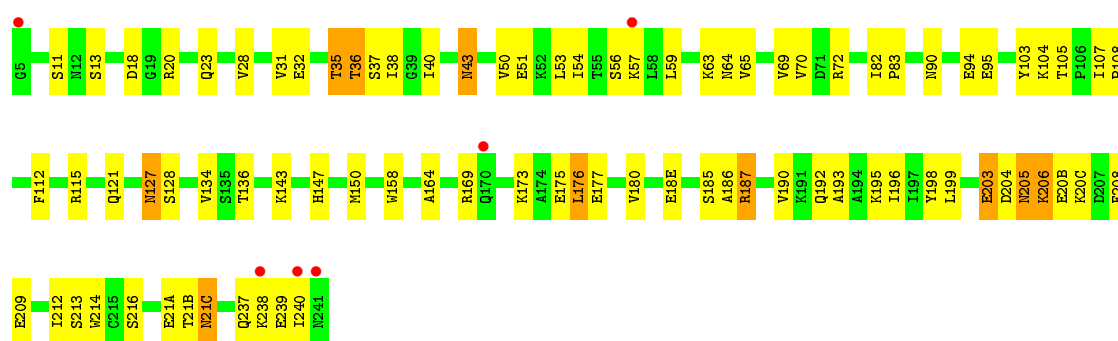


• Molecule 6: Proteasome component C1

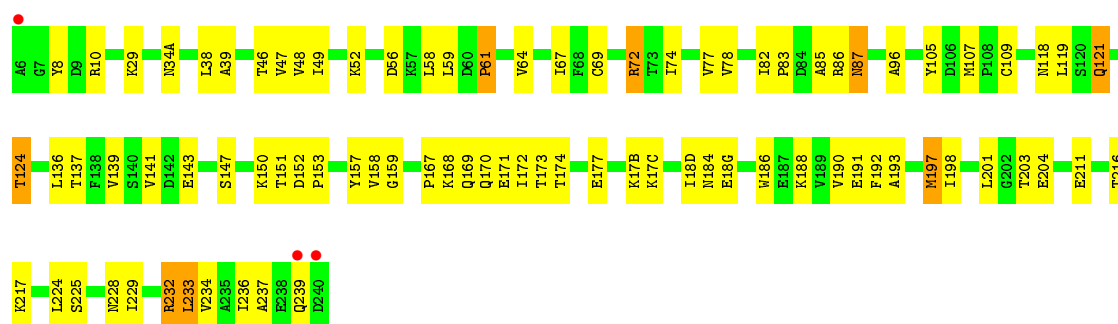




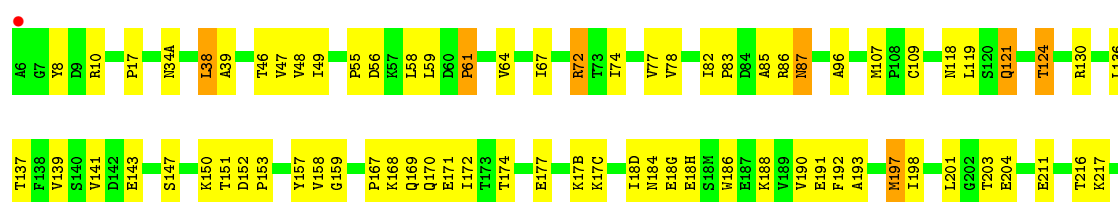
• Molecule 6: Proteasome component C1



• Molecule 7: Proteasome component C7-alpha

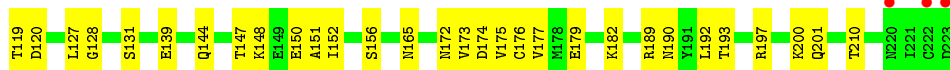
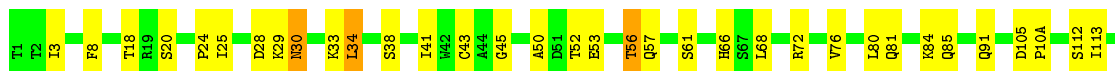


• Molecule 7: Proteasome component C7-alpha

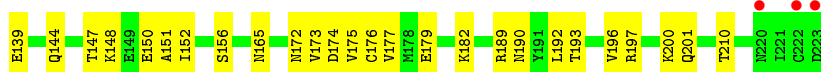
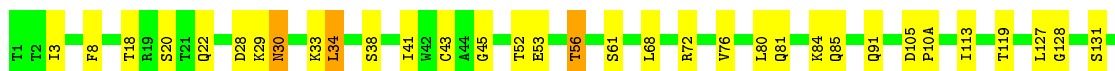




- Molecule 8: Proteasome component PUP1



- Molecule 8: Proteasome component PUP1



- Molecule 9: Proteasome component PUP3

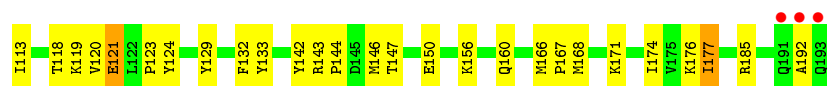


- Molecule 9: Proteasome component PUP3

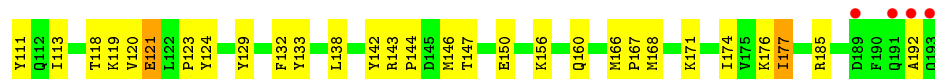
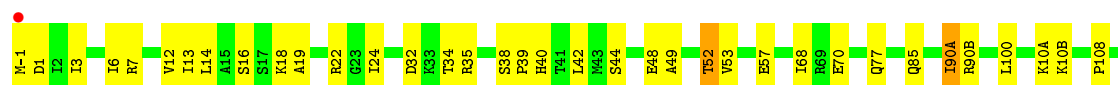


- Molecule 10: Proteasome component C11





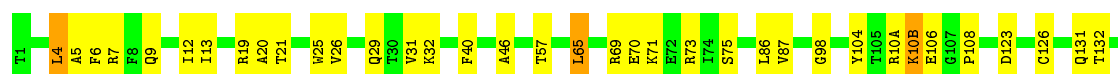
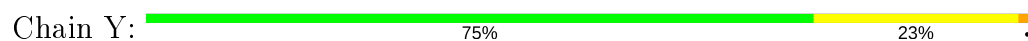
• Molecule 10: Proteasome component C11



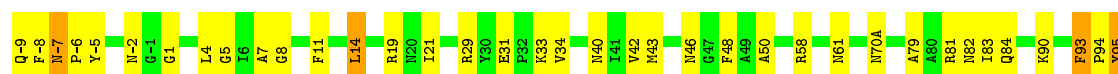
• Molecule 11: Proteasome component PRE2



• Molecule 11: Proteasome component PRE2

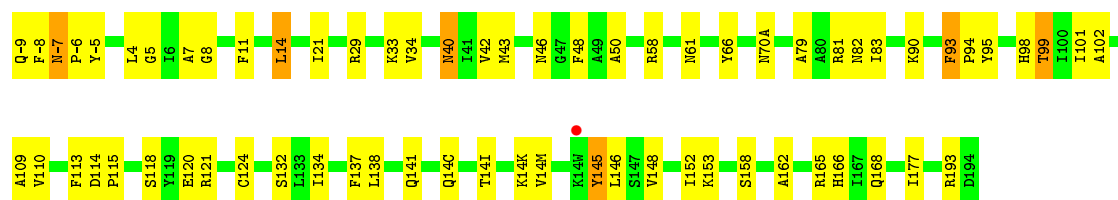


• Molecule 12: Proteasome component C5



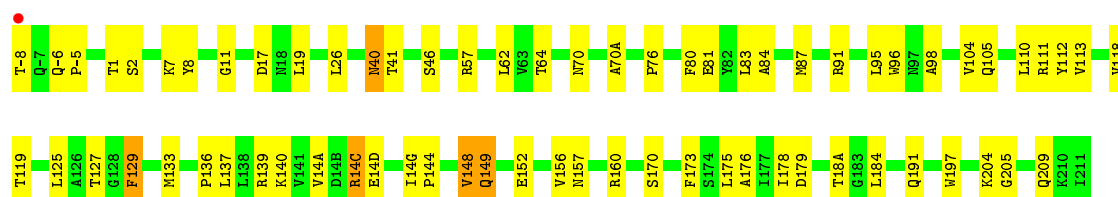
• Molecule 12: Proteasome component C5

Chain Z:  70% 27%



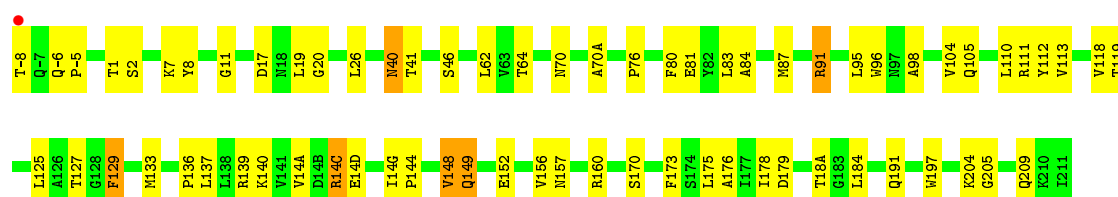
- Molecule 13: Proteasome component PRE4

Chain M:  70% 27%



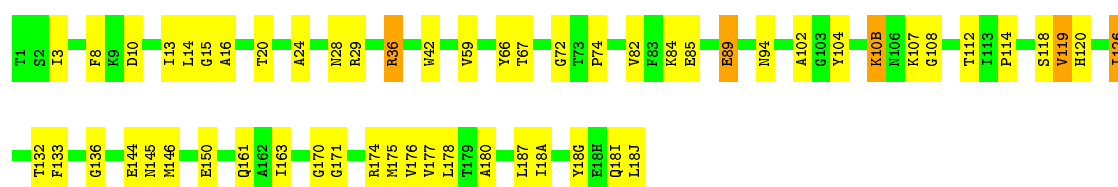
- Molecule 13: Proteasome component PRE4

Chain 1:  70% 27%



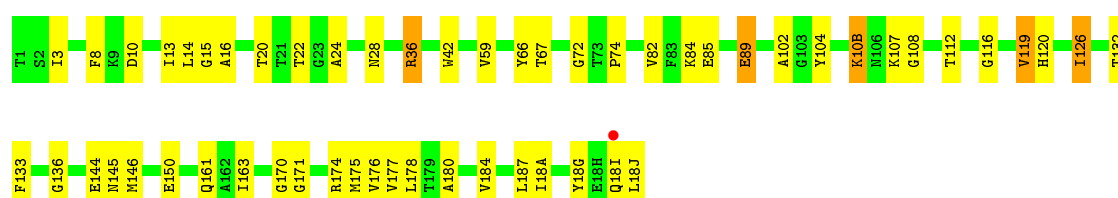
- Molecule 14: Proteasome component PRE3

Chain N:  71% 26%



- Molecule 14: Proteasome component PRE3

Chain 2:  72% 26%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.43 Å 300.96 Å 144.76 Å 90.00° 113.17° 90.00°	Depositor
Resolution (Å)	15.00 – 2.81 20.04 – 2.82	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-2.81) 97.9 (20.04-2.82)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.83 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.241 0.204 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.719	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50714	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: BIQ

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	0.39	0/1952	0.64	0/2642
1	O	0.37	0/1952	0.63	0/2642
2	B	0.37	0/1935	0.63	0/2618
2	P	0.37	0/1935	0.64	0/2618
3	C	0.36	0/1920	0.61	0/2598
3	Q	0.35	0/1920	0.61	0/2598
4	D	0.36	0/1887	0.63	0/2541
4	R	0.36	0/1887	0.63	0/2541
5	E	0.35	0/1823	0.60	0/2463
5	S	0.36	0/1823	0.60	0/2463
6	F	0.37	0/1937	0.61	0/2614
6	T	0.37	0/1937	0.62	0/2614
7	G	0.40	0/1959	0.63	0/2652
7	U	0.40	0/1959	0.63	0/2652
8	H	0.38	0/1716	0.68	0/2326
8	V	0.37	0/1716	0.67	0/2326
9	I	0.39	0/1611	0.66	0/2174
9	W	0.40	0/1611	0.67	0/2174
10	J	0.38	0/1613	0.64	0/2173
10	X	0.39	0/1613	0.65	0/2173
11	K	0.41	0/1681	0.65	0/2274
11	Y	0.39	0/1681	0.64	0/2274
12	L	0.40	0/1795	0.67	1/2420 (0.0%)
12	Z	0.40	0/1795	0.66	0/2420
13	1	0.41	0/1855	0.67	1/2514 (0.0%)
13	M	0.39	0/1855	0.66	1/2514 (0.0%)
14	2	0.40	0/1541	0.65	1/2087 (0.0%)
14	N	0.40	0/1541	0.65	0/2087
All	All	0.38	0/50450	0.64	4/68192 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
13	1	95	LEU	N-CA-C	-5.48	96.21	111.00
13	M	95	LEU	N-CA-C	-5.47	96.22	111.00
14	2	22	THR	N-CA-C	-5.15	97.09	111.00
12	L	95	TYR	N-CA-C	-5.13	97.16	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	50	0
1	O	1915	0	1926	52	0
2	B	1905	0	1901	94	0
2	P	1905	0	1901	96	0
3	C	1891	0	1900	101	0
3	Q	1891	0	1900	91	0
4	D	1862	0	1836	52	0
4	R	1862	0	1836	70	0
5	E	1795	0	1797	91	0
5	S	1795	0	1797	103	0
6	F	1897	0	1886	77	0
6	T	1897	0	1886	74	0
7	G	1921	0	1910	78	0
7	U	1921	0	1910	82	0
8	H	1685	0	1688	53	0
8	V	1685	0	1688	47	0
9	I	1581	0	1574	49	0
9	W	1581	0	1574	55	0
10	J	1585	0	1590	69	0
10	X	1585	0	1590	75	0
11	K	1644	0	1595	42	0
11	Y	1644	0	1595	40	0
12	L	1757	0	1711	57	0
12	Z	1757	0	1711	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	1	1824	0	1832	57	0
13	M	1824	0	1832	56	0
14	2	1512	0	1481	44	0
14	N	1512	0	1481	46	0
15	H	48	0	35	4	0
15	V	48	0	35	5	0
16	1	59	0	0	2	0
16	2	49	0	0	2	0
16	A	43	0	0	1	0
16	B	27	0	0	2	0
16	C	32	0	0	4	0
16	D	30	0	0	2	0
16	E	14	0	0	2	0
16	F	38	0	0	2	0
16	G	51	0	0	3	0
16	H	37	0	0	2	0
16	I	48	0	0	0	0
16	J	44	0	0	2	0
16	K	36	0	0	1	0
16	L	49	0	0	5	0
16	M	60	0	0	4	0
16	N	48	0	0	2	0
16	O	27	0	0	2	0
16	P	24	0	0	0	0
16	Q	22	0	0	3	0
16	R	25	0	0	3	0
16	S	16	0	0	1	0
16	T	36	0	0	3	0
16	U	47	0	0	5	0
16	V	39	0	0	3	0
16	W	44	0	0	4	0
16	X	38	0	0	5	0
16	Y	42	0	0	2	0
16	Z	45	0	0	3	0
All	All	50714	0	49324	1654	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 17.

All (1654) 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)
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:H	1.10	1.17
2:P:202:THR:HG22	2:P:204:SER:H	1.13	1.12
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.11	1.10
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.09	1.08
2:B:202:THR:HG22	2:B:204:SER:H	1.14	1.04
7:G:96:ALA:HA	7:G:107:MET:HE2	1.35	1.04
2:B:190:ILE:HG21	2:B:232:ILE:HD11	1.36	1.03
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.13	1.03
7:U:96:ALA:HA	7:U:107:MET:HE2	1.35	1.03
2:P:190:ILE:HG21	2:P:232:ILE:HD11	1.35	1.03
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.24	1.00
1:O:15:PHE:H	2:P:23:GLN:HE22	1.09	0.97
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.28	0.97
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.26	0.96
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.12	0.94
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.65	0.93
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.67	0.92
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.68	0.92
3:C:185:THR:HG22	3:C:187:GLU:H	1.33	0.92
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.69	0.91
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.31	0.91
3:C:163:GLN:NE2	3:C:164:THR:H	1.68	0.91
3:C:15:PHE:H	4:D:23:GLN:HE22	1.18	0.91
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.54	0.90
3:C:163:GLN:HE21	3:C:164:THR:N	1.68	0.90
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.70	0.90
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.68	0.90
2:B:15:PHE:H	3:C:23:GLN:HE22	1.19	0.89
1:A:15:PHE:H	2:B:23:GLN:HE22	1.14	0.89
3:C:185:THR:HB	3:C:188:GLU:HG2	1.55	0.88
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.57	0.87
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.87	0.87
2:P:163:ILE:HD13	2:P:164:SER:H	1.40	0.87
13:M:157:ASN:HD22	13:M:160:ARG:HH11	0.90	0.86
13:1:157:ASN:HD22	13:1:160:ARG:HH11	0.88	0.86
3:Q:163:GLN:HE21	3:Q:164:THR:H	0.86	0.85
5:S:15:PHE:H	6:T:23:GLN:HE22	1.23	0.85
14:N:161:GLN:NE2	14:2:136:GLY:HA2	1.91	0.85
2:B:163:ILE:HD13	2:B:164:SER:H	1.42	0.85
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.25	0.84
3:C:163:GLN:HE21	3:C:164:THR:H	0.86	0.84
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.43	0.82
5:E:207:LEU:H	5:E:207:LEU:HD23	1.44	0.82
1:O:124:THR:CG2	2:P:130:ARG:HH21	1.93	0.82
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.42	0.82
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.26	0.82
5:S:207:LEU:HD23	5:S:207:LEU:H	1.42	0.82
5:E:15:PHE:H	6:F:23:GLN:HE22	1.28	0.81
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.44	0.81
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.62	0.81
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.93	0.80
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.80	0.80
2:B:71:ASN:ND2	2:B:72:ASP:H	1.80	0.80
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.62	0.80
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.61	0.80
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.64	0.80
7:G:198:ILE:HG23	7:G:203:THR:O	1.81	0.80
3:Q:65:SER:HB2	16:Q:247:HOH:O	1.80	0.80
7:U:198:ILE:HG23	7:U:203:THR:O	1.81	0.80
2:P:71:ASN:ND2	2:P:72:ASP:H	1.79	0.80
2:B:124:THR:CG2	3:C:130:ARG:HH21	1.95	0.79
11:K:10(B):LYS:N	11:K:10(B):LYS:HD2	1.94	0.79
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.64	0.79
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.64	0.79
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.81	0.78
5:E:198:SER:HA	5:E:201:LEU:HG	1.65	0.78
5:S:198:SER:HA	5:S:201:LEU:HG	1.65	0.78
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.66	0.78
1:A:124:THR:CG2	2:B:130:ARG:HH21	1.96	0.78
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.32	0.78
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.00	0.77
12:Z:114:ASP:HB2	12:Z:118:SER:HB3	1.64	0.77
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.48	0.77
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.65	0.77
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.00	0.77
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.85	0.77
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.97	0.76
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.67	0.76
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.89	0.76
14:N:107:LYS:HG2	14:N:108:GLY:H	1.49	0.76
12:L:33:LYS:HD2	12:L:46:ASN:ND2	1.99	0.75
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:121:LEU:HB2	16:R:853:HOH:O	1.85	0.75
3:C:33:ARG:HB2	3:C:33:ARG:NH1	2.00	0.75
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.68	0.75
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.53	0.74
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.70	0.74
14:2:107:LYS:HG2	14:2:108:GLY:H	1.51	0.74
2:B:202:THR:HG22	2:B:204:SER:N	1.98	0.74
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.17	0.74
3:C:33:ARG:HB2	3:C:33:ARG:HH11	1.53	0.74
9:W:192:ARG:HG3	16:W:200:HOH:O	1.87	0.73
12:L:166:HIS:HD2	12:L:168:GLN:H	1.36	0.73
3:Q:33:ARG:HH11	3:Q:33:ARG:HB2	1.52	0.73
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.70	0.73
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.03	0.73
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.34	0.73
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.68	0.73
14:N:146:MET:HE3	14:N:150:GLU:HB3	1.70	0.73
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.36	0.73
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.03	0.73
2:P:202:THR:HG22	2:P:204:SER:N	1.97	0.73
4:D:177:LEU:HD13	5:E:58:LEU:HD11	1.71	0.72
4:R:156:THR:HG22	5:S:83:PRO:HD3	1.71	0.72
11:Y:10(B):LYS:N	11:Y:10(B):LYS:HD2	1.96	0.72
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.70	0.72
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.89	0.72
8:V:52:THR:O	8:V:56:THR:HB	1.90	0.71
8:V:128:GLY:O	8:V:131:SER:HB2	1.89	0.71
13:1:40:ASN:HD22	13:1:40:ASN:H	1.37	0.71
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.54	0.71
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.72	0.71
6:F:43:ASN:N	6:F:43:ASN:HD22	1.88	0.71
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.72	0.71
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.71	0.71
4:D:175:GLU:HG2	4:D:196:ILE:HD12	1.72	0.71
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.05	0.70
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	2.04	0.70
2:P:190:ILE:HG21	2:P:232:ILE:CD1	2.18	0.70
13:1:76:PRO:HD2	13:1:105:GLN:OE1	1.91	0.70
3:C:185:THR:HG22	3:C:187:GLU:N	2.06	0.70
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.38	0.70
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.40	0.70
12:Z:-9:GLN:HE21	13:1:-8:THR:HG21	1.56	0.70
5:E:18(D):ILE:HG23	5:E:18(E):LYS:HG3	1.73	0.70
8:H:52:THR:O	8:H:56:THR:HB	1.91	0.70
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:H	1.90	0.70
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.04	0.70
2:B:181:LYS:O	2:B:184:MET:HG3	1.92	0.70
10:J:-1:MET:HG2	10:J:1:ASP:H	1.57	0.70
6:T:43:ASN:HD22	6:T:43:ASN:N	1.88	0.70
4:R:175:GLU:HG2	4:R:196:ILE:HD12	1.73	0.69
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.72	0.69
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.26	0.69
2:B:190:ILE:HG21	2:B:232:ILE:CD1	2.19	0.69
11:K:142:TYR:O	11:K:143:LYS:HD2	1.92	0.69
5:S:18(D):ILE:HG23	5:S:18(E):LYS:HG3	1.73	0.69
8:H:128:GLY:O	8:H:131:SER:HB2	1.93	0.69
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG13	1.75	0.69
12:L:134:ILE:HD12	12:L:158:SER:HB3	1.73	0.69
12:Z:134:ILE:HD12	12:Z:158:SER:HB3	1.75	0.69
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.75	0.69
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.58	0.68
5:E:167:ALA:HB3	16:E:246:HOH:O	1.93	0.68
14:2:10(B):LYS:HD3	14:2:10(B):LYS:O	1.93	0.68
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.28	0.68
13:M:40:ASN:H	13:M:40:ASN:HD22	1.39	0.68
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG13	1.75	0.68
3:C:41:LYS:HG2	3:C:161:SER:O	1.92	0.68
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.73	0.68
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.23	0.68
9:W:29:ASN:ND2	9:W:30:LYS:HG3	2.09	0.68
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.59	0.68
9:I:29:ASN:ND2	9:I:30:LYS:HG3	2.08	0.68
5:S:207:LEU:H	5:S:207:LEU:CD2	2.06	0.68
2:B:51:GLU:OE2	2:B:202:THR:HG23	1.94	0.68
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.75	0.68
10:X:-1:MET:HG2	10:X:1:ASP:H	1.58	0.68
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.41	0.67
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.58	0.67
6:F:35:THR:HG21	6:F:51:GLU:O	1.94	0.67
7:U:59:LEU:O	7:U:61:PRO:HD3	1.94	0.67
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:86:ARG:HD2	16:G:256:HOH:O	1.95	0.67
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.24	0.67
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.10	0.67
14:N:10(B):LYS:HD3	14:N:10(B):LYS:O	1.95	0.67
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.95	0.67
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.94	0.67
13:M:14(C):ARG:HH11	13:M:14(C):ARG:HG3	1.60	0.67
5:S:207:LEU:N	5:S:207:LEU:HD23	2.10	0.67
4:R:161:ASN:N	5:S:58:LEU:O	2.26	0.67
14:2:13:ILE:HG12	14:2:177:VAL:HG13	1.77	0.66
3:Q:187:GLU:HG3	3:Q:232:TYR:OH	1.95	0.66
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.25	0.66
1:O:159:PRO:O	2:P:59:LEU:HD12	1.95	0.66
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.25	0.66
7:G:59:LEU:O	7:G:61:PRO:HD3	1.95	0.66
2:P:181:LYS:O	2:P:184:MET:HG3	1.94	0.66
3:Q:52:ARG:HD2	3:Q:208:LYS:O	1.95	0.66
4:R:207:LEU:C	4:R:207:LEU:HD23	2.16	0.66
6:F:192:GLN:O	6:F:196:ILE:HG12	1.95	0.66
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.43	0.66
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.61	0.66
7:U:72:ARG:HB2	7:U:72:ARG:HH11	1.60	0.66
11:K:21:THR:HG22	11:K:26:VAL:HA	1.77	0.66
5:E:207:LEU:H	5:E:207:LEU:CD2	2.08	0.66
2:P:51:GLU:OE2	2:P:202:THR:HG23	1.96	0.66
9:W:45:ILE:HB	9:W:52:VAL:HG13	1.76	0.66
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.31	0.66
2:B:190:ILE:CG2	2:B:232:ILE:HD11	2.20	0.66
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.26	0.66
13:M:149:GLN:NE2	13:M:149:GLN:H	1.92	0.66
2:P:190:ILE:CG2	2:P:232:ILE:HD11	2.19	0.66
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.78	0.66
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.60	0.66
6:T:192:GLN:O	6:T:196:ILE:HG12	1.96	0.66
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.61	0.66
13:1:149:GLN:H	13:1:149:GLN:NE2	1.94	0.65
7:G:72:ARG:NH1	7:G:72:ARG:HB2	2.11	0.65
3:C:52:ARG:HD2	3:C:208:LYS:O	1.97	0.65
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.77	0.65
12:Z:29:ARG:NH1	12:Z:193:ARG:HB3	2.11	0.65
5:E:207:LEU:HD23	5:E:207:LEU:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:121:GLN:O	1:O:124:THR:HB	1.95	0.65
10:X:32:ASP:OD2	10:X:34:THR:HG22	1.96	0.65
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.77	0.65
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.12	0.65
12:L:14(C):GLN:HG2	8:V:210:THR:HG21	1.79	0.65
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.43	0.65
13:M:76:PRO:HD2	13:M:105:GLN:OE1	1.96	0.65
6:T:35:THR:HG21	6:T:51:GLU:O	1.95	0.65
4:D:207:LEU:CD2	4:D:233:ILE:HD12	2.27	0.65
5:E:226:GLY:O	5:E:229:VAL:HG22	1.97	0.65
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.25	0.65
5:S:226:GLY:O	5:S:229:VAL:HG22	1.97	0.65
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.60	0.65
8:V:38:SER:OG	8:V:41:ILE:HD13	1.96	0.65
11:Y:21:THR:HG22	11:Y:26:VAL:HA	1.78	0.65
12:Z:14(I):THR:HG21	12:Z:14(M):VAL:HB	1.79	0.65
5:E:132:TYR:O	5:E:153:PRO:HB3	1.97	0.65
5:S:132:TYR:O	5:S:153:PRO:HB3	1.97	0.65
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.78	0.65
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.59	0.65
12:Z:114:ASP:HB3	12:Z:118:SER:H	1.62	0.65
8:H:34:LEU:HB2	16:H:1021:HOH:O	1.97	0.65
16:T:244:HOH:O	7:U:86:ARG:HD2	1.97	0.65
14:N:107:LYS:HG2	14:N:108:GLY:N	2.12	0.64
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.61	0.64
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.94	0.64
2:P:101:LYS:HZ1	10:X:85:GLN:HE22	1.46	0.64
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.61	0.64
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.80	0.64
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.61	0.64
2:B:121:GLN:O	2:B:124:THR:HB	1.98	0.64
13:M:14(D):GLU:O	13:M:14(G):ILE:HG12	1.98	0.64
8:H:45:GLY:O	15:H:1000:BIQ:H251	1.97	0.64
5:S:214:ILE:HG13	5:S:215:VAL:N	2.13	0.64
10:X:156:LYS:O	10:X:160:GLN:HG3	1.98	0.64
7:U:96:ALA:CA	7:U:107:MET:HE2	2.21	0.64
14:2:84:LYS:HG3	14:2:119:VAL:HG22	1.79	0.64
5:E:214:ILE:HG13	5:E:215:VAL:N	2.12	0.64
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.78	0.64
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.80	0.64
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.79	0.64
10:J:133:TYR:HD1	16:Y:236:HOH:O	1.81	0.64
4:D:102:TYR:O	12:L:81:ARG:HG3	1.97	0.64
2:P:121:GLN:O	2:P:124:THR:HB	1.97	0.64
4:D:207:LEU:HD23	4:D:207:LEU:C	2.18	0.64
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.79	0.64
3:Q:235:GLN:O	3:Q:239:GLU:HG2	1.98	0.64
4:R:102:TYR:O	12:Z:81:ARG:HG3	1.98	0.64
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.45	0.64
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.62	0.64
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.81	0.63
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.79	0.63
2:B:71:ASN:HD22	2:B:72:ASP:H	1.47	0.63
3:C:187:GLU:HG3	3:C:232:TYR:OH	1.98	0.63
7:G:72:ARG:HH11	7:G:72:ARG:HB2	1.63	0.63
3:C:71:ASP:HA	10:J:68:ILE:HD13	1.80	0.63
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.79	0.63
2:P:71:ASN:HD22	2:P:72:ASP:H	1.46	0.63
4:R:207:LEU:CD2	4:R:233:ILE:HD12	2.28	0.63
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.80	0.63
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.79	0.63
12:L:14(I):THR:HG21	12:L:14(M):VAL:HB	1.80	0.63
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.33	0.63
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.13	0.63
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.80	0.63
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.80	0.63
9:I:45:ILE:HB	9:I:52:VAL:HG13	1.80	0.63
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.33	0.63
11:K:143:LYS:HB2	11:K:146:LEU:HD13	1.80	0.63
4:R:192:LEU:O	4:R:196:ILE:HG12	1.99	0.63
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.62	0.63
14:N:13:ILE:HG12	14:N:177:VAL:HG13	1.80	0.63
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.34	0.63
2:P:101:LYS:HZ1	10:X:85:GLN:NE2	1.96	0.63
14:2:107:LYS:HG2	14:2:108:GLY:N	2.13	0.63
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.64	0.63
10:J:156:LYS:O	10:J:160:GLN:HG3	1.99	0.63
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.63	0.63
10:X:44:SER:OG	10:X:100:LEU:HB2	1.99	0.62
1:A:121:GLN:O	1:A:124:THR:HB	2.00	0.62
8:H:38:SER:OG	8:H:41:ILE:HD13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:32:ASP:OD2	10:J:34:THR:HG22	1.99	0.62
14:2:10(B):LYS:C	14:2:10(B):LYS:HD3	2.19	0.62
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.47	0.62
3:C:235:GLN:O	3:C:239:GLU:HG2	2.00	0.62
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.33	0.62
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.34	0.62
4:D:97:VAL:HG11	11:K:65:LEU:HD22	1.81	0.62
12:L:14(C):GLN:HG2	8:V:210:THR:CG2	2.29	0.62
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.80	0.62
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.34	0.62
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.79	0.62
3:C:232:TYR:O	3:C:236:ILE:HG13	1.98	0.62
7:G:96:ALA:CA	7:G:107:MET:HE2	2.22	0.62
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.80	0.62
7:U:8:TYR:C	7:U:10:ARG:H	2.03	0.62
13:1:14(D):GLU:O	13:1:14(G):ILE:HG12	2.00	0.62
4:D:12(G):GLU:HG2	4:D:125:GLU:H	1.63	0.62
5:S:201:LEU:O	5:S:202:ARG:HB2	1.98	0.62
11:Y:143:LYS:HB2	11:Y:146:LEU:HD13	1.79	0.62
6:F:43:ASN:ND2	6:F:185:SER:HA	2.15	0.62
8:V:45:GLY:O	15:V:1001:BIQ:H251	2.00	0.62
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.00	0.62
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.47	0.62
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.82	0.62
3:C:71:ASP:HA	10:J:68:ILE:CD1	2.29	0.62
10:J:-1:MET:HG2	10:J:1:ASP:N	2.14	0.62
1:O:225:THR:OG1	1:O:228:GLU:HG3	2.00	0.62
6:T:43:ASN:ND2	6:T:185:SER:HA	2.14	0.62
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.35	0.62
13:M:57:ARG:NE	16:M:247:HOH:O	2.33	0.62
7:U:121:GLN:O	7:U:124:THR:HB	2.00	0.62
4:R:97:VAL:HG11	11:Y:65:LEU:HD22	1.81	0.62
15:V:1001:BIQ:HN6	9:W:114:ASP:HB2	1.64	0.61
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.64	0.61
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.82	0.61
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.80	0.61
4:D:192:LEU:O	4:D:196:ILE:HG12	2.00	0.61
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.00	0.61
5:E:201:LEU:O	5:E:202:ARG:HB2	2.00	0.61
3:Q:232:TYR:O	3:Q:236:ILE:HG13	1.99	0.61
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.83	0.61
2:P:163:ILE:HD13	2:P:164:SER:N	2.11	0.61
10:J:168:MET:HE1	10:X:167:PRO:HB2	1.81	0.61
10:J:167:PRO:HB2	10:X:168:MET:HE1	1.82	0.61
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.01	0.61
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.15	0.61
10:J:44:SER:OG	10:J:100:LEU:HB2	2.01	0.61
9:W:43:LEU:HD21	9:W:45:ILE:HD11	1.82	0.61
10:X:-1:MET:HG2	10:X:1:ASP:N	2.15	0.61
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.82	0.61
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.00	0.61
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.16	0.61
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.81	0.61
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.36	0.61
2:P:185:LYS:HD3	2:P:186:VAL:N	2.16	0.60
3:Q:241:GLN:C	3:Q:243:GLN:H	2.03	0.60
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.83	0.60
6:T:187:ARG:HG3	6:T:187:ARG:HH11	1.64	0.60
6:T:186:ALA:O	6:T:190:VAL:HG23	2.02	0.60
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.49	0.60
9:W:6:MET:HB3	9:W:151:LEU:HD11	1.84	0.60
3:C:241:GLN:C	3:C:243:GLN:H	2.03	0.60
4:D:175:GLU:CG	4:D:196:ILE:HD12	2.31	0.60
12:L:29:ARG:NH1	12:L:193:ARG:HB3	2.16	0.60
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.82	0.60
14:N:10(B):LYS:HD3	14:N:10(B):LYS:C	2.22	0.60
2:B:185:LYS:HD3	2:B:186:VAL:N	2.17	0.60
6:F:69:VAL:HG12	16:F:248:HOH:O	2.01	0.60
6:T:54:ILE:HG12	6:T:208:PHE:HA	1.84	0.60
6:T:147:HIS:HD2	16:T:242:HOH:O	1.84	0.60
7:G:8:TYR:C	7:G:10:ARG:H	2.03	0.60
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.01	0.60
2:B:163:ILE:HD13	2:B:164:SER:N	2.13	0.60
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.83	0.60
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.84	0.60
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.81	0.60
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.81	0.60
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.36	0.60
1:A:173:LYS:O	1:A:177:GLU:HG3	2.03	0.59
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.37	0.59
1:O:110:LYS:HG2	16:O:245:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.37	0.59
8:V:196:VAL:HG23	16:V:1021:HOH:O	2.01	0.59
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.83	0.59
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.83	0.59
8:H:165:ASN:ND2	13:1:139:ARG:HH11	1.99	0.59
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.01	0.59
2:B:121:GLN:HG3	3:C:83:ALA:HB1	1.85	0.59
10:J:133:TYR:HE1	16:X:220:HOH:O	1.86	0.59
9:I:43:LEU:HD21	9:I:45:ILE:HD11	1.85	0.59
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.83	0.59
8:H:210:THR:HG21	12:Z:14(C):GLN:HG2	1.85	0.59
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.82	0.59
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.84	0.59
9:W:106:GLY:HA2	9:W:181:LYS:HD3	1.85	0.59
4:D:243:ALA:O	4:D:244:GLU:HB2	2.01	0.59
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.33	0.59
6:F:186:ALA:O	6:F:190:VAL:HG23	2.03	0.59
1:O:179:ARG:NH1	1:O:179:ARG:HB3	2.17	0.59
8:V:18:THR:HB	8:V:30:ASN:HA	1.83	0.59
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.18	0.59
12:L:93:PHE:N	12:L:94:PRO:HD3	2.17	0.59
4:R:243:ALA:O	4:R:244:GLU:HB2	2.02	0.59
6:T:203:GLU:O	6:T:206:LYS:HD2	2.03	0.59
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.84	0.59
4:D:207:LEU:HD21	4:D:233:ILE:HD12	1.84	0.59
13:M:139:ARG:HH11	8:V:165:ASN:ND2	1.97	0.59
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.49	0.59
10:J:168:MET:HE3	10:X:168:MET:HE3	1.85	0.59
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.85	0.59
3:C:173:ARG:O	3:C:177:GLU:HG3	2.03	0.59
6:F:173:LYS:O	6:F:177:GLU:HG3	2.02	0.58
15:H:1000:BIQ:HN6	9:I:114:ASP:HB2	1.68	0.58
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.85	0.58
4:R:207:LEU:HD21	4:R:233:ILE:HD12	1.84	0.58
6:T:43:ASN:ND2	6:T:43:ASN:N	2.52	0.58
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.03	0.58
9:I:6:MET:HB3	9:I:151:LEU:HD11	1.85	0.58
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.86	0.58
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.34	0.58
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.85	0.58
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:54:ILE:HG12	6:F:208:PHE:HA	1.85	0.58
1:A:97:HIS:HD2	8:H:61:SER:OG	1.87	0.58
4:R:85:ALA:O	4:R:89:ILE:HG12	2.03	0.58
1:O:33:GLN:HA	1:O:33:GLN:HE21	1.68	0.58
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.84	0.58
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.85	0.58
10:X:7:ARG:HG2	10:X:7:ARG:HH11	1.69	0.58
2:B:15:PHE:H	3:C:23:GLN:NE2	1.96	0.58
14:N:107:LYS:CG	14:N:108:GLY:H	2.17	0.58
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.85	0.58
6:F:43:ASN:N	6:F:43:ASN:ND2	2.51	0.58
6:F:72:ARG:HD2	13:M:64:THR:OG1	2.04	0.58
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.69	0.57
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.38	0.57
9:I:106:GLY:HA2	9:I:181:LYS:HD3	1.86	0.57
4:R:175:GLU:CG	4:R:196:ILE:HD12	2.33	0.57
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.69	0.57
4:D:85:ALA:O	4:D:89:ILE:HG12	2.04	0.57
8:H:210:THR:CG2	12:Z:14(C):GLN:HG2	2.34	0.57
12:L:114:ASP:HB3	12:L:118:SER:H	1.69	0.57
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.69	0.57
3:C:7:GLY:N	16:C:268:HOH:O	2.37	0.57
10:J:147:THR:OG1	10:J:150:GLU:HG3	2.04	0.57
3:C:41:LYS:HD3	3:C:161:SER:HA	1.85	0.57
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	2.02	0.57
5:S:47:VAL:HG22	5:S:214:ILE:HD12	1.86	0.57
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.33	0.57
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.85	0.57
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.69	0.57
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.86	0.57
3:Q:182:PRO:O	3:Q:184:ALA:N	2.38	0.57
7:G:172:ILE:HD12	7:G:197:MET:CE	2.35	0.57
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.86	0.57
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.87	0.57
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.03	0.57
9:I:29:ASN:HD22	9:I:29:ASN:H	1.52	0.57
9:W:29:ASN:H	9:W:29:ASN:HD22	1.53	0.57
12:L:148:VAL:O	12:L:152:ILE:HG13	2.05	0.57
5:E:47:VAL:HG22	5:E:214:ILE:HD12	1.87	0.56
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.40	0.56
11:K:19:ARG:HH21	11:K:29:GLN:HE22	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:177:LEU:HA	5:S:58:LEU:HD11	1.86	0.56
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.34	0.56
6:F:237:GLN:O	6:F:240:ILE:HG22	2.06	0.56
7:G:121:GLN:O	7:G:124:THR:HB	2.04	0.56
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.17	0.56
2:P:225:LYS:HG3	2:P:228:GLU:OE1	2.04	0.56
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.86	0.56
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.06	0.56
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.40	0.56
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.87	0.56
3:C:182:PRO:O	3:C:184:ALA:N	2.38	0.56
6:F:203:GLU:O	6:F:206:LYS:HD2	2.05	0.56
8:H:18:THR:HB	8:H:30:ASN:HA	1.86	0.56
11:K:7:ARG:HD2	11:K:108:PRO:O	2.05	0.56
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.40	0.56
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.18	0.56
2:P:6:ARG:HD2	4:R:9:ASP:N	2.20	0.56
6:T:237:GLN:O	6:T:240:ILE:HG22	2.05	0.56
7:G:141:VAL:HG21	7:G:216:THR:HA	1.87	0.56
1:O:60:MET:HE2	16:U:255:HOH:O	2.06	0.56
4:R:121:LEU:HD13	5:S:130:ARG:HH21	1.71	0.56
5:S:73:HIS:HE1	5:S:107:LEU:O	1.87	0.56
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.87	0.56
6:T:72:ARG:HD2	13:1:64:THR:OG1	2.04	0.56
7:U:83:PRO:HG2	16:U:262:HOH:O	2.06	0.56
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.51	0.56
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	1.87	0.56
2:B:225:LYS:HG3	2:B:228:GLU:OE1	2.06	0.56
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.86	0.56
2:B:55:THR:HG22	2:B:59:LEU:HD23	1.88	0.56
9:W:29:ASN:H	9:W:29:ASN:ND2	2.04	0.56
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.88	0.56
11:Y:19:ARG:HH21	11:Y:29:GLN:HE22	1.52	0.56
13:1:7:LYS:HG3	13:1:14(G):ILE:HD12	1.88	0.56
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.87	0.56
6:T:173:LYS:O	6:T:177:GLU:HG3	2.05	0.56
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.71	0.56
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.36	0.56
9:I:43:LEU:CG	9:I:45:ILE:HD11	2.36	0.56
9:W:14:ILE:HG13	9:W:34:ILE:HD12	1.88	0.56
9:W:43:LEU:CG	9:W:45:ILE:HD11	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	2.03	0.56
11:K:156:LYS:HB2	11:K:175:LEU:HD11	1.88	0.56
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.16	0.56
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.35	0.55
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.36	0.55
9:I:29:ASN:H	9:I:29:ASN:ND2	2.03	0.55
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.86	0.55
10:J:52:THR:CG2	10:J:53:VAL:N	2.69	0.55
14:N:126:ILE:HD13	14:N:126:ILE:H	1.72	0.55
5:E:73:HIS:HE1	5:E:107:LEU:O	1.89	0.55
16:D:268:HOH:O	5:E:86:ARG:HD3	2.07	0.55
8:V:53:GLU:O	8:V:56:THR:HG22	2.06	0.55
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.04	0.55
4:R:53:ARG:HG2	4:R:53:ARG:O	2.05	0.55
4:R:72:ARG:HG3	16:R:1302:HOH:O	2.05	0.55
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.88	0.55
13:1:46:SER:OG	13:1:98:ALA:HB3	2.06	0.55
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.07	0.55
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.87	0.55
2:B:196:THR:O	2:B:200:THR:HG23	2.07	0.55
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.34	0.55
12:L:14(I):THR:O	12:L:14(K):LYS:HB2	2.07	0.55
7:U:141:VAL:HG21	7:U:216:THR:HA	1.88	0.55
8:V:34:LEU:HD22	8:V:174:ASP:HB3	1.88	0.55
13:1:113:VAL:HG23	13:1:119:THR:HG22	1.87	0.55
10:J:168:MET:HE1	10:X:167:PRO:CB	2.37	0.55
7:U:87:ASN:HD22	7:U:87:ASN:C	2.09	0.55
6:F:36:THR:HG22	6:F:51:GLU:OE2	2.07	0.55
13:M:7:LYS:HG3	13:M:14(G):ILE:HD12	1.89	0.55
2:P:71:ASN:ND2	2:P:72:ASP:N	2.52	0.55
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.41	0.55
5:S:15:PHE:H	6:T:23:GLN:NE2	2.01	0.55
9:W:14:ILE:CG1	9:W:34:ILE:HD12	2.36	0.55
14:2:107:LYS:CG	14:2:108:GLY:H	2.18	0.55
1:A:197:LEU:HD23	1:A:210:ILE:HD12	1.87	0.55
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.21	0.55
8:V:172:ASN:HD22	8:V:193:THR:HA	1.71	0.55
12:Z:14(I):THR:O	12:Z:14(K):LYS:HB2	2.07	0.55
12:Z:79:ALA:O	12:Z:83:ILE:HG12	2.07	0.55
2:P:239:THR:OXT	2:P:239:THR:HG22	2.07	0.55
9:W:174:VAL:HG21	9:W:186:LYS:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.07	0.55
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.10	0.55
3:C:190:VAL:O	3:C:194:VAL:HG23	2.07	0.55
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.89	0.55
7:U:172:ILE:HD12	7:U:197:MET:CE	2.36	0.55
12:L:79:ALA:O	12:L:83:ILE:HG12	2.07	0.54
1:O:173:LYS:O	1:O:177:GLU:HG3	2.06	0.54
2:P:55:THR:HG22	2:P:59:LEU:HD23	1.88	0.54
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.36	0.54
4:R:160:TYR:HA	5:S:59:SER:HA	1.88	0.54
5:S:68:ILE:HB	5:S:76:LEU:CD2	2.37	0.54
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.37	0.54
9:W:43:LEU:CD2	9:W:45:ILE:HD11	2.36	0.54
7:G:225:SER:O	7:G:229:ILE:HG13	2.06	0.54
12:L:5:GLY:O	12:L:124:CYS:HA	2.07	0.54
13:M:113:VAL:HG23	13:M:119:THR:HG22	1.88	0.54
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.89	0.54
10:X:143:ARG:O	10:X:146:MET:HG3	2.07	0.54
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.41	0.54
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.06	0.54
3:C:206:GLY:CA	3:C:209:ASN:HB2	2.36	0.54
8:H:34:LEU:HD22	8:H:174:ASP:HB3	1.89	0.54
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.89	0.54
7:U:225:SER:O	7:U:229:ILE:HG13	2.08	0.54
10:X:52:THR:CG2	10:X:53:VAL:N	2.70	0.54
13:1:40:ASN:HD22	13:1:40:ASN:N	1.99	0.54
7:G:233:LEU:O	7:G:236:ILE:HG13	2.08	0.54
1:O:197:LEU:HD23	1:O:210:ILE:HD12	1.89	0.54
5:E:65:LYS:HG3	5:E:65:LYS:O	2.07	0.54
5:S:190:ILE:CG2	5:S:212:ILE:HD13	2.38	0.54
6:T:54:ILE:HD11	6:T:209:GLU:HB2	1.89	0.54
6:T:43:ASN:ND2	6:T:43:ASN:H	2.04	0.54
7:U:224:LEU:HB3	7:U:228:ASN:HB2	1.90	0.54
1:A:69:LEU:HD23	1:A:69:LEU:C	2.27	0.54
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.38	0.54
13:M:40:ASN:HD22	13:M:40:ASN:N	1.99	0.54
2:P:71:ASN:HD22	2:P:72:ASP:N	2.06	0.54
5:S:68:ILE:HB	5:S:76:LEU:HD21	1.89	0.54
6:T:20(B):GLU:CD	6:T:20(C):LYS:HE3	2.28	0.54
7:U:168:LYS:O	7:U:172:ILE:HG12	2.07	0.54
11:Y:7:ARG:HG2	11:Y:108:PRO:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:40:ASN:ND2	16:Z:219:HOH:O	2.39	0.54
3:C:216:LYS:HD2	3:C:220:ASP:OD1	2.08	0.54
16:B:254:HOH:O	3:C:33:ARG:HD2	2.07	0.54
4:D:53:ARG:HG2	4:D:53:ARG:O	2.08	0.54
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.89	0.54
10:J:7:ARG:HG2	10:J:7:ARG:HH11	1.73	0.54
11:K:195:LEU:O	11:K:199:VAL:HG23	2.07	0.54
3:Q:216:LYS:HD2	3:Q:220:ASP:OD1	2.07	0.54
4:R:186:LEU:O	4:R:190:GLU:HG3	2.08	0.54
7:G:38:LEU:HD12	7:G:38:LEU:C	2.28	0.54
5:S:190:ILE:HG23	5:S:212:ILE:HD13	1.89	0.54
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.05	0.54
10:X:113:ILE:HA	10:X:118:THR:O	2.08	0.54
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.21	0.54
1:A:86:ARG:HH21	7:G:118:ASN:ND2	2.05	0.54
2:B:21:LEU:O	2:B:25:GLU:HG2	2.07	0.54
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.90	0.54
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.90	0.54
1:O:232:ARG:HG3	1:O:232:ARG:HH11	1.71	0.54
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.88	0.54
6:F:20(B):GLU:CD	6:F:20(C):LYS:HE3	2.29	0.54
9:I:14:ILE:CG1	9:I:34:ILE:HD12	2.38	0.54
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.90	0.54
7:U:233:LEU:O	7:U:236:ILE:HG13	2.08	0.54
12:Z:114:ASP:CB	12:Z:118:SER:HB3	2.37	0.54
5:E:190:ILE:HG23	5:E:212:ILE:HD13	1.90	0.53
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.89	0.53
6:F:54:ILE:HD11	6:F:209:GLU:HB2	1.91	0.53
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.90	0.53
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.90	0.53
9:I:174:VAL:HG21	9:I:186:LYS:HE3	1.90	0.53
9:I:43:LEU:HG	9:I:45:ILE:HD11	1.88	0.53
11:K:12:ILE:HB	11:K:178:VAL:HB	1.89	0.53
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.43	0.53
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.08	0.53
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.73	0.53
2:B:71:ASN:ND2	2:B:72:ASP:N	2.53	0.53
4:D:12(F):GLY:HA3	16:E:243:HOH:O	2.08	0.53
5:E:68:ILE:HB	5:E:76:LEU:HD21	1.91	0.53
6:F:43:ASN:H	6:F:43:ASN:ND2	2.06	0.53
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:48:LEU:HG	9:I:50:THR:HG22	1.91	0.53
14:N:14:LEU:O	14:N:175:MET:HA	2.07	0.53
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.90	0.53
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.43	0.53
4:D:186:LEU:O	4:D:190:GLU:HG3	2.09	0.53
7:U:136:LEU:O	7:U:150:LYS:HA	2.07	0.53
12:Z:148:VAL:O	12:Z:152:ILE:HG13	2.08	0.53
2:P:196:THR:O	2:P:200:THR:HG23	2.08	0.53
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.08	0.53
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.39	0.53
6:F:203:GLU:C	6:F:205:ASN:H	2.11	0.53
9:I:43:LEU:CD2	9:I:45:ILE:HD11	2.38	0.53
10:J:111:TYR:CE1	10:J:121:GLU:HG3	2.43	0.53
14:2:146:MET:CE	14:2:150:GLU:HB3	2.38	0.53
14:2:14:LEU:O	14:2:175:MET:HA	2.08	0.53
10:X:24:ILE:HD13	11:Y:132:THR:HG21	1.90	0.53
7:G:236:ILE:HD12	7:G:237:ALA:N	2.24	0.53
1:O:69:LEU:HD23	1:O:69:LEU:C	2.29	0.53
5:S:65:LYS:HG3	5:S:65:LYS:O	2.08	0.53
7:U:236:ILE:HD12	7:U:237:ALA:N	2.24	0.53
9:W:43:LEU:HG	9:W:45:ILE:HD11	1.90	0.53
3:C:227:GLU:OE1	3:C:227:GLU:N	2.41	0.53
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.89	0.53
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.90	0.53
2:B:239:THR:OXT	2:B:239:THR:HG22	2.09	0.53
4:D:170:GLU:N	4:D:170:GLU:OE1	2.40	0.53
10:J:6:ILE:HD11	10:J:142:TYR:CD1	2.44	0.53
11:K:7:ARG:HG2	11:K:108:PRO:HB2	1.91	0.53
12:L:-7:ASN:ND2	12:L:-5:TYR:H	2.07	0.53
6:T:127:ASN:HD22	6:T:128:SER:N	2.07	0.53
14:2:146:MET:HE3	14:2:150:GLU:HB3	1.91	0.52
6:F:127:ASN:HD22	6:F:128:SER:N	2.07	0.52
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.09	0.52
12:L:145:TYR:CD1	12:L:146:LEU:N	2.77	0.52
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.08	0.52
4:R:170:GLU:OE1	4:R:170:GLU:N	2.40	0.52
5:S:40:LEU:HD23	5:S:40:LEU:N	2.24	0.52
6:T:43:ASN:HD21	6:T:185:SER:HA	1.74	0.52
12:Z:83:ILE:HB	12:Z:113:PHE:CE2	2.44	0.52
14:2:126:ILE:H	14:2:126:ILE:HD13	1.73	0.52
5:E:194:VAL:O	5:E:197:ILE:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:158:VAL:HG22	7:G:159:GLY:N	2.24	0.52
7:G:87:ASN:HD22	7:G:87:ASN:C	2.13	0.52
8:H:179:GLU:OE2	8:H:182:LYS:HE2	2.10	0.52
8:V:172:ASN:ND2	8:V:193:THR:HA	2.25	0.52
16:V:1036:HOH:O	9:W:150:ASP:HA	2.09	0.52
10:X:6:ILE:HD11	10:X:142:TYR:CE1	2.44	0.52
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.38	0.52
5:E:190:ILE:CG2	5:E:212:ILE:HD13	2.39	0.52
5:E:40:LEU:HD23	5:E:40:LEU:N	2.25	0.52
6:F:21(B):THR:O	6:F:21(C):ASN:HB2	2.09	0.52
8:H:33:LYS:HD3	15:H:1000:BIQ:H253	1.92	0.52
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.44	0.52
7:U:186:TRP:O	7:U:190:VAL:HG23	2.10	0.52
9:W:130:ALA:HB2	9:W:166:ASP:HB2	1.91	0.52
3:C:186:VAL:O	3:C:190:VAL:HG23	2.10	0.52
7:G:136:LEU:O	7:G:150:LYS:HA	2.08	0.52
7:G:168:LYS:O	7:G:172:ILE:HG12	2.10	0.52
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.40	0.52
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.30	0.52
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.40	0.52
10:X:6:ILE:HD11	10:X:142:TYR:CD1	2.45	0.52
1:A:32:LYS:HE2	1:A:32:LYS:HA	1.91	0.52
5:E:15:PHE:H	6:F:23:GLN:NE2	2.02	0.52
9:I:44:GLY:O	9:I:45:ILE:HD13	2.09	0.52
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.45	0.52
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.77	0.52
2:B:95:HIS:CD2	2:B:115:ARG:HG2	2.44	0.52
2:B:6:ARG:HB2	5:E:127:TYR:OH	2.10	0.52
6:F:43:ASN:HD21	6:F:185:SER:HA	1.75	0.52
10:J:6:ILE:HD11	10:J:142:TYR:CE1	2.45	0.52
10:J:24:ILE:HD13	11:K:132:THR:HG21	1.92	0.52
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.45	0.52
4:R:229:THR:O	4:R:233:ILE:HG12	2.09	0.52
6:T:203:GLU:C	6:T:205:ASN:H	2.12	0.52
10:X:3:ILE:HG22	10:X:100:LEU:CD1	2.39	0.52
9:I:130:ALA:HB2	9:I:166:ASP:HB2	1.92	0.52
2:P:95:HIS:CD2	2:P:115:ARG:HG2	2.44	0.52
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.39	0.52
10:X:111:TYR:CE1	10:X:121:GLU:HG3	2.45	0.52
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.91	0.52
14:N:146:MET:CE	14:N:150:GLU:HB3	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:163:GLN:HE22	3:Q:173:ARG:NE	2.08	0.52
1:O:97:HIS:HD2	8:V:61:SER:OG	1.92	0.52
5:S:104:ASN:HB2	13:1:81:GLU:HG2	1.91	0.52
2:B:41:MET:HE3	16:B:240:HOH:O	2.10	0.52
5:E:227:GLU:CD	5:E:227:GLU:N	2.63	0.52
12:L:83:ILE:HB	12:L:113:PHE:CE2	2.45	0.52
8:V:81:GLN:O	8:V:85:GLN:HG3	2.10	0.52
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.10	0.51
14:2:59:VAL:HG22	14:2:82:VAL:HG12	1.91	0.51
6:F:127:ASN:HD22	6:F:127:ASN:C	2.12	0.51
8:H:165:ASN:HD22	13:1:139:ARG:NH1	2.03	0.51
10:J:143:ARG:O	10:J:146:MET:HG3	2.10	0.51
13:M:46:SER:OG	13:M:98:ALA:HB3	2.09	0.51
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.40	0.51
14:2:8:PHE:CE1	14:2:10:ASP:HB2	2.45	0.51
3:C:55:THR:C	3:C:56:LEU:HD22	2.31	0.51
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.91	0.51
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.10	0.51
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.45	0.51
6:T:53:LEU:HD11	6:T:205:ASN:OD1	2.10	0.51
7:G:69:CYS:HB3	16:G:276:HOH:O	2.11	0.51
10:J:167:PRO:CB	10:X:168:MET:HE1	2.40	0.51
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.40	0.51
2:P:21(A):LYS:O	2:P:21(B):GLY:C	2.49	0.51
5:S:227:GLU:N	5:S:227:GLU:CD	2.63	0.51
7:U:227:GLU:HG2	16:U:282:HOH:O	2.11	0.51
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.92	0.51
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.91	0.51
2:B:71:ASN:HD22	2:B:72:ASP:N	2.07	0.51
4:D:229:THR:O	4:D:233:ILE:HG12	2.11	0.51
5:E:107:LEU:HD11	5:E:111:ARG:HG2	1.92	0.51
5:E:68:ILE:HB	5:E:76:LEU:CD2	2.39	0.51
7:G:192:PHE:CD1	7:G:192:PHE:C	2.83	0.51
10:J:113:ILE:HA	10:J:118:THR:O	2.11	0.51
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.92	0.51
9:W:48:LEU:HG	9:W:50:THR:HG22	1.92	0.51
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.91	0.51
5:E:58:LEU:HD12	5:E:58:LEU:N	2.25	0.51
11:K:10(A):ARG:HH11	11:K:10(A):ARG:HG2	1.75	0.51
2:P:224:PHE:N	2:P:224:PHE:HD2	2.08	0.51
6:T:21(B):THR:O	6:T:21(C):ASN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:71:ASP:HA	10:X:68:ILE:HD13	1.92	0.51
11:Y:40:PHE:HB3	11:Y:73:ARG:NH2	2.26	0.51
1:A:4:MET:SD	1:A:5:THR:N	2.68	0.51
9:I:14:ILE:HG13	9:I:34:ILE:HD12	1.91	0.51
10:J:168:MET:CE	10:X:168:MET:HE3	2.40	0.51
4:R:90:GLU:OE2	11:Y:69:ARG:NH1	2.44	0.51
13:1:-6:GLN:O	13:1:-6:GLN:HG3	2.11	0.51
2:B:234:VAL:HA	2:B:239:THR:HA	1.93	0.51
4:D:112:LEU:C	4:D:112:LEU:HD13	2.31	0.51
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.37	0.51
8:H:53:GLU:O	8:H:56:THR:HG22	2.11	0.51
13:M:-6:GLN:O	13:M:-6:GLN:HG3	2.10	0.51
1:O:33:GLN:CA	1:O:33:GLN:HE21	2.24	0.51
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.93	0.51
3:C:175:PHE:O	3:C:179:ASN:HB2	2.10	0.51
3:C:79:SER:HA	16:C:260:HOH:O	2.09	0.51
7:G:186:TRP:O	7:G:190:VAL:HG23	2.11	0.51
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.40	0.51
5:S:194:VAL:O	5:S:197:ILE:HG22	2.10	0.51
7:U:158:VAL:HG22	7:U:159:GLY:N	2.26	0.51
1:A:197:LEU:CD2	1:A:210:ILE:HD12	2.41	0.51
2:B:224:PHE:HD2	2:B:224:PHE:N	2.09	0.51
10:X:13:ILE:HD12	10:X:177:ILE:HD13	1.93	0.51
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.11	0.51
2:B:224:PHE:CD2	2:B:224:PHE:N	2.79	0.51
7:G:77:VAL:HG12	7:G:137:THR:HB	1.93	0.51
8:V:33:LYS:HD3	15:V:1001:BIQ:H253	1.92	0.51
9:W:23:GLN:HB2	16:W:228:HOH:O	2.11	0.51
2:B:27:ALA:O	2:B:31:ILE:HG12	2.12	0.50
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.92	0.50
2:P:224:PHE:N	2:P:224:PHE:CD2	2.79	0.50
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.93	0.50
13:M:139:ARG:NH1	8:V:165:ASN:HD22	2.02	0.50
2:P:235:LYS:C	2:P:237:GLY:H	2.14	0.50
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.25	0.50
11:Y:10(A):ARG:HH11	11:Y:10(A):ARG:HG2	1.76	0.50
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.42	0.50
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.74	0.50
7:G:77:VAL:CG1	7:G:137:THR:HB	2.42	0.50
12:L:31:GLU:HA	16:L:212:HOH:O	2.11	0.50
2:P:27:ALA:O	2:P:31:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:38:LEU:C	7:U:38:LEU:HD12	2.31	0.50
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.93	0.50
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.75	0.50
8:H:41:ILE:HG13	8:H:76:VAL:HG22	1.93	0.50
8:H:200:LYS:HE3	9:I:140:SER:O	2.12	0.50
8:V:20:SER:HB3	8:V:28:ASP:HB3	1.93	0.50
10:X:14:LEU:HD12	10:X:42:LEU:HD23	1.94	0.50
12:Z:99:THR:HG23	12:Z:113:PHE:HB2	1.92	0.50
8:H:20:SER:HB3	8:H:28:ASP:HB3	1.94	0.50
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.11	0.50
1:A:85:TYR:O	1:A:89:VAL:HG23	2.11	0.50
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.47	0.50
8:H:172:ASN:HD22	8:H:193:THR:HA	1.76	0.50
6:T:69:VAL:HG12	16:T:264:HOH:O	2.12	0.50
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.12	0.50
8:V:34:LEU:HB2	16:V:1019:HOH:O	2.10	0.50
6:F:170:GLN:HB2	16:F:265:HOH:O	2.12	0.50
1:O:197:LEU:CD2	1:O:210:ILE:HD12	2.42	0.50
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.12	0.50
6:T:36:THR:HG22	6:T:51:GLU:OE2	2.11	0.50
14:2:66:TYR:CD2	14:2:74:PRO:HB3	2.47	0.50
11:K:32:LYS:N	11:K:32:LYS:HD2	2.27	0.50
2:B:185:LYS:HD2	2:B:187:ASP:H	1.77	0.49
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.42	0.49
7:U:77:VAL:HG12	7:U:137:THR:HB	1.93	0.49
13:1:152:GLU:O	13:1:156:VAL:HG23	2.11	0.49
5:E:17:PRO:HA	6:F:26:TYR:CD2	2.47	0.49
7:G:49:ILE:HD13	7:G:193:ALA:HB1	1.92	0.49
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.47	0.49
7:G:72:ARG:HH11	7:G:72:ARG:CB	2.24	0.49
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.94	0.49
13:M:17:ASP:HA	13:M:173:PHE:CB	2.43	0.49
5:S:39:GLY:O	5:S:162:GLY:HA2	2.11	0.49
7:U:192:PHE:C	7:U:192:PHE:CD1	2.84	0.49
2:B:38:ILE:HD13	2:B:164:SER:HB3	1.94	0.49
10:J:6:ILE:CG2	10:J:13:ILE:HB	2.42	0.49
1:O:4:MET:SD	1:O:5:THR:N	2.70	0.49
3:Q:57:LYS:NZ	16:Q:250:HOH:O	2.46	0.49
5:S:221:PHE:CE1	5:S:223:ILE:HD11	2.47	0.49
5:S:54:ASN:ND2	5:S:56:ASP:O	2.43	0.49
4:D:17:PRO:HD2	16:D:271:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:HD12	7:G:173:THR:HG23	1.95	0.49
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.95	0.49
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.47	0.49
3:Q:71:ASP:HA	10:X:68:ILE:CD1	2.43	0.49
6:T:127:ASN:HD22	6:T:127:ASN:C	2.14	0.49
10:J:168:MET:CE	10:X:168:MET:CE	2.90	0.49
10:X:16:SER:HB2	16:X:226:HOH:O	2.13	0.49
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.94	0.49
2:B:190:ILE:HG23	2:B:212:PHE:CE2	2.48	0.49
2:B:235:LYS:C	2:B:237:GLY:H	2.15	0.49
10:J:3:ILE:HG22	10:J:100:LEU:CD1	2.42	0.49
10:J:133:TYR:OH	10:X:24:ILE:HG12	2.12	0.49
5:E:104:ASN:HB2	13:M:81:GLU:HG2	1.93	0.49
4:R:68:VAL:HG21	4:R:89:ILE:HD12	1.94	0.49
7:U:203:THR:HG22	7:U:204:GLU:N	2.27	0.49
4:D:243:ALA:O	4:D:244:GLU:CB	2.60	0.49
5:E:231:LYS:HD2	5:E:231:LYS:H	1.77	0.49
6:F:53:LEU:HD11	6:F:205:ASN:OD1	2.12	0.49
8:H:172:ASN:ND2	8:H:193:THR:HA	2.28	0.49
2:B:101:LYS:NZ	10:J:85:GLN:NE2	2.60	0.49
12:L:166:HIS:CD2	12:L:168:GLN:H	2.24	0.49
1:O:15:PHE:H	2:P:23:GLN:NE2	1.93	0.49
2:P:185:LYS:HD2	2:P:187:ASP:H	1.77	0.49
6:T:192:GLN:HE21	6:T:195:LYS:CE	2.23	0.49
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.42	0.49
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.95	0.49
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.13	0.49
2:P:51:GLU:OE2	2:P:209:ARG:NH2	2.46	0.49
1:O:17:PRO:HA	2:P:26:TYR:CD1	2.48	0.49
5:S:231:LYS:HD2	5:S:231:LYS:H	1.78	0.49
11:Y:32:LYS:N	11:Y:32:LYS:HD2	2.28	0.49
3:C:227:GLU:CD	3:C:227:GLU:H	2.16	0.49
5:E:15:PHE:N	6:F:23:GLN:HE22	2.04	0.49
3:Q:201:VAL:HG11	3:Q:210:ILE:HG13	1.94	0.49
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.12	0.49
6:T:175:GLU:OE1	6:T:199:LEU:HD23	2.13	0.49
8:V:179:GLU:OE2	8:V:182:LYS:HE2	2.11	0.49
10:J:144:PRO:CG	11:Y:207:ASN:HD21	2.25	0.49
8:H:81:GLN:O	8:H:85:GLN:HG3	2.13	0.49
14:N:94:ASN:ND2	16:N:228:HOH:O	2.39	0.49
4:R:15:PHE:HB2	5:S:23:GLN:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:243:ALA:O	4:R:244:GLU:CB	2.61	0.49
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.93	0.49
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.95	0.49
10:X:6:ILE:CG2	10:X:13:ILE:HB	2.43	0.49
2:B:21(A):LYS:O	2:B:21(B):GLY:C	2.50	0.48
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.95	0.48
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.47	0.48
2:P:194:LEU:O	2:P:198:SER:HB2	2.13	0.48
3:Q:175:PHE:O	3:Q:179:ASN:HB2	2.13	0.48
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.28	0.48
11:Y:4:LEU:CD1	11:Y:159:ILE:HD11	2.43	0.48
3:C:201:VAL:HG11	3:C:210:ILE:HG13	1.95	0.48
11:K:131:GLN:HG3	11:K:132:THR:N	2.28	0.48
14:N:59:VAL:HG22	14:N:82:VAL:HG12	1.95	0.48
7:U:72:ARG:CB	7:U:72:ARG:HH11	2.24	0.48
9:W:33:LYS:O	9:W:44:GLY:HA2	2.14	0.48
11:Y:131:GLN:HG3	11:Y:132:THR:N	2.28	0.48
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.48	0.48
4:R:175:GLU:OE1	4:R:175:GLU:HA	2.13	0.48
5:S:58:LEU:N	5:S:58:LEU:HD12	2.28	0.48
7:U:49:ILE:HD13	7:U:193:ALA:HB1	1.94	0.48
7:U:77:VAL:CG1	7:U:137:THR:HB	2.42	0.48
4:D:68:VAL:HG21	4:D:89:ILE:HD12	1.95	0.48
6:F:199:LEU:HD12	6:F:240:ILE:HD13	1.95	0.48
2:P:234:VAL:HA	2:P:239:THR:HA	1.94	0.48
2:P:27:ALA:O	2:P:30:SER:HB3	2.13	0.48
2:B:186:VAL:O	2:B:190:ILE:HG13	2.14	0.48
5:E:38:VAL:HG12	5:E:39:GLY:N	2.29	0.48
7:G:8:TYR:C	7:G:10:ARG:N	2.67	0.48
1:O:85:TYR:O	1:O:89:VAL:HG23	2.13	0.48
2:P:186:VAL:O	2:P:190:ILE:HG13	2.13	0.48
4:R:32:LYS:O	4:R:167:SER:HA	2.13	0.48
13:1:104:VAL:HG23	13:1:178:ILE:CG2	2.41	0.48
5:E:185:ASN:C	5:E:185:ASN:HD22	2.16	0.48
7:G:203:THR:HG22	7:G:204:GLU:N	2.27	0.48
12:L:98:HIS:HD2	16:L:200:HOH:O	1.95	0.48
5:S:107:LEU:HD11	5:S:111:ARG:HG2	1.94	0.48
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.49	0.48
3:Q:15:PHE:N	4:R:23:GLN:HE22	1.95	0.48
13:1:184:LEU:C	13:1:184:LEU:HD23	2.34	0.48
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.14	0.48
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.96	0.48
2:B:15:PHE:N	3:C:23:GLN:HE22	1.99	0.48
5:E:221:PHE:CE1	5:E:223:ILE:HD11	2.49	0.48
12:L:48:PHE:CZ	12:L:50:ALA:HB3	2.49	0.48
2:P:190:ILE:HG23	2:P:212:PHE:CE2	2.48	0.48
6:F:192:GLN:HE21	6:F:195:LYS:CE	2.26	0.48
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.42	0.48
2:P:224:PHE:H	2:P:224:PHE:HD2	1.62	0.48
2:P:73:LYS:C	2:P:74:ILE:HD12	2.35	0.48
3:Q:40:VAL:HG12	3:Q:162:ALA:CB	2.43	0.48
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.49	0.48
2:P:6:ARG:HD3	4:R:9:ASP:HB3	1.94	0.48
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.78	0.48
3:Q:168:ASN:O	3:Q:172:VAL:HG12	2.14	0.48
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.96	0.48
6:T:56:SER:OG	6:T:57:LYS:N	2.45	0.48
12:L:153:LYS:HG2	8:V:201:GLN:HG3	1.95	0.48
2:B:51:GLU:OE2	2:B:209:ARG:NH2	2.47	0.47
3:C:15:PHE:N	4:D:23:GLN:HE22	2.00	0.47
6:F:238:LYS:HZ2	6:F:239:GLU:HG3	1.79	0.47
13:M:14(A):VAL:O	13:M:14(A):VAL:HG23	2.13	0.47
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.13	0.47
3:Q:97:GLN:HA	3:Q:97:GLN:NE2	2.29	0.47
5:S:15:PHE:N	6:T:23:GLN:HE22	2.02	0.47
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.96	0.47
2:B:191:GLU:O	2:B:195:LYS:HG2	2.14	0.47
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.79	0.47
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.96	0.47
6:F:36:THR:CG2	6:F:51:GLU:OE2	2.63	0.47
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.28	0.47
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.49	0.47
12:Z:99:THR:CG2	16:Z:200:HOH:O	2.62	0.47
2:B:4:GLY:HA3	5:E:127:TYR:CE1	2.48	0.47
5:E:142:ASP:HB2	16:M:258:HOH:O	2.13	0.47
7:G:158:VAL:HG22	7:G:159:GLY:H	1.79	0.47
2:P:21:LEU:O	2:P:25:GLU:HG2	2.14	0.47
5:S:70:CYS:SG	5:S:92:LEU:HD23	2.54	0.47
8:V:41:ILE:HG13	8:V:76:VAL:HG22	1.96	0.47
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.14	0.47
6:F:56:SER:OG	6:F:57:LYS:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.96	0.47
4:R:215:ILE:HD13	4:R:215:ILE:C	2.34	0.47
7:U:158:VAL:HG22	7:U:159:GLY:H	1.79	0.47
7:U:17:PRO:HD3	16:U:263:HOH:O	2.14	0.47
7:U:78:VAL:HG11	7:U:85:ALA:CB	2.44	0.47
13:1:157:ASN:HB3	16:1:249:HOH:O	2.14	0.47
3:C:225:SER:OG	3:C:228:GLU:HG3	2.14	0.47
5:E:194:VAL:HG13	5:E:207:LEU:CD1	2.44	0.47
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.14	0.47
4:R:159:ARG:O	5:S:60:SER:N	2.47	0.47
13:1:104:VAL:CG2	13:1:178:ILE:HG22	2.41	0.47
3:C:163:GLN:HE22	3:C:173:ARG:NE	2.10	0.47
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.50	0.47
8:H:152:ILE:O	8:H:156:SER:HB2	2.15	0.47
9:I:33:LYS:O	9:I:44:GLY:HA2	2.15	0.47
12:L:21:ILE:HD11	12:L:168:GLN:NE2	2.29	0.47
13:M:152:GLU:O	13:M:156:VAL:HG23	2.14	0.47
3:Q:112:LEU:HD13	3:Q:112:LEU:O	2.14	0.47
3:Q:39:GLY:HA2	3:Q:47:VAL:O	2.14	0.47
4:R:65:GLU:HA	16:R:750:HOH:O	2.14	0.47
5:S:38:VAL:HG12	5:S:39:GLY:N	2.29	0.47
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.79	0.47
10:X:7:ARG:NH1	10:X:7:ARG:HG2	2.30	0.47
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.13	0.47
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.80	0.47
10:J:18:LYS:CG	10:J:174:ILE:HG13	2.44	0.47
11:K:208:ASN:HB3	16:K:236:HOH:O	2.15	0.47
12:L:114:ASP:CB	12:L:118:SER:HB3	2.39	0.47
6:T:238:LYS:HZ2	6:T:239:GLU:HG3	1.80	0.47
7:U:87:ASN:ND2	7:U:87:ASN:C	2.67	0.47
2:B:141:TYR:C	2:B:141:TYR:CD1	2.88	0.47
4:D:175:GLU:HA	4:D:175:GLU:OE1	2.14	0.47
8:H:156:SER:HB3	16:H:1030:HOH:O	2.14	0.47
9:I:113:PHE:CD2	9:I:113:PHE:N	2.82	0.47
5:S:194:VAL:HG13	5:S:207:LEU:CD1	2.45	0.47
7:U:151:THR:HG22	7:U:157:TYR:CB	2.42	0.47
7:G:39:ALA:CB	7:G:48:VAL:HG12	2.43	0.47
10:J:168:MET:HE2	10:X:168:MET:HE2	1.97	0.47
1:O:207:ASN:HB2	16:O:261:HOH:O	2.15	0.47
3:Q:55:THR:O	3:Q:56:LEU:HD22	2.15	0.47
5:S:77:SER:OG	5:S:137:LEU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:227:GLU:CD	5:S:227:GLU:H	2.18	0.47
7:U:8:TYR:C	7:U:10:ARG:N	2.67	0.47
10:X:18:LYS:CG	10:X:174:ILE:HG13	2.45	0.47
13:1:175:LEU:HD23	13:1:176:ALA:N	2.30	0.47
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.63	0.47
10:J:64:GLN:NE2	16:J:215:HOH:O	2.39	0.47
13:M:184:LEU:C	13:M:184:LEU:HD23	2.36	0.47
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.97	0.47
3:Q:227:GLU:N	3:Q:227:GLU:OE1	2.44	0.47
6:T:199:LEU:HD12	6:T:240:ILE:HD13	1.96	0.47
8:V:22:GLN:HE22	15:V:1001:BIQ:H32	1.80	0.47
2:P:101:LYS:NZ	10:X:85:GLN:HE22	2.06	0.47
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.15	0.47
10:J:6:ILE:HG22	10:J:13:ILE:HB	1.97	0.47
14:N:29:ARG:HG2	16:N:223:HOH:O	2.15	0.47
5:S:185:ASN:C	5:S:185:ASN:HD22	2.18	0.47
9:W:113:PHE:HA	9:W:118:CYS:O	2.15	0.47
3:C:55:THR:O	3:C:56:LEU:HD22	2.15	0.46
2:P:146:TYR:OH	2:P:21(A):LYS:HB2	2.14	0.46
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.41	0.46
13:1:113:VAL:HA	13:1:118:VAL:O	2.15	0.46
13:1:14(C):ARG:CG	13:1:14(C):ARG:HH11	2.28	0.46
14:2:36:ARG:HG3	14:2:42:TRP:CZ2	2.50	0.46
7:G:74:ILE:HD12	7:G:109:CYS:HA	1.97	0.46
10:J:14:LEU:HD12	10:J:42:LEU:HD23	1.96	0.46
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.30	0.46
14:N:36:ARG:HG3	14:N:42:TRP:CZ2	2.51	0.46
2:P:191:GLU:O	2:P:195:LYS:HG2	2.16	0.46
3:Q:206:GLY:CA	3:Q:209:ASN:HB2	2.37	0.46
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.28	0.46
10:J:24:ILE:HG12	10:X:133:TYR:OH	2.16	0.46
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.18	0.46
3:C:40:VAL:HG12	3:C:162:ALA:CB	2.43	0.46
3:C:35:THR:HB	3:C:51:GLU:HG3	1.97	0.46
5:E:2(C):VAL:HG13	5:E:2(D):ASP:N	2.30	0.46
6:F:175:GLU:OE1	6:F:199:LEU:HD23	2.16	0.46
7:G:151:THR:HG22	7:G:157:TYR:CB	2.44	0.46
3:Q:227:GLU:H	3:Q:227:GLU:CD	2.18	0.46
5:S:2(C):VAL:HG13	5:S:2(D):ASP:N	2.30	0.46
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.97	0.46
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:39:ALA:CB	7:U:48:VAL:HG12	2.44	0.46
9:W:159:LEU:CD2	9:W:173:ALA:HB1	2.46	0.46
16:X:220:HOH:O	11:Y:132:THR:HG22	2.16	0.46
12:Z:21:ILE:HD11	12:Z:168:GLN:NE2	2.31	0.46
3:C:39:GLY:HA2	3:C:47:VAL:O	2.15	0.46
4:D:32:LYS:O	4:D:167:SER:HA	2.15	0.46
6:F:195:LYS:O	6:F:199:LEU:HD13	2.16	0.46
8:H:175:VAL:HG12	8:H:176:CYS:N	2.31	0.46
9:I:29:ASN:HD22	9:I:29:ASN:N	2.11	0.46
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.98	0.46
5:S:194:VAL:HG13	5:S:207:LEU:HD11	1.98	0.46
14:2:3:ILE:HG22	14:2:16:ALA:CB	2.46	0.46
5:E:194:VAL:CG1	5:E:207:LEU:HD11	2.45	0.46
1:A:4:MET:HG2	6:F:126:TYR:CE2	2.51	0.46
9:I:122:ALA:HB3	9:I:125:ILE:CD1	2.46	0.46
12:L:34:VAL:HB	16:L:232:HOH:O	2.15	0.46
2:P:235:LYS:N	2:P:235:LYS:HD3	2.31	0.46
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	2.30	0.46
6:T:36:THR:CG2	6:T:51:GLU:OE2	2.64	0.46
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.27	0.46
13:1:14(A):VAL:O	13:1:14(A):VAL:HG23	2.15	0.46
13:1:17:ASP:HA	13:1:173:PHE:CB	2.45	0.46
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.51	0.46
5:E:4:PHE:CG	5:E:5:ARG:N	2.83	0.46
5:E:70:CYS:SG	5:E:92:LEU:HD23	2.56	0.46
6:F:127:ASN:ND2	6:F:127:ASN:C	2.68	0.46
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.15	0.46
5:S:179:THR:O	5:S:179:THR:HG22	2.14	0.46
10:X:35:ARG:HD3	10:X:35:ARG:HA	1.72	0.46
5:E:2(C):VAL:O	5:E:226:GLY:HA2	2.16	0.46
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.97	0.46
9:W:44:GLY:O	9:W:45:ILE:HD13	2.15	0.46
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.98	0.46
2:B:27:ALA:O	2:B:30:SER:HB3	2.15	0.46
5:E:39:GLY:O	5:E:162:GLY:HA2	2.16	0.46
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.98	0.46
1:A:97:HIS:CD2	8:H:61:SER:OG	2.67	0.46
13:M:129:PHE:HE2	14:2:24:ALA:HB3	1.79	0.46
2:P:181:LYS:HE2	2:P:183:ASP:OD1	2.15	0.46
5:S:136:LEU:HD12	5:S:151:PHE:CD2	2.51	0.46
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:122:ALA:HB3	9:W:125:ILE:CD1	2.46	0.46
10:X:6:ILE:HG22	10:X:13:ILE:HB	1.97	0.46
13:1:83:LEU:O	13:1:87:MET:HG2	2.15	0.46
8:H:29:LYS:HE2	12:Z:165:ARG:CZ	2.46	0.46
10:J:48:GLU:OE1	10:J:48:GLU:HA	2.16	0.46
13:M:104:VAL:CG2	13:M:178:ILE:HG22	2.43	0.46
3:Q:225:SER:OG	3:Q:228:GLU:HG3	2.15	0.46
5:S:194:VAL:CG1	5:S:207:LEU:HD11	2.46	0.46
9:W:101:VAL:O	9:W:110:ILE:HA	2.16	0.46
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.15	0.46
1:A:207:ASN:HA	1:A:233:LEU:CD1	2.45	0.46
2:B:181:LYS:HE2	2:B:183:ASP:OD1	2.15	0.46
3:C:112:LEU:HD13	3:C:112:LEU:O	2.15	0.46
2:B:161:LYS:HG3	3:C:59:GLN:O	2.15	0.46
2:P:141:TYR:C	2:P:141:TYR:CD1	2.89	0.46
3:Q:31:VAL:HG11	3:Q:135:SER:HB2	1.98	0.46
4:R:59:LEU:HD13	4:R:59:LEU:C	2.37	0.46
10:X:166:MET:CE	10:X:168:MET:HB2	2.46	0.46
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.16	0.46
2:B:52:ARG:HH22	2:B:63(A):SER:HB3	1.80	0.45
5:E:214:ILE:HG13	5:E:215:VAL:H	1.79	0.45
6:F:28:VAL:O	6:F:32:GLU:HG3	2.17	0.45
14:N:104:TYR:OH	14:N:180:ALA:HB2	2.16	0.45
2:P:52:ARG:HH22	2:P:63(A):SER:HB3	1.81	0.45
6:T:31:VAL:HG22	6:T:134:VAL:HA	1.98	0.45
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.31	0.45
7:U:191:GLU:HG3	7:U:232:ARG:HG3	1.98	0.45
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.26	0.45
5:E:227:GLU:CD	5:E:227:GLU:H	2.18	0.45
5:E:54:ASN:ND2	5:E:56:ASP:O	2.42	0.45
6:F:31:VAL:HG22	6:F:134:VAL:HA	1.99	0.45
8:H:139:GLU:OE2	8:H:139:GLU:HA	2.16	0.45
13:M:40:ASN:ND2	13:M:40:ASN:N	2.64	0.45
14:N:85:GLU:O	14:N:89:GLU:HB2	2.15	0.45
14:N:89:GLU:HA	14:N:89:GLU:OE1	2.16	0.45
1:O:40:ILE:HD12	1:O:193:ALA:HB2	1.99	0.45
2:P:74:ILE:N	2:P:74:ILE:CD1	2.78	0.45
4:R:122:ARG:HG2	4:R:122:ARG:HH11	1.81	0.45
4:R:86:ARG:HD3	4:R:86:ARG:HA	1.69	0.45
6:T:40:ILE:HD12	6:T:193:ALA:HB2	1.99	0.45
12:Z:99:THR:HG22	16:Z:200:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:TYR:OH	2:B:21(A):LYS:HB2	2.17	0.45
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.98	0.45
1:O:161:LYS:HD2	2:P:58:LEU:HA	1.98	0.45
1:O:62:GLU:C	1:O:64:LEU:H	2.19	0.45
3:Q:62(A):ILE:HG13	3:Q:63:THR:N	2.31	0.45
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.80	0.45
8:V:18:THR:HB	8:V:30:ASN:HD22	1.81	0.45
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.79	0.45
14:2:89:GLU:HA	14:2:89:GLU:OE1	2.15	0.45
8:H:18:THR:HB	8:H:30:ASN:HD22	1.81	0.45
10:J:168:MET:CE	10:X:168:MET:HG2	2.46	0.45
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.52	0.45
1:O:207:ASN:HA	1:O:233:LEU:CD1	2.46	0.45
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.98	0.45
4:R:21:LEU:HD21	5:S:130:ARG:HD2	1.99	0.45
5:S:214:ILE:HG13	5:S:215:VAL:H	1.80	0.45
10:X:44:SER:HG	10:X:100:LEU:HB2	1.81	0.45
10:X:90(B):ARG:NH1	16:X:204:HOH:O	2.41	0.45
14:2:85:GLU:O	14:2:89:GLU:HB2	2.16	0.45
1:A:177:GLU:HG2	2:B:58:LEU:HD21	1.96	0.45
5:E:194:VAL:HG13	5:E:207:LEU:HD11	1.98	0.45
6:F:103:TYR:O	6:F:104:LYS:HB3	2.17	0.45
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.99	0.45
10:J:166:MET:CE	10:J:168:MET:HB2	2.46	0.45
1:O:198:LYS:HE3	1:O:236:LEU:HD11	1.98	0.45
14:2:3:ILE:HG22	14:2:16:ALA:HB2	1.97	0.45
14:2:15:GLY:HA2	14:2:174:ARG:O	2.17	0.45
3:C:97:GLN:NE2	3:C:97:GLN:HA	2.32	0.45
4:D:59:LEU:C	4:D:59:LEU:HD13	2.36	0.45
9:I:159:LEU:CD2	9:I:173:ALA:HB1	2.47	0.45
3:Q:46:VAL:HG22	3:Q:146:PRO:HB2	1.99	0.45
5:S:134:VAL:O	5:S:153:PRO:HG3	2.16	0.45
6:T:103:TYR:O	6:T:104:LYS:HB3	2.17	0.45
6:T:70:VAL:HG11	6:T:112:PHE:CE1	2.51	0.45
15:V:1001:BIQ:H122	9:W:114:ASP:OD1	2.17	0.45
8:V:139:GLU:OE2	8:V:139:GLU:HA	2.17	0.45
5:E:136:LEU:HD12	5:E:151:PHE:CD2	2.52	0.45
5:E:179:THR:HG22	5:E:179:THR:O	2.17	0.45
3:Q:55:THR:O	3:Q:56:LEU:HD13	2.17	0.45
8:V:200:LYS:HE3	9:W:140:SER:O	2.17	0.45
10:X:143:ARG:HG2	10:X:143:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.37	0.45
1:A:169:SER:O	1:A:173:LYS:HG3	2.16	0.45
3:C:168:ASN:O	3:C:172:VAL:HG12	2.17	0.45
8:H:147:THR:HG23	8:H:150:GLU:OE1	2.17	0.45
13:M:70:ASN:ND2	13:M:70(A):ALA:HA	2.32	0.45
8:H:201:GLN:HG3	12:Z:153:LYS:HG2	1.98	0.45
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.70	0.45
13:1:1:THR:OG1	13:1:2:SER:N	2.50	0.45
1:A:198:LYS:HE3	1:A:236:LEU:HD11	1.98	0.45
2:B:224:PHE:HD2	2:B:224:PHE:H	1.62	0.45
7:G:52:LYS:HA	16:G:257:HOH:O	2.16	0.45
7:G:78:VAL:HG11	7:G:85:ALA:CB	2.47	0.45
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.52	0.45
11:K:75:SER:HB2	11:K:106:GLU:OE2	2.17	0.45
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.51	0.45
5:S:4:PHE:CG	5:S:5:ARG:N	2.84	0.45
6:F:18:ASP:OD1	6:F:20:ARG:HD3	2.17	0.45
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.52	0.45
6:T:136:THR:O	6:T:150:MET:HA	2.17	0.45
7:U:188:LYS:HA	7:U:188:LYS:HD3	1.82	0.45
6:T:176:LEU:HB3	7:U:58:LEU:HD21	1.99	0.45
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.52	0.45
2:B:20:ARG:HH11	2:B:20:ARG:HG2	1.83	0.44
12:L:165:ARG:CZ	8:V:29:LYS:HE2	2.47	0.44
13:M:14(C):ARG:CG	13:M:14(C):ARG:HH11	2.29	0.44
1:O:26:TYR:CD1	7:U:17:PRO:HA	2.52	0.44
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.17	0.44
6:T:175:GLU:CB	6:T:196:ILE:HD12	2.47	0.44
14:2:104:TYR:OH	14:2:180:ALA:HB2	2.16	0.44
1:A:62:GLU:C	1:A:64:LEU:H	2.20	0.44
1:A:62:GLU:H	1:A:62:GLU:CD	2.21	0.44
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.51	0.44
9:I:101:VAL:O	9:I:110:ILE:HA	2.17	0.44
13:M:113:VAL:HA	13:M:118:VAL:O	2.16	0.44
13:M:14(G):ILE:N	13:M:144:PRO:HD2	2.33	0.44
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.99	0.44
1:O:159:PRO:HB2	2:P:60:GLU:HB3	1.99	0.44
3:Q:241:GLN:C	3:Q:243:GLN:N	2.70	0.44
4:R:112:LEU:C	4:R:112:LEU:HD13	2.37	0.44
5:S:18(F):ILE:O	5:S:18(F):ILE:HG22	2.17	0.44
10:X:10(B):LYS:NZ	10:X:10(B):LYS:HB2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.99	0.44
13:1:140:LYS:HG3	16:1:219:HOH:O	2.17	0.44
12:L:-7:ASN:C	12:L:-7:ASN:HD22	2.21	0.44
14:N:67:THR:HA	14:N:72:GLY:O	2.17	0.44
2:P:209:ARG:HH11	2:P:209:ARG:HG2	1.83	0.44
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.99	0.44
9:W:19:ARG:HB2	9:W:171:TRP:HB2	2.00	0.44
13:1:8:TYR:CZ	13:1:148:VAL:HG13	2.52	0.44
1:A:150:GLN:O	1:A:157:TYR:HA	2.17	0.44
3:C:195:ARG:HD3	16:C:270:HOH:O	2.17	0.44
4:D:215:ILE:HD13	4:D:215:ILE:C	2.37	0.44
6:F:176:LEU:O	6:F:180:VAL:HG23	2.17	0.44
7:G:87:ASN:ND2	7:G:87:ASN:C	2.71	0.44
10:J:10(B):LYS:HB2	10:J:10(B):LYS:NZ	2.32	0.44
1:O:150:GLN:O	1:O:157:TYR:HA	2.17	0.44
2:P:122:GLY:C	2:P:124:THR:H	2.21	0.44
6:T:127:ASN:ND2	6:T:127:ASN:C	2.70	0.44
12:Z:48:PHE:CZ	12:Z:50:ALA:HB3	2.53	0.44
1:A:40:ILE:HD12	1:A:193:ALA:HB2	1.99	0.44
6:F:40:ILE:HD12	6:F:193:ALA:HB2	2.00	0.44
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.33	0.44
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.53	0.44
6:T:18:ASP:OD1	6:T:20:ARG:HD3	2.16	0.44
7:U:49:ILE:N	7:U:49:ILE:HD12	2.33	0.44
13:1:133:MET:C	13:1:136:PRO:HD2	2.38	0.44
5:E:221:PHE:HE1	5:E:223:ILE:HD11	1.83	0.44
12:L:84:GLN:HG3	12:L:117:GLY:O	2.18	0.44
2:P:38:ILE:HD13	2:P:164:SER:HB3	1.98	0.44
3:Q:45:CYS:HA	3:Q:141:PHE:HZ	1.82	0.44
4:R:81:LEU:HD12	4:R:133:GLY:HA3	2.00	0.44
5:S:41:ARG:NH1	5:S:42:SER:O	2.51	0.44
1:A:141:HIS:HA	1:A:146:GLY:O	2.17	0.44
3:C:120:GLN:O	3:C:124:THR:HG23	2.18	0.44
5:E:97:ASN:HD22	5:E:97:ASN:HA	1.67	0.44
7:G:191:GLU:HG3	7:G:232:ARG:HG3	2.00	0.44
11:K:10(A):ARG:NH1	11:K:10(A):ARG:HG2	2.32	0.44
11:K:86:LEU:HD13	11:K:86:LEU:C	2.38	0.44
2:P:229:ILE:O	2:P:233:LEU:HB2	2.18	0.44
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.63	0.44
11:Y:172:SER:HA	11:Y:192:VAL:HG23	2.00	0.44
3:C:241:GLN:C	3:C:243:GLN:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:LYS:CG	3:C:208:LYS:HZ1	2.30	0.44
4:D:177:LEU:CD1	5:E:58:LEU:HD11	2.46	0.44
6:F:136:THR:O	6:F:150:MET:HA	2.18	0.44
6:F:203:GLU:HA	6:F:203:GLU:OE1	2.17	0.44
1:O:27:ALA:O	1:O:31:VAL:HG23	2.18	0.44
5:S:52:LYS:HD3	5:S:211:SER:HB2	2.00	0.44
6:T:176:LEU:O	6:T:180:VAL:HG23	2.17	0.44
6:T:63:LYS:O	6:T:65:VAL:HG23	2.18	0.44
8:V:152:ILE:O	8:V:156:SER:HB2	2.18	0.44
10:X:185:ARG:HG2	10:X:185:ARG:HH11	1.82	0.44
5:E:18(F):ILE:O	5:E:18(F):ILE:HG22	2.18	0.44
7:G:17(C):LYS:HE3	7:G:17(C):LYS:HB2	1.78	0.44
10:J:168:MET:HG2	10:X:168:MET:CE	2.47	0.44
10:J:7:ARG:HG2	10:J:7:ARG:NH1	2.33	0.44
11:K:174:ASN:HD21	11:K:189:ASN:HB2	1.83	0.44
12:L:109:ALA:HA	16:L:227:HOH:O	2.18	0.44
12:L:42:VAL:HG23	12:L:102:ALA:HB3	2.00	0.44
13:M:8:TYR:CZ	13:M:148:VAL:HG13	2.53	0.44
2:P:136:PHE:O	2:P:150:THR:HA	2.18	0.44
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.22	0.44
7:U:204:GLU:HG3	16:U:283:HOH:O	2.18	0.44
7:U:78:VAL:HG11	7:U:85:ALA:HB2	2.00	0.44
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.00	0.44
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.53	0.44
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.17	0.44
11:Y:174:ASN:HD21	11:Y:189:ASN:HB2	1.83	0.44
13:1:70:ASN:ND2	13:1:70(A):ALA:HA	2.32	0.43
1:A:117:ALA:HB1	1:A:155:GLY:O	2.18	0.43
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.47	0.43
11:K:5:ALA:HA	11:K:13:ILE:O	2.18	0.43
1:O:141:HIS:HA	1:O:146:GLY:O	2.18	0.43
2:B:161:LYS:HE3	3:C:59:GLN:O	2.18	0.43
2:B:209:ARG:HG2	2:B:209:ARG:HH11	1.81	0.43
3:C:45:CYS:HA	3:C:141:PHE:HZ	1.82	0.43
5:E:134:VAL:O	5:E:153:PRO:HG3	2.18	0.43
6:F:63:LYS:O	6:F:65:VAL:HG23	2.18	0.43
7:G:49:ILE:HD12	7:G:49:ILE:N	2.33	0.43
8:H:128:GLY:O	8:H:131:SER:CB	2.65	0.43
8:H:72:ARG:NH1	8:H:72:ARG:HG3	2.32	0.43
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.33	0.43
10:J:76:PRO:HD2	16:J:210:HOH:O	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:11:GLY:HA3	13:M:178:ILE:O	2.17	0.43
1:O:62:GLU:CD	1:O:62:GLU:H	2.21	0.43
4:R:159:ARG:HB3	5:S:60:SER:HB3	1.99	0.43
6:T:203:GLU:OE1	6:T:203:GLU:HA	2.18	0.43
7:U:56:ASP:HB3	7:U:59:LEU:HG	2.00	0.43
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:NH1	2.33	0.43
12:Z:42:VAL:HG23	12:Z:102:ALA:HB3	2.01	0.43
13:1:14(G):ILE:N	13:1:144:PRO:HD2	2.32	0.43
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	2.00	0.43
4:D:81:LEU:HD12	4:D:133:GLY:HA3	2.00	0.43
6:F:70:VAL:HG11	6:F:112:PHE:CE1	2.52	0.43
6:F:180:VAL:HG21	7:G:58:LEU:HD23	1.99	0.43
6:F:90:ASN:O	6:F:94:GLU:HG3	2.17	0.43
8:H:112:SER:OG	8:H:120:ASP:HB2	2.18	0.43
2:P:66:LYS:O	2:P:77:ALA:HA	2.18	0.43
9:W:113:PHE:CD2	9:W:113:PHE:N	2.85	0.43
13:1:40:ASN:ND2	13:1:40:ASN:N	2.64	0.43
3:C:62(A):ILE:HG13	3:C:63:THR:N	2.32	0.43
5:E:58:LEU:CD1	5:E:58:LEU:N	2.81	0.43
6:F:240:ILE:HD12	6:F:240:ILE:HA	1.91	0.43
7:G:56:ASP:HB3	7:G:59:LEU:HG	2.00	0.43
7:G:105:TYR:OH	8:H:66:HIS:HE1	2.02	0.43
9:I:29:ASN:ND2	9:I:29:ASN:N	2.65	0.43
10:J:185:ARG:HH11	10:J:185:ARG:HG2	1.84	0.43
11:K:172:SER:HA	11:K:192:VAL:HG23	2.00	0.43
6:T:195:LYS:O	6:T:199:LEU:HD13	2.19	0.43
9:W:143:GLU:HG3	9:W:146:LEU:HD21	2.01	0.43
13:1:137:LEU:O	13:1:140:LYS:HB2	2.19	0.43
2:B:39:GLY:O	2:B:162:ALA:HA	2.18	0.43
5:E:77:SER:OG	5:E:137:LEU:HB2	2.18	0.43
6:F:176:LEU:HB3	7:G:58:LEU:HD21	2.00	0.43
9:I:124:PHE:O	9:I:125:ILE:HD12	2.19	0.43
11:K:4:LEU:C	11:K:4:LEU:HD22	2.39	0.43
2:P:141:TYR:CE2	2:P:145:GLY:HA2	2.54	0.43
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.54	0.43
5:S:2(C):VAL:O	5:S:226:GLY:HA2	2.18	0.43
7:U:171:GLU:OE1	7:U:171:GLU:N	2.52	0.43
7:U:18(H):GLU:H	7:U:18(H):GLU:CD	2.22	0.43
13:1:11:GLY:HA3	13:1:178:ILE:O	2.18	0.43
3:C:71:ASP:OD1	3:C:100:ARG:NH1	2.51	0.43
4:D:207:LEU:HD21	4:D:233:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:ASP:OD2	10:J:10(B):LYS:HE2	2.19	0.43
12:L:19:ARG:NE	12:L:171:ASP:OD2	2.44	0.43
5:S:160:LEU:HD22	6:T:59:LEU:HD12	2.01	0.43
7:U:143:GLU:HA	7:U:217:LYS:NZ	2.34	0.43
14:N:133:PHE:HA	14:2:132:THR:O	2.19	0.43
1:A:13:THR:O	2:B:130:ARG:HD3	2.19	0.43
2:B:74:ILE:CD1	2:B:74:ILE:N	2.81	0.43
5:E:18(C):PHE:HA	5:E:18(F):ILE:CG1	2.47	0.43
5:E:41:ARG:NH1	5:E:42:SER:O	2.51	0.43
6:F:175:GLU:CB	6:F:196:ILE:HD12	2.49	0.43
9:I:113:PHE:HA	9:I:118:CYS:O	2.18	0.43
9:I:29:ASN:HD22	9:I:30:LYS:HG3	1.84	0.43
10:J:19:ALA:HB2	10:J:171:LYS:HG2	1.99	0.43
13:M:175:LEU:HD23	13:M:176:ALA:N	2.33	0.43
14:N:126:ILE:HD13	14:N:126:ILE:N	2.34	0.43
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.48	0.43
7:U:139:VAL:HA	7:U:147:SER:O	2.19	0.43
8:V:3:ILE:HD11	8:V:127:LEU:HB2	2.01	0.43
10:X:40:HIS:CD2	10:X:10(A):LYS:HD3	2.54	0.43
10:X:166:MET:HA	10:X:167:PRO:HD3	1.81	0.43
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.17	0.43
3:C:100:ARG:NH1	3:C:106:PRO:HB3	2.34	0.43
3:C:31:VAL:HG11	3:C:135:SER:HB2	2.00	0.43
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.54	0.43
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.53	0.43
8:H:189:ARG:O	8:H:190:ASN:HB2	2.19	0.43
2:P:39:GLY:O	2:P:162:ALA:HA	2.19	0.43
5:S:4:PHE:O	5:S:6:ASN:N	2.52	0.43
7:U:46:THR:HG21	7:U:139:VAL:HB	2.00	0.43
7:U:172:ILE:HD11	7:U:201:LEU:HD21	2.01	0.43
8:V:113:ILE:HG12	8:V:119:THR:HG22	2.01	0.43
8:V:84:LYS:HG3	8:V:85:GLN:N	2.34	0.43
10:X:19:ALA:HB2	10:X:171:LYS:HG2	2.00	0.43
10:X:32:ASP:CG	10:X:34:THR:HG22	2.39	0.43
12:Z:109:ALA:HB2	12:Z:121:ARG:NH2	2.34	0.43
12:Z:113:PHE:N	12:Z:113:PHE:CD1	2.86	0.43
2:B:17:PRO:HA	3:C:26:TYR:CZ	2.53	0.43
5:E:2(B):THR:H	5:E:2(E):ASN:HB3	1.84	0.43
7:G:152:ASP:HB2	7:G:153:PRO:HD2	2.01	0.43
7:G:172:ILE:HD11	7:G:201:LEU:HD21	1.99	0.43
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.54	0.43
14:N:15:GLY:HA2	14:N:174:ARG:O	2.18	0.43
1:O:35:VAL:HG11	1:O:51:GLU:HB3	2.01	0.43
5:E:179:THR:O	5:E:18(B):THR:HB	2.19	0.43
12:L:113:PHE:CD1	12:L:113:PHE:N	2.86	0.43
12:L:177:ILE:N	12:L:177:ILE:HD12	2.34	0.43
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.17	0.43
13:M:133:MET:C	13:M:136:PRO:HD2	2.39	0.43
3:Q:136:THR:O	3:Q:150:GLN:HA	2.19	0.43
4:R:207:LEU:HD21	4:R:233:ILE:CD1	2.49	0.43
5:S:179:THR:O	5:S:18(B):THR:HB	2.18	0.43
7:U:152:ASP:HB2	7:U:153:PRO:HD2	2.00	0.43
7:U:18(D):ILE:N	7:U:18(D):ILE:HD12	2.34	0.43
8:V:147:THR:HG23	8:V:150:GLU:OE1	2.19	0.43
9:W:183:GLU:HA	16:W:229:HOH:O	2.19	0.43
10:X:12:VAL:CG2	10:X:108:PRO:HB2	2.49	0.43
10:X:124:TYR:CD2	10:X:138:LEU:HD13	2.54	0.43
11:Y:25:TRP:CH2	12:Z:132:SER:HA	2.54	0.43
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	2.10	0.43
2:B:20:ARG:NH1	2:B:20:ARG:HG2	2.34	0.42
2:B:235:LYS:HD3	2:B:235:LYS:N	2.33	0.42
2:B:71:ASN:HB3	2:B:74:ILE:H	1.84	0.42
5:E:11:ASP:OD1	5:E:13:VAL:HG12	2.20	0.42
15:H:1000:BIQ:H122	9:I:114:ASP:OD1	2.18	0.42
6:T:18:ASP:N	6:T:18:ASP:OD2	2.44	0.42
7:U:82:ILE:N	7:U:83:PRO:HD2	2.34	0.42
8:V:175:VAL:HG12	8:V:176:CYS:N	2.33	0.42
10:X:52:THR:HG22	10:X:53:VAL:H	1.84	0.42
14:2:116:GLY:HA3	16:2:190:HOH:O	2.18	0.42
1:A:110:LYS:HG2	16:A:246:HOH:O	2.18	0.42
3:C:186:VAL:HG21	3:C:216:LYS:HE2	2.00	0.42
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.82	0.42
7:G:143:GLU:HA	7:G:217:LYS:NZ	2.34	0.42
13:M:175:LEU:C	13:M:175:LEU:HD23	2.39	0.42
14:N:3:ILE:HG22	14:N:16:ALA:HB2	2.00	0.42
1:O:13:THR:O	2:P:130:ARG:HD3	2.19	0.42
2:P:202:THR:HG22	2:P:203:ASP:N	2.34	0.42
3:Q:55:THR:HG22	3:Q:56:LEU:CD2	2.44	0.42
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.34	0.42
2:B:194:LEU:O	2:B:198:SER:HB2	2.19	0.42
2:B:63:THR:O	2:B:63:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:SER:HB2	16:C:252:HOH:O	2.19	0.42
10:J:12:VAL:CG2	10:J:108:PRO:HB2	2.50	0.42
1:O:169:SER:O	1:O:173:LYS:HG3	2.20	0.42
2:P:71:ASN:HB3	2:P:74:ILE:H	1.84	0.42
3:Q:134:VAL:HG12	3:Q:135:SER:N	2.33	0.42
6:T:240:ILE:HA	6:T:240:ILE:HD12	1.91	0.42
5:S:160:LEU:CD2	6:T:59:LEU:HD12	2.49	0.42
12:Z:134:ILE:HD11	12:Z:162:ALA:HB2	2.01	0.42
12:Z:-8:PHE:CB	13:1:-8:THR:HG23	2.49	0.42
1:A:27:ALA:O	1:A:31:VAL:HG23	2.19	0.42
2:B:6:ARG:HG2	3:C:10:ARG:NH2	2.34	0.42
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.54	0.42
3:C:197:LEU:O	3:C:201:VAL:HG23	2.19	0.42
3:C:52:ARG:HH21	3:C:211:GLU:HB3	1.84	0.42
5:E:2(C):VAL:CG1	5:E:2(D):ASP:N	2.83	0.42
8:H:3:ILE:HD11	8:H:127:LEU:HB2	2.01	0.42
8:H:50:ALA:CB	9:I:116:ILE:HG13	2.50	0.42
13:M:191:GLN:HE21	13:M:191:GLN:HB3	1.57	0.42
13:M:83:LEU:O	13:M:87:MET:HG2	2.20	0.42
3:Q:120:GLN:O	3:Q:124:THR:HG23	2.20	0.42
5:S:2(C):VAL:CG1	5:S:2(D):ASP:N	2.82	0.42
2:B:229:ILE:O	2:B:233:LEU:HB2	2.19	0.42
4:D:185:THR:HG23	4:D:188:GLU:OE1	2.19	0.42
5:E:4:PHE:O	5:E:6:ASN:N	2.53	0.42
6:F:50:VAL:HG22	6:F:51:GLU:N	2.35	0.42
7:G:18(D):ILE:N	7:G:18(D):ILE:HD12	2.34	0.42
6:F:158:TRP:CZ3	7:G:64:VAL:HA	2.54	0.42
11:K:6:PHE:HA	11:K:123:ASP:O	2.19	0.42
2:P:63:THR:HG22	2:P:63:THR:O	2.18	0.42
3:Q:52:ARG:HH21	3:Q:211:GLU:HB3	1.84	0.42
7:U:47:VAL:HG12	7:U:49:ILE:CD1	2.50	0.42
8:V:18:THR:CB	8:V:30:ASN:HD22	2.33	0.42
10:X:48:GLU:HA	10:X:48:GLU:OE1	2.19	0.42
12:Z:93:PHE:N	12:Z:94:PRO:CD	2.81	0.42
2:B:202:THR:HG22	2:B:203:ASP:N	2.34	0.42
3:C:105:ASP:OD2	3:C:106:PRO:HD2	2.20	0.42
3:C:134:VAL:HG12	3:C:135:SER:N	2.34	0.42
3:C:136:THR:O	3:C:150:GLN:HA	2.19	0.42
3:C:57:LYS:HD2	3:C:58:LEU:N	2.35	0.42
7:G:82:ILE:HG22	7:G:83:PRO:HD3	2.01	0.42
8:H:148:LYS:HE3	8:H:177:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:18:THR:CB	8:H:30:ASN:HD22	2.33	0.42
9:I:19:ARG:HB2	9:I:171:TRP:HB2	2.01	0.42
10:J:13:ILE:HD12	10:J:177:ILE:HD13	2.01	0.42
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.00	0.42
11:K:70:GLU:O	11:K:71:LYS:C	2.57	0.42
5:S:11:ASP:OD1	5:S:13:VAL:HG12	2.19	0.42
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.50	0.42
6:T:28:VAL:O	6:T:32:GLU:HG3	2.19	0.42
9:W:29:ASN:N	9:W:29:ASN:HD22	2.12	0.42
10:X:129:TYR:O	10:X:132:PHE:HB2	2.20	0.42
14:2:67:THR:HA	14:2:72:GLY:O	2.19	0.42
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.31	0.42
7:G:78:VAL:HG11	7:G:85:ALA:HB2	2.02	0.42
10:J:40:HIS:CD2	10:J:10(A):LYS:HD3	2.54	0.42
11:K:40:PHE:CD1	11:K:73:ARG:CZ	3.02	0.42
1:O:122:GLU:C	1:O:124:THR:H	2.23	0.42
4:R:160:TYR:HA	5:S:58:LEU:O	2.20	0.42
5:S:97:ASN:HA	5:S:97:ASN:HD22	1.66	0.42
9:W:66:TYR:CZ	9:W:70:GLU:HG3	2.54	0.42
13:1:80:PHE:CE1	13:1:111:ARG:HD3	2.54	0.42
9:I:14:ILE:HG12	9:I:34:ILE:HD12	2.01	0.42
13:M:1:THR:OG1	13:M:2:SER:N	2.51	0.42
14:N:114:PRO:HD2	14:N:118:SER:O	2.20	0.42
5:S:52:LYS:O	5:S:63:TYR:HD2	2.03	0.42
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.34	0.42
6:T:212:ILE:HG22	6:T:213:SER:N	2.35	0.42
7:U:82:ILE:CG2	7:U:83:PRO:HD3	2.49	0.42
9:W:29:ASN:N	9:W:29:ASN:ND2	2.65	0.42
10:X:35:ARG:NH1	10:X:57:GLU:HG2	2.34	0.42
14:N:132:THR:O	14:2:133:PHE:HA	2.20	0.42
4:D:31:ILE:HD13	4:D:135:ALA:HB2	2.01	0.42
5:E:172:ALA:HB2	5:E:196:ALA:O	2.20	0.42
9:I:22:SER:O	9:I:23:GLN:HB2	2.19	0.42
10:J:143:ARG:HG2	10:J:143:ARG:HH11	1.85	0.42
6:T:90:ASN:O	6:T:94:GLU:HG3	2.20	0.42
7:U:74:ILE:HD12	7:U:109:CYS:HA	2.00	0.42
7:U:234:VAL:O	7:U:237:ALA:HB3	2.19	0.42
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.40	0.42
14:2:126:ILE:N	14:2:126:ILE:HD13	2.34	0.42
14:2:184:VAL:HG21	16:2:194:HOH:O	2.20	0.42
7:G:171:GLU:OE1	7:G:171:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:28:SER:CB	10:J:120:VAL:HG21	2.49	0.42
10:J:166:MET:HA	10:J:167:PRO:HD3	1.81	0.42
10:J:22:ARG:HA	10:J:22:ARG:HD3	1.95	0.42
10:J:35:ARG:HA	10:J:35:ARG:HD3	1.71	0.42
2:P:24:VAL:HG11	2:P:154:SER:HB3	2.02	0.42
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	2.02	0.42
5:S:162:GLY:O	5:S:163:THR:HB	2.20	0.42
3:C:46:VAL:HG22	3:C:146:PRO:HB2	2.02	0.41
2:B:160:TRP:CZ3	3:C:59:GLN:HG2	2.55	0.41
8:H:24:PRO:HG2	8:H:25:ILE:HD12	2.01	0.41
10:J:32:ASP:CG	10:J:34:THR:HG22	2.40	0.41
4:R:117:CYS:SG	4:R:157:PHE:HB3	2.60	0.41
13:I:112:TYR:HE1	13:I:127:THR:HG22	1.85	0.41
2:B:66:LYS:O	2:B:77:ALA:HA	2.20	0.41
3:C:55:THR:O	3:C:56:LEU:HD13	2.20	0.41
5:E:52:LYS:HD3	5:E:211:SER:HB2	2.02	0.41
14:N:107:LYS:CG	14:N:108:GLY:N	2.79	0.41
1:O:117:ALA:HB1	1:O:155:GLY:O	2.20	0.41
5:S:221:PHE:HE1	5:S:223:ILE:HD11	1.82	0.41
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.83	0.41
6:T:186:ALA:HB3	6:T:21(A):GLU:HG3	2.01	0.41
7:U:236:ILE:HD12	7:U:236:ILE:C	2.41	0.41
8:V:148:LYS:HE3	8:V:177:VAL:HG11	2.02	0.41
9:W:20:LEU:C	9:W:20:LEU:HD13	2.40	0.41
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.55	0.41
2:B:136:PHE:O	2:B:150:THR:HA	2.19	0.41
6:F:186:ALA:HB3	6:F:21(A):GLU:HG3	2.02	0.41
7:G:47:VAL:HG12	7:G:49:ILE:CD1	2.51	0.41
11:K:97:MET:O	11:K:114:ASP:HA	2.20	0.41
13:M:1:THR:HG22	16:M:213:HOH:O	2.20	0.41
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.34	0.41
5:S:172:ALA:HB2	5:S:196:ALA:O	2.20	0.41
5:S:64:GLN:HA	16:S:242:HOH:O	2.19	0.41
7:U:18(H):GLU:N	7:U:18(H):GLU:CD	2.74	0.41
9:W:16:CYS:SG	9:W:34:ILE:HG12	2.60	0.41
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.35	0.41
10:X:90(A):ILE:HA	10:X:90(A):ILE:HD13	1.89	0.41
9:I:143:GLU:HG3	9:I:146:LEU:HD21	2.02	0.41
9:I:159:LEU:HD21	9:I:173:ALA:HB1	2.02	0.41
13:M:112:TYR:HE1	13:M:127:THR:HG22	1.84	0.41
2:P:233:LEU:HD12	2:P:233:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:31:ILE:HD13	4:R:135:ALA:HB2	2.02	0.41
5:S:58:LEU:N	5:S:58:LEU:CD1	2.83	0.41
7:U:82:ILE:HG22	7:U:83:PRO:HD3	2.01	0.41
9:W:14:ILE:CG2	9:W:176:TYR:HB2	2.51	0.41
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.50	0.41
11:Y:75:SER:HB2	11:Y:106:GLU:OE2	2.20	0.41
13:1:191:GLN:HB3	13:1:191:GLN:HE21	1.58	0.41
1:A:21(B):ASN:CB	1:A:21(F):LEU:HD12	2.51	0.41
1:A:4:MET:HG2	6:F:126:TYR:CZ	2.55	0.41
3:C:57:LYS:HG3	3:C:208:LYS:HZ1	1.86	0.41
4:D:12:VAL:CG2	4:D:12(A):GLY:HA2	2.50	0.41
7:G:188:LYS:HD3	7:G:191:GLU:OE2	2.20	0.41
11:K:46:ALA:HB3	11:K:98:GLY:O	2.20	0.41
13:M:57:ARG:CD	16:M:247:HOH:O	2.68	0.41
4:R:12:VAL:CG2	4:R:12(A):GLY:HA2	2.51	0.41
11:Y:70:GLU:O	11:Y:71:LYS:C	2.59	0.41
13:1:175:LEU:HD23	13:1:175:LEU:C	2.41	0.41
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.56	0.41
3:C:20:HIS:HB3	3:C:25:GLU:OE1	2.21	0.41
5:E:150:GLU:O	5:E:157:VAL:HA	2.21	0.41
5:E:57:GLU:C	5:E:58:LEU:HD12	2.41	0.41
6:F:49:ALA:HA	6:F:211:GLU:O	2.20	0.41
10:J:168:MET:HE3	10:X:168:MET:CE	2.48	0.41
13:M:80:PHE:CE1	13:M:111:ARG:HD3	2.56	0.41
12:L:-8:PHE:CB	13:M:-8:THR:HG23	2.51	0.41
5:S:198:SER:HA	5:S:201:LEU:CG	2.43	0.41
9:W:36:HIS:HB3	9:W:42:PHE:CD2	2.55	0.41
11:Y:138:LEU:HD13	11:Y:158:SER:OG	2.21	0.41
3:C:57:LYS:O	3:C:58:LEU:HB2	2.20	0.41
4:D:91:HIS:CG	4:D:119:LEU:HD11	2.56	0.41
9:I:16:CYS:SG	9:I:34:ILE:HG12	2.61	0.41
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.71	0.41
5:S:67:ILE:HG21	5:S:223:ILE:HD12	2.01	0.41
5:S:52:LYS:HB3	5:S:63:TYR:O	2.21	0.41
6:T:50:VAL:HG22	6:T:51:GLU:N	2.35	0.41
2:P:143:ASP:OD2	10:X:10(B):LYS:HE2	2.21	0.41
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.35	0.41
3:C:241:GLN:O	3:C:243:GLN:N	2.50	0.41
7:G:139:VAL:HA	7:G:147:SER:O	2.20	0.41
7:G:82:ILE:N	7:G:83:PRO:HD2	2.35	0.41
8:H:53:GLU:O	8:H:57:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:-2:ASN:HA	12:L:21:ILE:O	2.20	0.41
3:Q:241:GLN:O	3:Q:243:GLN:N	2.50	0.41
6:T:13:SER:HB2	7:U:130:ARG:HD3	2.02	0.41
9:W:22:SER:O	9:W:23:GLN:HB2	2.21	0.41
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.36	0.41
14:N:144:GLU:O	14:N:145:ASN:HB2	2.21	0.41
3:Q:18(A):ASP:OD2	3:Q:18(C):LYS:HG2	2.20	0.41
3:Q:38:VAL:HG22	3:Q:39:GLY:N	2.36	0.41
3:Q:44:ASN:O	3:Q:45:CYS:HB3	2.21	0.41
5:S:4:PHE:O	5:S:5:ARG:C	2.59	0.41
9:W:124:PHE:O	9:W:125:ILE:HD12	2.21	0.41
1:A:7:ARG:NH1	5:E:127:TYR:HD2	2.19	0.41
5:E:139:ILE:HD12	5:E:215:VAL:HG12	2.02	0.41
8:H:84:LYS:HG3	8:H:85:GLN:N	2.35	0.41
10:J:52:THR:HG22	10:J:53:VAL:H	1.86	0.41
12:L:8:GLY:HA3	12:L:11:PHE:CZ	2.56	0.41
13:M:-5:PRO:HD3	13:M:96:TRP:CE2	2.56	0.41
14:N:24:ALA:HB3	13:1:129:PHE:HE2	1.85	0.41
2:P:4:GLY:HA3	5:S:127:TYR:CZ	2.56	0.41
8:V:189:ARG:O	8:V:190:ASN:HB2	2.21	0.41
9:W:130:ALA:HB2	9:W:166:ASP:CB	2.51	0.41
10:X:7:ARG:HD3	16:X:195:HOH:O	2.21	0.41
2:B:73:LYS:C	2:B:74:ILE:HD12	2.41	0.41
3:C:224:LEU:HD12	3:C:224:LEU:N	2.36	0.41
3:C:44:ASN:O	3:C:45:CYS:HB3	2.20	0.41
5:E:67:ILE:HG21	5:E:223:ILE:HD12	2.03	0.41
5:E:52:LYS:CB	5:E:63:TYR:HB3	2.51	0.41
6:F:212:ILE:HG22	6:F:213:SER:N	2.36	0.41
7:G:29:LYS:HA	7:G:29:LYS:HD2	1.75	0.41
11:K:12:ILE:HG13	11:K:108:PRO:HB3	2.03	0.41
13:M:14(G):ILE:HB	13:M:144:PRO:CD	2.51	0.41
3:Q:57:LYS:CG	3:Q:208:LYS:HZ1	2.34	0.41
3:Q:224:LEU:HD12	3:Q:224:LEU:N	2.36	0.41
8:V:18:THR:HG21	8:V:30:ASN:ND2	2.35	0.41
9:W:29:ASN:C	9:W:29:ASN:HD22	2.24	0.41
2:B:21(C):ASP:OD2	2:B:219:GLU:HB3	2.21	0.40
8:H:84:LYS:HE2	8:H:119:THR:HG23	2.02	0.40
9:I:149:GLU:H	9:I:149:GLU:CD	2.24	0.40
9:I:93:GLY:N	9:I:94:PRO:CD	2.83	0.40
12:L:42:VAL:CG2	12:L:102:ALA:HB3	2.51	0.40
12:L:-7:ASN:C	12:L:-7:ASN:ND2	2.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:21(C):ASP:OD2	2:P:219:GLU:HB3	2.21	0.40
3:Q:106:PRO:HG2	3:Q:143:PRO:HG2	1.99	0.40
4:R:101:LEU:CD1	11:Y:57:THR:HG22	2.51	0.40
4:R:105:GLU:OE1	12:Z:66:TYR:OH	2.33	0.40
5:S:2(B):THR:H	5:S:2(E):ASN:HB3	1.85	0.40
8:V:128:GLY:O	8:V:131:SER:CB	2.66	0.40
8:V:72:ARG:NH1	8:V:72:ARG:HG3	2.34	0.40
9:W:23:GLN:CB	16:W:228:HOH:O	2.67	0.40
10:X:22:ARG:HA	10:X:22:ARG:HD3	1.94	0.40
14:2:144:GLU:O	14:2:145:ASN:HB2	2.21	0.40
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	2.02	0.40
3:C:106:PRO:HG2	3:C:143:PRO:HG2	2.00	0.40
6:F:18:ASP:N	6:F:18:ASP:OD2	2.44	0.40
7:G:234:VAL:O	7:G:237:ALA:HB3	2.21	0.40
10:J:129:TYR:O	10:J:132:PHE:HB2	2.21	0.40
10:J:147:THR:HG23	10:J:150:GLU:OE2	2.21	0.40
2:P:101:LYS:HZ2	10:X:85:GLN:HE21	1.68	0.40
3:Q:185:THR:HG22	3:Q:186:VAL:N	2.35	0.40
4:R:185:THR:HG23	4:R:188:GLU:OE1	2.21	0.40
4:R:97:VAL:HG13	16:Y:226:HOH:O	2.21	0.40
5:S:139:ILE:HD12	5:S:215:VAL:HG12	2.03	0.40
9:W:93:GLY:N	9:W:94:PRO:CD	2.84	0.40
12:Z:42:VAL:CG2	12:Z:102:ALA:HB3	2.51	0.40
12:Z:114:ASP:OD2	12:Z:115:PRO:HD2	2.21	0.40
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.89	0.40
5:E:162:GLY:O	5:E:163:THR:HB	2.21	0.40
6:F:179:LEU:HD11	6:F:192:GLN:HG3	2.03	0.40
11:K:76:VAL:N	11:K:106:GLU:OE2	2.49	0.40
13:M:137:LEU:O	13:M:140:LYS:HB2	2.20	0.40
6:T:175:GLU:HB2	6:T:196:ILE:HD12	2.03	0.40
9:W:28:SER:CB	10:X:120:VAL:HG21	2.51	0.40
13:1:19:LEU:HD12	13:1:20:GLY:H	1.87	0.40
3:C:62(A):ILE:O	3:C:63:THR:C	2.60	0.40
6:F:175:GLU:HB2	6:F:196:ILE:HD12	2.04	0.40
5:E:17:PRO:HA	6:F:26:TYR:CE2	2.56	0.40
9:I:137:MET:CE	9:I:141:LEU:HD11	2.51	0.40
10:J:12:VAL:HG23	10:J:108:PRO:HB2	2.03	0.40
11:K:138:LEU:HD13	11:K:158:SER:OG	2.22	0.40
11:K:25:TRP:HH2	12:L:135:MET:HB2	1.86	0.40
1:O:21(B):ASN:CB	1:O:21(F):LEU:HD12	2.51	0.40
3:Q:108:THR:HG23	16:Q:255:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:15:PHE:H	4:R:23:GLN:NE2	1.95	0.40
5:S:230:ALA:C	5:S:232:TYR:H	2.25	0.40
5:S:7:ASN:HA	5:S:7:ASN:HD22	1.76	0.40
7:U:17(C):LYS:HE3	7:U:17(C):LYS:HB2	1.76	0.40
3:C:134:VAL:CG1	3:C:135:SER:N	2.84	0.40
7:G:46:THR:HG21	7:G:139:VAL:HB	2.03	0.40
8:H:18:THR:HG21	8:H:30:ASN:ND2	2.37	0.40
8:H:41:ILE:N	8:H:41:ILE:HD12	2.37	0.40
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.57	0.40
12:L:1:GLY:N	16:L:220:HOH:O	2.55	0.40
3:Q:134:VAL:CG1	3:Q:135:SER:N	2.84	0.40
5:S:152:GLN:HA	5:S:153:PRO:HD3	1.96	0.40
9:W:55:LEU:HD23	9:W:55:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	232 (94%)	13 (5%)	3 (1%)	13	37
1	O	248/250 (99%)	231 (93%)	13 (5%)	4 (2%)	9	29
2	B	242/244 (99%)	224 (93%)	12 (5%)	6 (2%)	5	18
2	P	242/244 (99%)	222 (92%)	14 (6%)	6 (2%)	5	18
3	C	239/241 (99%)	216 (90%)	18 (8%)	5 (2%)	7	22
3	Q	239/241 (99%)	216 (90%)	18 (8%)	5 (2%)	7	22
4	D	240/242 (99%)	226 (94%)	10 (4%)	4 (2%)	9	27
4	R	240/242 (99%)	224 (93%)	12 (5%)	4 (2%)	9	27
5	E	231/233 (99%)	209 (90%)	15 (6%)	7 (3%)	4	14
5	S	231/233 (99%)	208 (90%)	16 (7%)	7 (3%)	4	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	242/244 (99%)	227 (94%)	13 (5%)	2 (1%)	19	47
6	T	242/244 (99%)	226 (93%)	13 (5%)	3 (1%)	13	37
7	G	241/243 (99%)	226 (94%)	13 (5%)	2 (1%)	19	47
7	U	241/243 (99%)	227 (94%)	11 (5%)	3 (1%)	13	37
8	H	220/222 (99%)	207 (94%)	12 (6%)	1 (0%)	29	59
8	V	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	29	59
9	I	202/204 (99%)	192 (95%)	10 (5%)	0	100	100
9	W	202/204 (99%)	192 (95%)	10 (5%)	0	100	100
10	J	196/198 (99%)	189 (96%)	5 (3%)	2 (1%)	15	42
10	X	196/198 (99%)	187 (95%)	7 (4%)	2 (1%)	15	42
11	K	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
11	Y	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
12	L	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	29	59
12	Z	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	29	59
13	1	231/233 (99%)	218 (94%)	13 (6%)	0	100	100
13	M	231/233 (99%)	217 (94%)	14 (6%)	0	100	100
14	2	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
14	N	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
All	All	6312/6368 (99%)	5921 (94%)	322 (5%)	69 (1%)	14	39

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	58	LEU
4	D	12(G)	GLU
5	E	5	ARG
5	E	202	ARG
3	Q	58	LEU
4	R	12(G)	GLU
5	S	5	ARG
5	S	202	ARG
1	A	5	THR
2	B	54	VAL
2	B	20(A)	SER
2	B	21(B)	GLY
2	B	21(C)	ASP

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Mol	Chain	Res	Type
3	C	183	PRO
3	C	203	THR
5	E	64	GLN
5	E	217	LYS
7	G	239	GLN
10	J	192	ALA
1	O	5	THR
2	P	54	VAL
2	P	20(A)	SER
2	P	21(B)	GLY
2	P	21(C)	ASP
3	Q	183	PRO
3	Q	203	THR
5	S	64	GLN
5	S	217	LYS
7	U	239	GLN
8	V	91	GLN
10	X	192	ALA
3	C	184	ALA
5	E	203	ASP
8	H	91	GLN
3	Q	184	ALA
5	S	203	ASP
6	T	206	LYS
1	A	56	SER
1	A	167	LYS
2	B	184	MET
4	D	12(C)	GLY
4	D	12(F)	GLY
5	E	180	LEU
5	E	231	LYS
6	F	64	ASN
6	F	206	LYS
10	J	49	ALA
1	O	56	SER
1	O	167	LYS
2	P	6	ARG
2	P	184	MET
4	R	12(C)	GLY
4	R	12(F)	GLY
5	S	180	LEU
5	S	231	LYS

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Mol	Chain	Res	Type
6	T	64	ASN
3	C	242	GLU
4	D	120	ALA
12	L	93	PHE
1	O	53	LYS
3	Q	242	GLU
4	R	120	ALA
6	T	143	LYS
10	X	49	ALA
12	Z	93	PHE
2	B	6	ARG
7	U	61	PRO
7	U	55	PRO
7	G	61	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	203 (97%)	6 (3%)	42	74
1	O	209/209 (100%)	203 (97%)	6 (3%)	42	74
2	B	203/203 (100%)	190 (94%)	13 (6%)	17	44
2	P	203/203 (100%)	190 (94%)	13 (6%)	17	44
3	C	213/213 (100%)	203 (95%)	10 (5%)	26	57
3	Q	213/213 (100%)	203 (95%)	10 (5%)	26	57
4	D	198/198 (100%)	188 (95%)	10 (5%)	24	54
4	R	198/198 (100%)	188 (95%)	10 (5%)	24	54
5	E	192/192 (100%)	175 (91%)	17 (9%)	9	27
5	S	192/192 (100%)	175 (91%)	17 (9%)	9	27
6	F	201/201 (100%)	185 (92%)	16 (8%)	12	32
6	T	201/201 (100%)	185 (92%)	16 (8%)	12	32
7	G	207/207 (100%)	197 (95%)	10 (5%)	25	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	207/207 (100%)	196 (95%)	11 (5%)	22	52
8	H	181/181 (100%)	174 (96%)	7 (4%)	32	64
8	V	181/181 (100%)	174 (96%)	7 (4%)	32	64
9	I	172/172 (100%)	167 (97%)	5 (3%)	42	74
9	W	172/172 (100%)	167 (97%)	5 (3%)	42	74
10	J	175/175 (100%)	169 (97%)	6 (3%)	37	69
10	X	175/175 (100%)	169 (97%)	6 (3%)	37	69
11	K	169/169 (100%)	162 (96%)	7 (4%)	30	63
11	Y	169/169 (100%)	162 (96%)	7 (4%)	30	63
12	L	185/185 (100%)	175 (95%)	10 (5%)	22	51
12	Z	185/185 (100%)	175 (95%)	10 (5%)	22	51
13	1	199/199 (100%)	191 (96%)	8 (4%)	31	64
13	M	199/199 (100%)	191 (96%)	8 (4%)	31	64
14	2	162/162 (100%)	155 (96%)	7 (4%)	29	60
14	N	162/162 (100%)	155 (96%)	7 (4%)	29	60
All	All	5332/5332 (100%)	5067 (95%)	265 (5%)	24	55

All (265) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	64	LEU
1	A	124	THR
1	A	158	PHE
1	A	179	ARG
1	A	229	ILE
2	B	58	LEU
2	B	71	ASN
2	B	74	ILE
2	B	121	GLN
2	B	135	SER
2	B	150	THR
2	B	163	ILE
2	B	185	LYS
2	B	187	ASP
2	B	192	LEU
2	B	212	PHE

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Mol	Chain	Res	Type
2	B	218	ASN
2	B	224	PHE
3	C	10	ARG
3	C	25	GLU
3	C	57	LYS
3	C	121	GLN
3	C	135	SER
3	C	150	GLN
3	C	172	VAL
3	C	174	GLU
3	C	208	LYS
3	C	227	GLU
4	D	28	LEU
4	D	76	CYS
4	D	110	GLU
4	D	126	ARG
4	D	170	GLU
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	244	GLU
5	E	11	ASP
5	E	12	THR
5	E	32	LYS
5	E	56	ASP
5	E	57	GLU
5	E	76	LEU
5	E	97	ASN
5	E	104	ASN
5	E	121	GLN
5	E	185	ASN
5	E	189	LEU
5	E	199	GLN
5	E	207	LEU
5	E	214	ILE
5	E	227	GLU
5	E	231	LYS
5	E	233	ILE
6	F	11	SER
6	F	35	THR
6	F	36	THR

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Mol	Chain	Res	Type
6	F	43	ASN
6	F	105	THR
6	F	121	GLN
6	F	127	ASN
6	F	169	ARG
6	F	176	LEU
6	F	18(E)	GLU
6	F	187	ARG
6	F	203	GLU
6	F	204	ASP
6	F	205	ASN
6	F	214	TRP
6	F	21(C)	ASN
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	124	THR
7	G	169	GLN
7	G	184	ASN
7	G	197	MET
7	G	232	ARG
7	G	233	LEU
8	H	30	ASN
8	H	34	LEU
8	H	43	CYS
8	H	56	THR
8	H	68	LEU
8	H	144	GLN
8	H	197	ARG
9	I	29	ASN
9	I	61	TYR
9	I	113	PHE
9	I	116	ILE
9	I	160	LEU
10	J	52	THR
10	J	70	GLU
10	J	77	GLN
10	J	90(A)	ILE
10	J	121	GLU
10	J	177	ILE
11	K	4	LEU

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Mol	Chain	Res	Type
11	K	9	GLN
11	K	65	LEU
11	K	87	VAL
11	K	104	TYR
11	K	10(B)	LYS
11	K	138	LEU
12	L	-7	ASN
12	L	14	LEU
12	L	40	ASN
12	L	58	ARG
12	L	70(A)	ASN
12	L	82	ASN
12	L	98	HIS
12	L	99	THR
12	L	120	GLU
12	L	145	TYR
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	129	PHE
13	M	14(C)	ARG
13	M	148	VAL
13	M	149	GLN
13	M	204	LYS
14	N	36	ARG
14	N	89	GLU
14	N	10(B)	LYS
14	N	119	VAL
14	N	126	ILE
14	N	18(A)	ILE
14	N	18(I)	GLN
1	O	33	GLN
1	O	64	LEU
1	O	124	THR
1	O	158	PHE
1	O	179	ARG
1	O	229	ILE
2	P	58	LEU
2	P	71	ASN
2	P	74	ILE
2	P	121	GLN
2	P	135	SER

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Mol	Chain	Res	Type
2	P	150	THR
2	P	163	ILE
2	P	185	LYS
2	P	187	ASP
2	P	192	LEU
2	P	212	PHE
2	P	218	ASN
2	P	224	PHE
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	121	GLN
3	Q	135	SER
3	Q	150	GLN
3	Q	172	VAL
3	Q	174	GLU
3	Q	208	LYS
3	Q	227	GLU
4	R	28	LEU
4	R	76	CYS
4	R	110	GLU
4	R	126	ARG
4	R	170	GLU
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	244	GLU
5	S	11	ASP
5	S	12	THR
5	S	32	LYS
5	S	56	ASP
5	S	57	GLU
5	S	76	LEU
5	S	97	ASN
5	S	104	ASN
5	S	121	GLN
5	S	185	ASN
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU
5	S	214	ILE

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Mol	Chain	Res	Type
5	S	227	GLU
5	S	231	LYS
5	S	233	ILE
6	T	11	SER
6	T	35	THR
6	T	36	THR
6	T	43	ASN
6	T	105	THR
6	T	121	GLN
6	T	127	ASN
6	T	169	ARG
6	T	176	LEU
6	T	18(E)	GLU
6	T	187	ARG
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
6	T	214	TRP
6	T	21(C)	ASN
7	U	38	LEU
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	124	THR
7	U	169	GLN
7	U	184	ASN
7	U	197	MET
7	U	232	ARG
7	U	233	LEU
8	V	30	ASN
8	V	34	LEU
8	V	43	CYS
8	V	56	THR
8	V	68	LEU
8	V	144	GLN
8	V	197	ARG
9	W	29	ASN
9	W	61	TYR
9	W	113	PHE
9	W	116	ILE
9	W	160	LEU

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Mol	Chain	Res	Type
10	X	52	THR
10	X	70	GLU
10	X	77	GLN
10	X	90(A)	ILE
10	X	121	GLU
10	X	177	ILE
11	Y	4	LEU
11	Y	9	GLN
11	Y	65	LEU
11	Y	87	VAL
11	Y	104	TYR
11	Y	10(B)	LYS
11	Y	138	LEU
12	Z	-7	ASN
12	Z	14	LEU
12	Z	40	ASN
12	Z	58	ARG
12	Z	70(A)	ASN
12	Z	82	ASN
12	Z	98	HIS
12	Z	99	THR
12	Z	120	GLU
12	Z	145	TYR
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	129	PHE
13	1	14(C)	ARG
13	1	148	VAL
13	1	149	GLN
13	1	204	LYS
14	2	36	ARG
14	2	89	GLU
14	2	10(B)	LYS
14	2	119	VAL
14	2	126	ILE
14	2	18(A)	ILE
14	2	18(I)	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (206) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
2	B	23	GLN
2	B	71	ASN
2	B	95	HIS
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	238	GLN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	147	GLN
4	D	161	ASN
4	D	211	GLN
4	D	218	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	64	GLN
5	E	73	HIS
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	185	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN

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Mol	Chain	Res	Type
6	F	192	GLN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
7	G	228	ASN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
9	I	81	GLN
9	I	161	ASN
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	140	HIS
10	J	141	HIS
10	J	186	GLN
10	J	193	GLN
11	K	9	GLN
11	K	85	ASN
11	K	174	ASN
11	K	207	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	40	ASN
12	L	46	ASN
12	L	61	ASN
12	L	70(A)	ASN
12	L	82	ASN
12	L	85	HIS
12	L	98	HIS
12	L	123	GLN

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Mol	Chain	Res	Type
12	L	1(I)	ASN
12	L	166	HIS
12	L	168	GLN
13	M	-7	GLN
13	M	10	ASN
13	M	18	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	191	GLN
14	N	69	GLN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
2	P	33	HIS
2	P	71	ASN
2	P	95	HIS
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN
3	Q	82	ASN
3	Q	97	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	238	GLN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	114	GLN
4	R	147	GLN

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Mol	Chain	Res	Type
4	R	161	ASN
4	R	211	GLN
4	R	218	GLN
4	R	226	ASN
5	S	7	ASN
5	S	64	GLN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	185	ASN
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	147	HIS
6	T	192	GLN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	170	GLN
7	U	178	ASN
7	U	184	ASN
7	U	228	ASN
8	V	30	ASN
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	64	ASN
9	W	81	GLN
9	W	161	ASN
10	X	54	GLN

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Mol	Chain	Res	Type
10	X	62	ASN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	140	HIS
10	X	141	HIS
10	X	186	GLN
10	X	193	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	207	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	61	ASN
12	Z	70(A)	ASN
12	Z	82	ASN
12	Z	123	GLN
12	Z	1(I)	ASN
12	Z	166	HIS
12	Z	168	GLN
13	1	10	ASN
13	1	18	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN
13	1	191	GLN
14	2	69	GLN
14	2	145	ASN
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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	BIQ	H	1000	-	50,51,51	1.75	13 (26%)	66,69,69	2.08	15 (22%)
15	BIQ	V	1001	-	50,51,51	1.79	14 (28%)	66,69,69	2.10	14 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BIQ	H	1000	-	-	14/51/53/53	0/3/4/4
15	BIQ	V	1001	-	-	13/51/53/53	0/3/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	1001	BIQ	C37-C32	3.89	1.47	1.40
15	V	1001	BIQ	C37-N38	-3.72	1.38	1.45
15	H	1000	BIQ	C37-C32	3.53	1.46	1.40
15	H	1000	BIQ	C37-N38	-3.42	1.39	1.45
15	V	1001	BIQ	C5-N6	3.37	1.43	1.34
15	H	1000	BIQ	C42-C30	3.35	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	1001	BIQ	C42-C30	3.33	1.45	1.38
15	H	1000	BIQ	O31-C32	3.25	1.46	1.39
15	V	1001	BIQ	O31-C32	3.17	1.46	1.39
15	H	1000	BIQ	C5-N6	3.06	1.42	1.34
15	V	1001	BIQ	C43-C42	2.65	1.43	1.38
15	H	1000	BIQ	O4-C5	2.60	1.40	1.35
15	V	1001	BIQ	C36-C37	2.56	1.44	1.39
15	V	1001	BIQ	O4-C5	2.56	1.40	1.35
15	H	1000	BIQ	C43-C42	2.51	1.43	1.38
15	H	1000	BIQ	C7-N6	2.44	1.51	1.45
15	V	1001	BIQ	C33-C32	2.20	1.42	1.38
15	H	1000	BIQ	C45-C2	2.19	1.43	1.38
15	V	1001	BIQ	C7-N6	2.15	1.50	1.45
15	V	1001	BIQ	C1-C2	2.13	1.43	1.38
15	V	1001	BIQ	C28-C27	2.10	1.43	1.38
15	H	1000	BIQ	C46-C45	2.10	1.43	1.38
15	V	1001	BIQ	O31-C30	2.06	1.44	1.39
15	H	1000	BIQ	O31-C30	2.05	1.44	1.39
15	H	1000	BIQ	O39-N38	2.04	1.26	1.22
15	V	1001	BIQ	C36-C35	2.01	1.42	1.38
15	H	1000	BIQ	C8-N10	2.01	1.38	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	1000	BIQ	C12-C11-N10	9.54	129.28	110.60
15	V	1001	BIQ	C12-C11-N10	9.38	128.96	110.60
15	V	1001	BIQ	C7-C8-N10	5.10	127.88	116.70
15	H	1000	BIQ	C11-N10-C8	4.86	132.09	121.67
15	V	1001	BIQ	C11-N10-C8	4.82	132.00	121.67
15	H	1000	BIQ	C41-C7-N6	-4.78	100.72	110.79
15	H	1000	BIQ	C7-C8-N10	4.73	127.07	116.70
15	V	1001	BIQ	O9-C8-N10	-4.08	115.38	122.93
15	V	1001	BIQ	C41-C7-N6	-4.03	102.29	110.79
15	H	1000	BIQ	O9-C8-N10	-3.93	115.66	122.93
15	V	1001	BIQ	C26-C19-N18	3.50	118.16	110.79
15	H	1000	BIQ	C26-C19-N18	3.32	117.79	110.79
15	H	1000	BIQ	C23-N22-C20	3.15	128.20	122.59
15	H	1000	BIQ	C41-C7-C8	3.09	118.27	110.25
15	V	1001	BIQ	C41-C7-C8	3.08	118.25	110.25
15	V	1001	BIQ	C34-C41-C7	3.06	121.84	113.39
15	H	1000	BIQ	C34-C41-C7	3.06	121.82	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	1001	BIQ	C32-O31-C30	-2.82	110.96	118.00
15	V	1001	BIQ	C23-N22-C20	2.76	127.51	122.59
15	V	1001	BIQ	O31-C32-C37	2.66	122.70	117.49
15	H	1000	BIQ	C24-C23-N22	-2.56	104.22	112.32
15	V	1001	BIQ	O4-C3-C2	2.53	115.48	109.39
15	H	1000	BIQ	C32-O31-C30	-2.53	111.70	118.00
15	H	1000	BIQ	O31-C32-C37	2.49	122.38	117.49
15	V	1001	BIQ	C36-C37-N38	2.40	119.04	116.47
15	V	1001	BIQ	C24-C23-N22	-2.39	104.76	112.32
15	H	1000	BIQ	C11-C12-C13	2.26	116.73	112.24
15	H	1000	BIQ	C20-C19-N18	-2.20	105.17	111.16
15	H	1000	BIQ	O4-C3-C2	2.00	114.21	109.39

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	V	1001	BIQ	C16-C11-C12-C13
15	H	1000	BIQ	O9-C8-N10-C11
15	V	1001	BIQ	O9-C8-N10-C11
15	V	1001	BIQ	C7-C8-N10-C11
15	H	1000	BIQ	C7-C8-N10-C11
15	H	1000	BIQ	C11-C12-C13-N14
15	V	1001	BIQ	C11-C12-C13-N14
15	H	1000	BIQ	C16-C11-C12-C13
15	V	1001	BIQ	C12-C11-N10-C8
15	H	1000	BIQ	C11-C12-C13-O15
15	V	1001	BIQ	C11-C12-C13-O15
15	H	1000	BIQ	N10-C11-C16-N18
15	V	1001	BIQ	N10-C11-C16-N18
15	V	1001	BIQ	C41-C7-N6-C5
15	H	1000	BIQ	C12-C11-N10-C8
15	H	1000	BIQ	C36-C37-N38-O39
15	V	1001	BIQ	C36-C37-N38-O39
15	H	1000	BIQ	N6-C7-C8-N10
15	V	1001	BIQ	N6-C7-C8-N10
15	H	1000	BIQ	C41-C7-N6-C5
15	V	1001	BIQ	N6-C7-C8-O9
15	V	1001	BIQ	N10-C11-C16-O17
15	H	1000	BIQ	N6-C7-C8-O9
15	H	1000	BIQ	N10-C11-C16-O17
15	H	1000	BIQ	C35-C34-C41-C7

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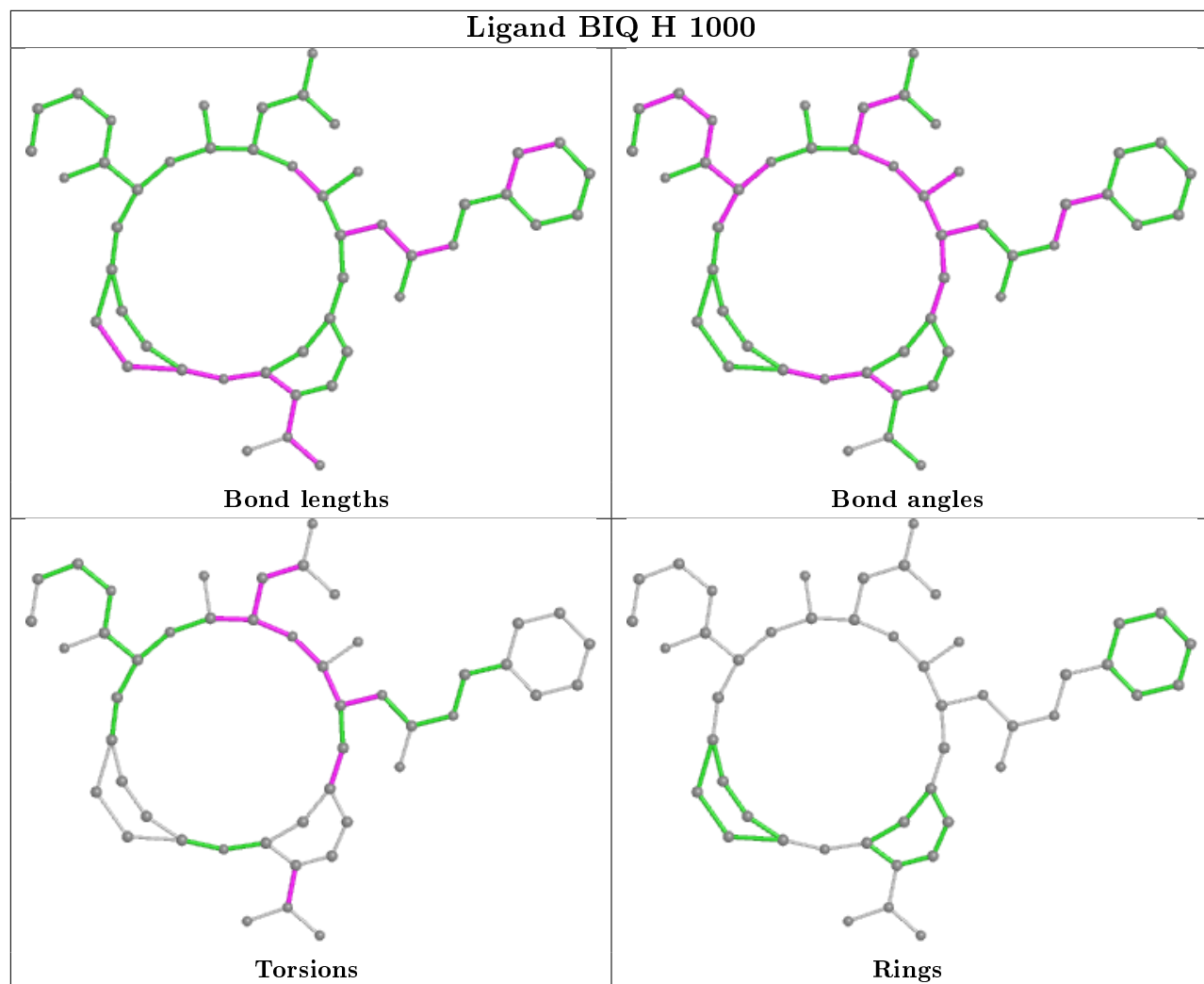
Mol	Chain	Res	Type	Atoms
15	H	1000	BIQ	C33-C34-C41-C7
15	V	1001	BIQ	C35-C34-C41-C7

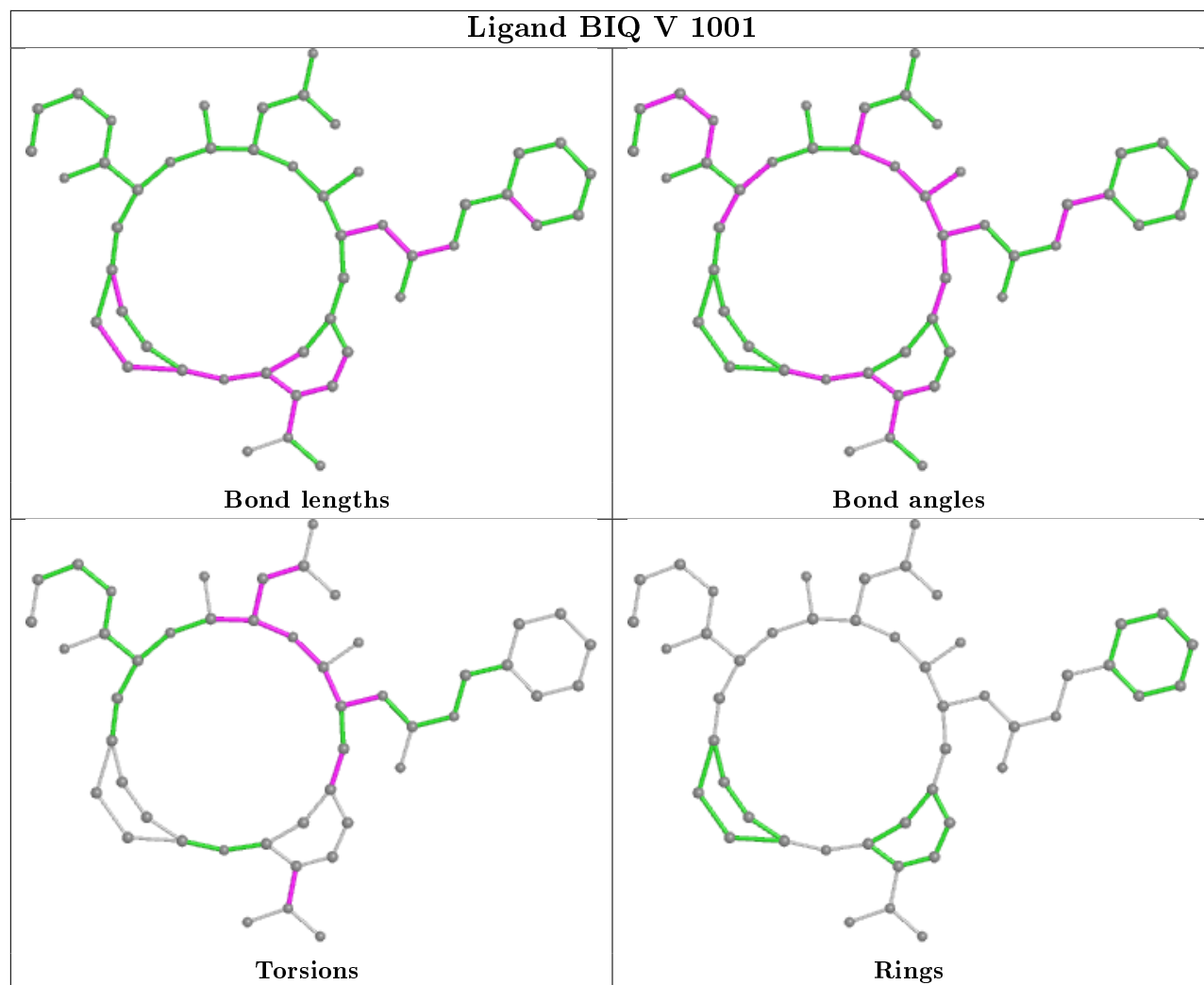
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	1000	BIQ	4	0
15	V	1001	BIQ	5	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.39	2 (0%) 86 82	33, 45, 76, 103	0
1	O	250/250 (100%)	-0.31	5 (2%) 65 56	33, 52, 81, 106	0
2	B	244/244 (100%)	-0.19	9 (3%) 41 31	31, 52, 87, 116	0
2	P	244/244 (100%)	-0.11	14 (5%) 23 15	35, 55, 91, 118	0
3	C	241/241 (100%)	-0.10	10 (4%) 37 27	33, 57, 109, 123	0
3	Q	241/241 (100%)	0.04	12 (4%) 28 20	37, 60, 110, 122	0
4	D	242/242 (100%)	-0.11	8 (3%) 46 36	35, 56, 89, 121	0
4	R	242/242 (100%)	-0.01	12 (4%) 28 20	36, 60, 91, 121	0
5	E	233/233 (100%)	-0.17	5 (2%) 63 54	39, 59, 85, 110	0
5	S	233/233 (100%)	0.07	17 (7%) 15 8	38, 63, 89, 108	0
6	F	244/244 (100%)	-0.33	4 (1%) 72 65	34, 54, 88, 105	0
6	T	244/244 (100%)	-0.21	6 (2%) 57 47	34, 55, 91, 107	0
7	G	243/243 (100%)	-0.40	3 (1%) 79 73	29, 47, 75, 114	0
7	U	243/243 (100%)	-0.36	2 (0%) 86 82	30, 49, 74, 114	0
8	H	222/222 (100%)	-0.57	3 (1%) 75 69	26, 43, 61, 92	0
8	V	222/222 (100%)	-0.57	3 (1%) 75 69	30, 44, 63, 96	0
9	I	204/204 (100%)	-0.64	1 (0%) 91 88	28, 44, 61, 80	0
9	W	204/204 (100%)	-0.62	1 (0%) 91 88	31, 45, 64, 79	0
10	J	198/198 (100%)	-0.45	3 (1%) 73 67	29, 45, 62, 120	0
10	X	198/198 (100%)	-0.39	5 (2%) 57 47	33, 48, 63, 122	0
11	K	212/212 (100%)	-0.49	0 100 100	27, 47, 63, 74	0
11	Y	212/212 (100%)	-0.50	1 (0%) 91 88	29, 48, 67, 74	0
12	L	222/222 (100%)	-0.55	2 (0%) 84 80	27, 45, 69, 88	0
12	Z	222/222 (100%)	-0.53	1 (0%) 91 88	30, 45, 69, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	-0.59	1 (0%)	92	91	28, 43, 57, 64	0
13	M	233/233 (100%)	-0.58	1 (0%)	92	91	29, 45, 60, 67	0
14	2	196/196 (100%)	-0.52	1 (0%)	91	88	24, 43, 66, 78	0
14	N	196/196 (100%)	-0.58	0	100	100	28, 42, 66, 76	0
All	All	6368/6368 (100%)	-0.35	132 (2%)	63	54	24, 49, 83, 123	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	U	240	ASP	9.8
3	C	55	THR	9.7
4	D	12(D)	ALA	9.3
4	R	12(D)	ALA	9.2
4	R	12(F)	GLY	8.9
3	C	56	LEU	8.0
4	R	12(E)	SER	7.8
4	D	12(F)	GLY	7.6
10	X	193	GLN	7.4
2	P	217	ALA	7.3
4	D	12(E)	SER	7.3
2	B	217	ALA	7.2
10	J	193	GLN	6.8
2	B	218	ASN	6.7
1	A	4	MET	6.7
7	U	6	ALA	6.5
10	X	192	ALA	6.5
7	G	240	ASP	6.4
2	P	218	ASN	6.0
4	D	12(C)	GLY	6.0
4	R	12(C)	GLY	5.9
10	J	192	ALA	5.8
7	G	6	ALA	5.8
3	Q	54	SER	5.7
4	D	126	ARG	5.7
5	E	203	ASP	5.2
3	Q	63	THR	5.1
5	S	203	ASP	5.0
3	Q	55	THR	4.8
6	F	5	GLY	4.8
4	D	12(G)	GLU	4.8
4	R	126	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	54	VAL	4.6
2	P	219	GLU	4.5
2	P	21(C)	ASP	4.4
1	O	4	MET	4.3
3	Q	56	LEU	4.2
8	V	223	ASP	4.2
2	B	21(B)	GLY	4.0
9	I	-8	SER	4.0
8	H	222	CYS	4.0
5	E	4	PHE	4.0
1	O	236	LEU	4.0
5	S	5	ARG	3.9
10	X	191	GLN	3.8
3	Q	242	GLU	3.8
5	S	206	SER	3.8
1	O	235	ALA	3.6
2	B	239	THR	3.6
8	H	223	ASP	3.6
10	X	189	ASP	3.6
1	O	5	THR	3.5
5	S	4	PHE	3.5
5	S	58	LEU	3.5
6	T	241	ASN	3.5
5	E	5	ARG	3.5
5	S	178	ARG	3.5
2	P	21(B)	GLY	3.5
12	Z	14(W)	LYS	3.4
3	Q	203	THR	3.4
3	Q	241	GLN	3.4
5	S	55	ALA	3.4
5	S	60	SER	3.4
1	A	5	THR	3.3
4	D	125	GLU	3.3
3	C	54	SER	3.3
4	R	125	GLU	3.3
10	J	191	GLN	3.3
3	Q	64	PRO	3.2
8	V	222	CYS	3.2
6	F	204	ASP	3.2
10	X	-1	MET	3.2
2	P	63	THR	3.2
5	S	54	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
9	W	-8	SER	3.1
4	R	12(G)	GLU	3.1
13	1	-8	THR	3.1
4	R	127	LEU	3.1
5	S	63	TYR	3.1
2	P	54	VAL	3.0
3	Q	243	GLN	3.0
4	R	9	ASP	3.0
6	T	5	GLY	3.0
4	R	12(B)	GLU	2.9
2	P	239	THR	2.9
2	P	62	ASP	2.9
13	M	-8	THR	2.9
3	C	203	THR	2.9
2	B	21(C)	ASP	2.8
3	Q	61	THR	2.7
3	C	242	GLU	2.7
5	S	57	GLU	2.7
6	T	240	ILE	2.7
3	C	237	GLU	2.7
5	S	56	ASP	2.6
6	F	205	ASN	2.6
12	L	145	TYR	2.6
11	Y	211	GLY	2.5
5	S	64	GLN	2.5
1	O	55	SER	2.5
14	2	18(I)	GLN	2.5
3	C	59	GLN	2.5
2	B	21(A)	LYS	2.4
8	V	220	ASN	2.4
4	D	9	ASP	2.4
12	L	14(W)	LYS	2.4
3	C	53	ARG	2.3
2	P	220	TYR	2.3
2	P	20(A)	SER	2.3
3	Q	62(A)	ILE	2.2
5	S	59	SER	2.2
5	S	195	GLU	2.2
2	P	183	ASP	2.2
6	T	57	LYS	2.2
3	C	243	GLN	2.2
2	P	21(A)	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
5	S	2(E)	ASN	2.1
8	H	220	ASN	2.1
5	E	57	GLU	2.1
3	C	240	LYS	2.1
2	B	219	GLU	2.1
2	B	20(A)	SER	2.1
3	Q	58	LEU	2.1
2	P	53	LYS	2.1
7	G	239	GLN	2.1
5	E	6	ASN	2.1
4	R	243	ALA	2.0
5	S	6	ASN	2.0
6	F	20(B)	GLU	2.0
6	T	170	GLN	2.0
6	T	238	LYS	2.0
4	R	178	ASN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

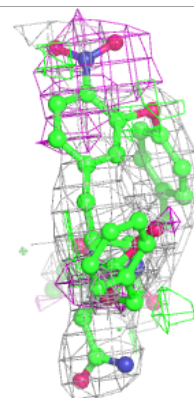
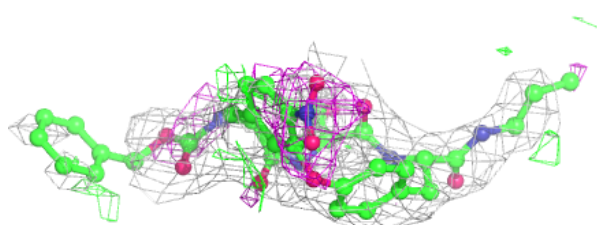
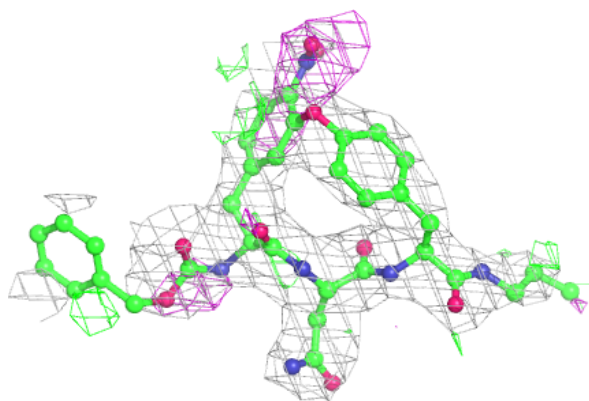
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	BIQ	V	1001	48/48	0.81	0.31	36,57,68,71	6
15	BIQ	H	1000	48/48	0.84	0.29	28,54,64,67	7

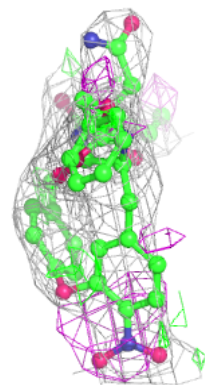
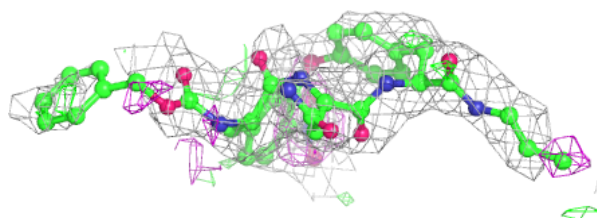
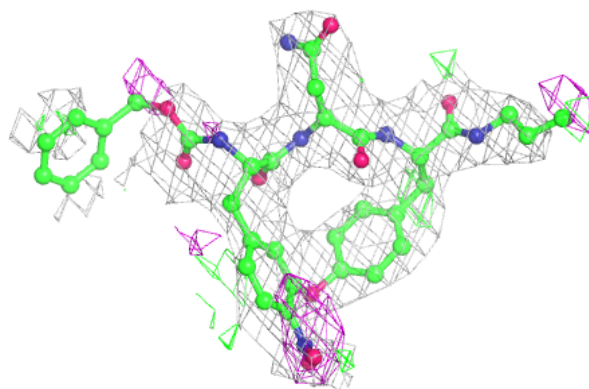
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BIQ V 1001:

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

**Electron density around BIQ H 1000:**

$2mF_o-DF_c$ (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.