



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:57 am BST

PDB ID : 3MG0
Title : Structure of yeast 20S proteasome with bortezomib
Authors : Sintchak, M.D.
Deposited on : 2010-04-05
Resolution : 2.68 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

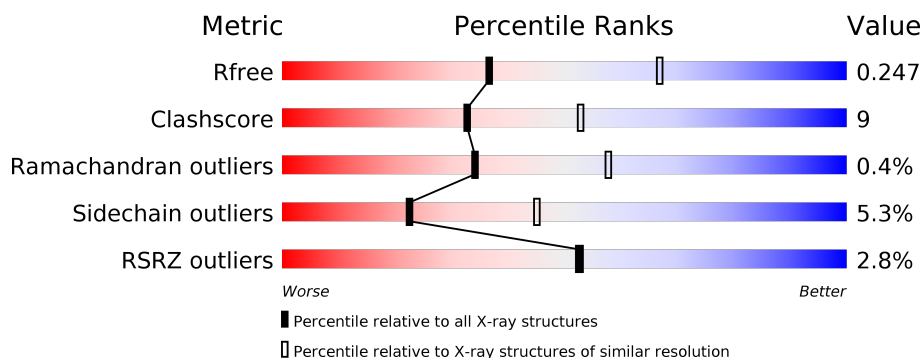
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> <div></div> </div>
1	O	250	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>13%</div> </div> <div></div> </div>
2	B	244	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>24%</div> </div> <div></div> </div>
2	P	244	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>21%</div> </div> <div></div> </div>
3	C	241	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>21%</div> </div> <div></div> </div>
3	Q	241	<div> <div>11%</div> <div> <div></div> <div>76%</div> <div>22%</div> </div> <div></div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	242	
4	R	242	
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	196	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50753 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			

Continued on next page...

Continued from previous page...

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			

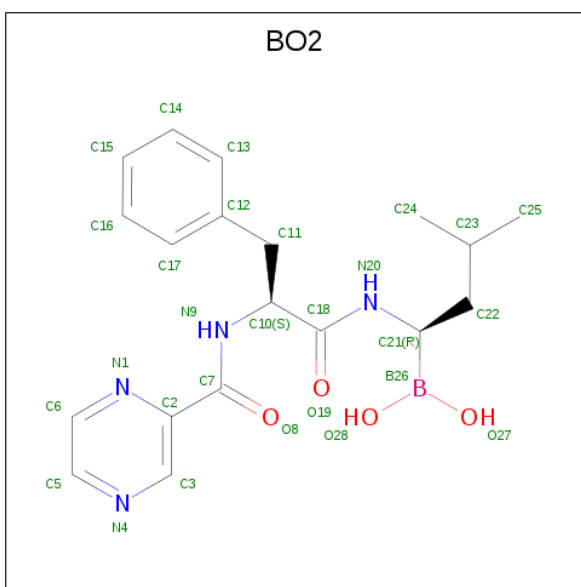
- Molecule 13 is a protein called Proteasome component PRE4.

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 N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (three-letter code: BO2) (formula: C₁₉H₂₅BN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	H	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
15	K	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
15	N	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
15	V	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
15	Y	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
15	2	1	Total	B	C	N	O	0	0
			28	1	19	4	4		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	49	Total	O	0	0
			49	49		
16	B	31	Total	O	0	0
			31	31		
16	C	32	Total	O	0	0
			32	32		
16	D	25	Total	O	0	0
			25	25		
16	E	14	Total	O	0	0
			14	14		
16	F	35	Total	O	0	0
			35	35		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	46	Total O 46 46	0	0
16	H	41	Total O 41 41	0	0
16	I	52	Total O 52 52	0	0
16	J	45	Total O 45 45	0	0
16	K	33	Total O 33 33	0	0
16	L	42	Total O 42 42	0	0
16	M	53	Total O 53 53	0	0
16	N	46	Total O 46 46	0	0
16	O	24	Total O 24 24	0	0
16	P	23	Total O 23 23	0	0
16	Q	19	Total O 19 19	0	0
16	R	24	Total O 24 24	0	0
16	S	17	Total O 17 17	0	0
16	T	32	Total O 32 32	0	0
16	U	53	Total O 53 53	0	0
16	V	35	Total O 35 35	0	0
16	W	44	Total O 44 44	0	0
16	X	38	Total O 38 38	0	0
16	Y	30	Total O 30 30	0	0
16	Z	38	Total O 38 38	0	0
16	1	63	Total O 63 63	0	0

Continued on next page...

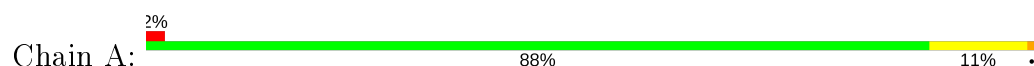
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	2	53	Total	O	0	0
			53	53		

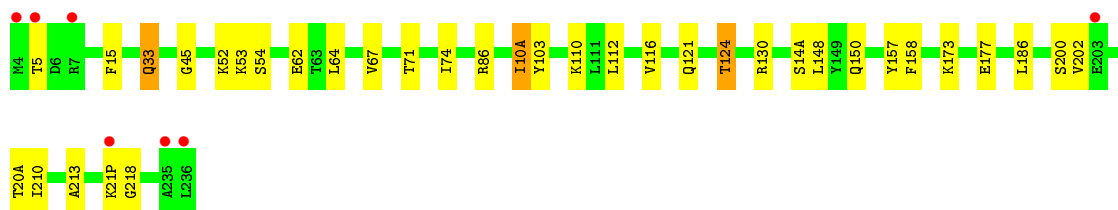
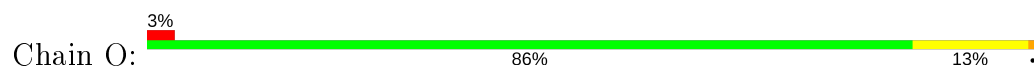
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

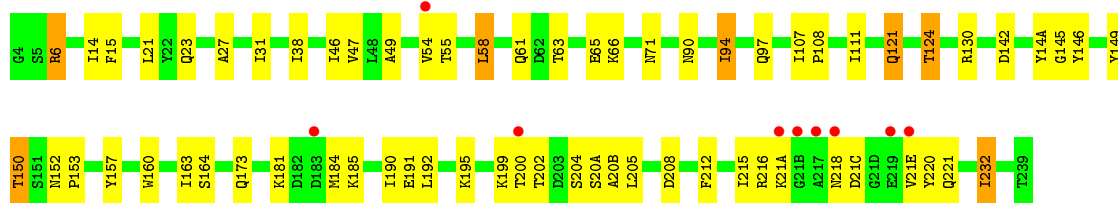
- Molecule 1: Proteasome component Y7



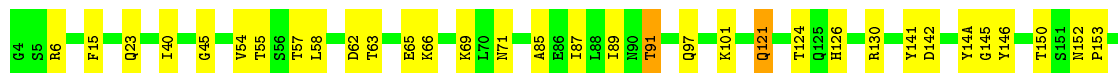
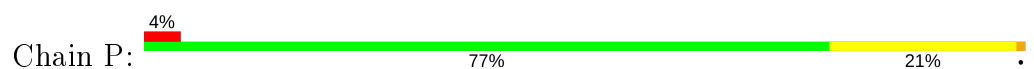
- Molecule 1: Proteasome component Y7



- Molecule 2: Proteasome component Y13

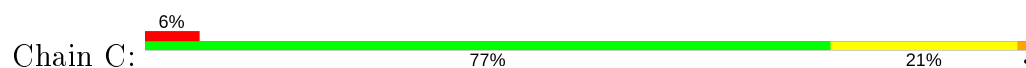


- Molecule 2: Proteasome component Y13

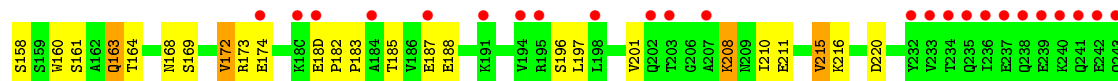
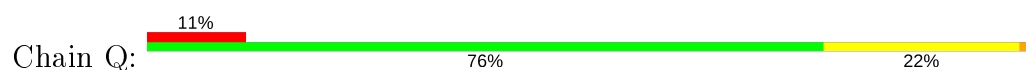




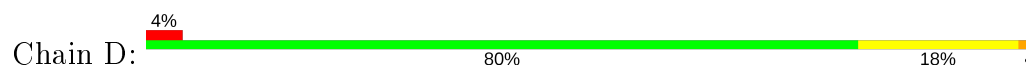
- Molecule 3: Proteasome component PRE6



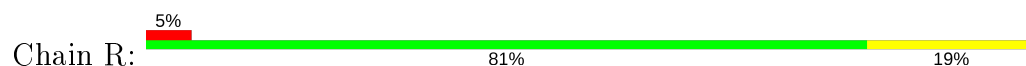
- Molecule 3: Proteasome component PRE6



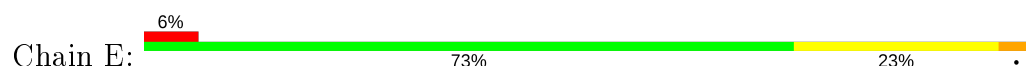
- Molecule 4: Proteasome component PUP2

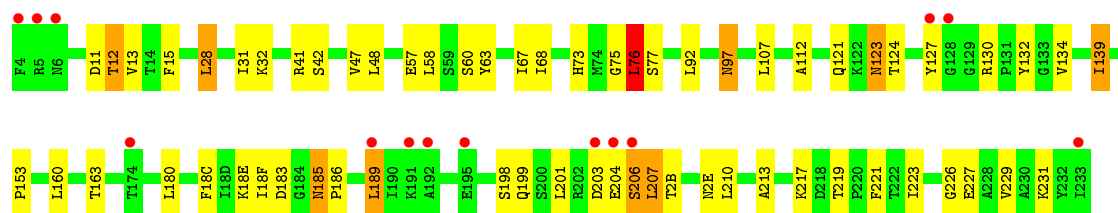


- Molecule 4: Proteasome component PUP2

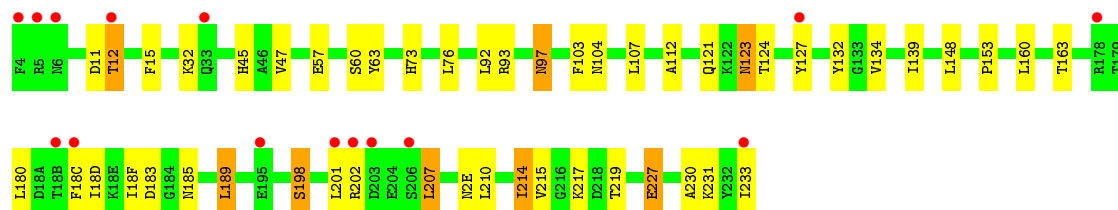
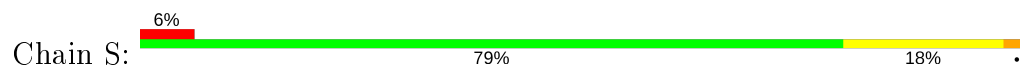


- Molecule 5: Proteasome component PRE5

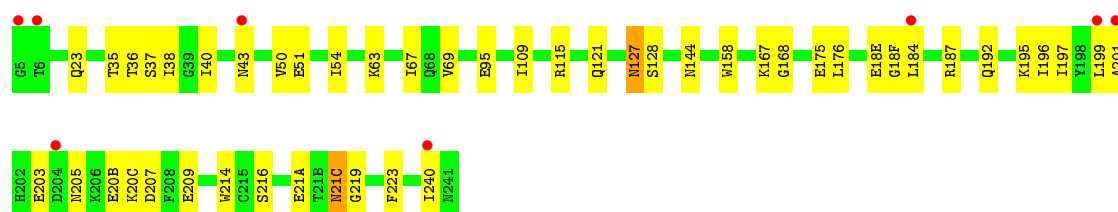
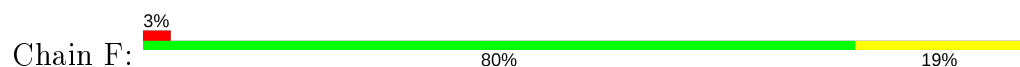




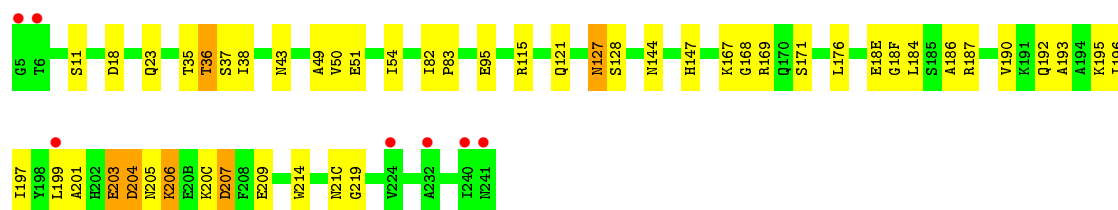
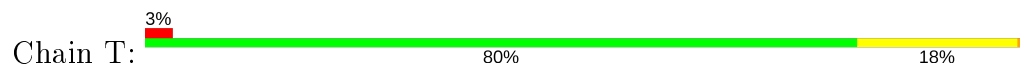
• Molecule 5: Proteasome component PRE5



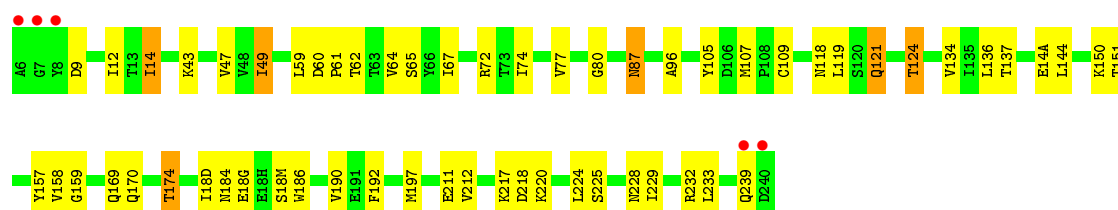
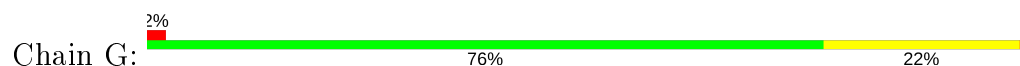
• Molecule 6: Proteasome component C1



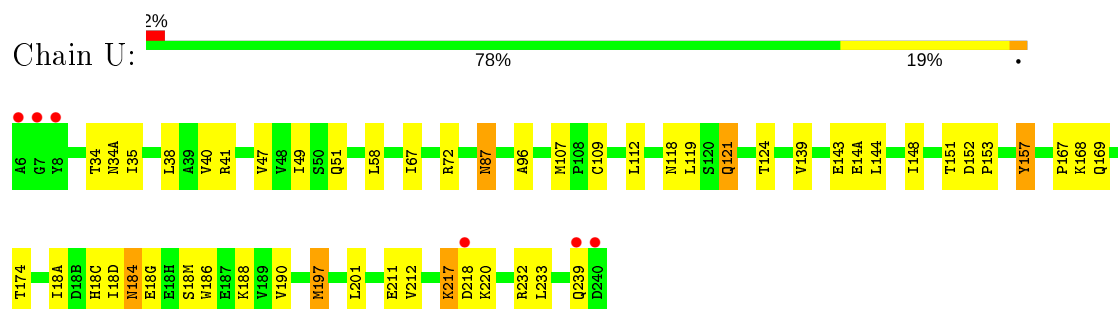
• Molecule 6: Proteasome component C1



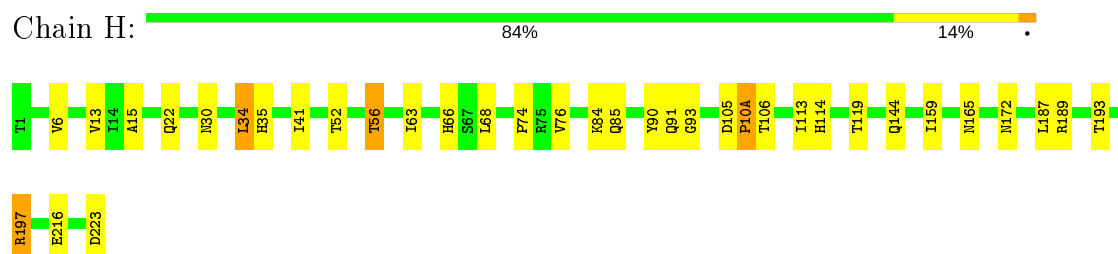
• Molecule 7: Proteasome component C7-alpha



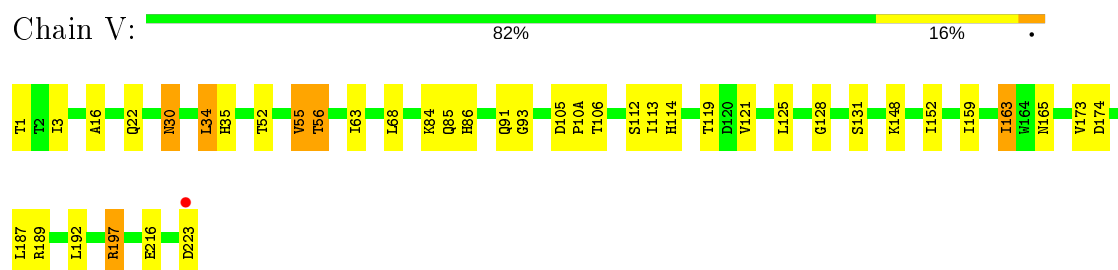
- Molecule 7: Proteasome component C7-alpha



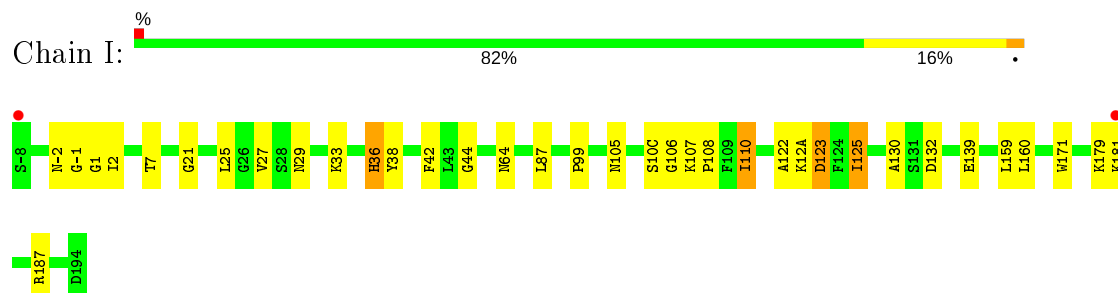
- Molecule 8: Proteasome component PUP1



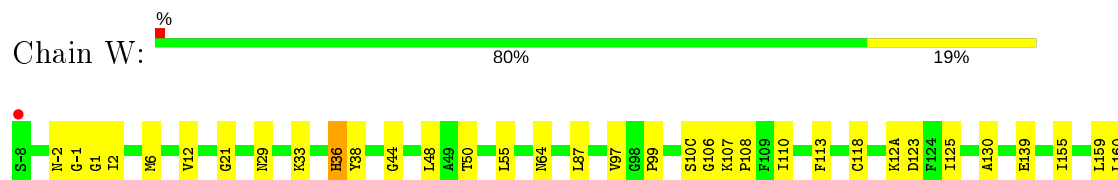
- Molecule 8: Proteasome component PUP1



- Molecule 9: Proteasome component PUP3

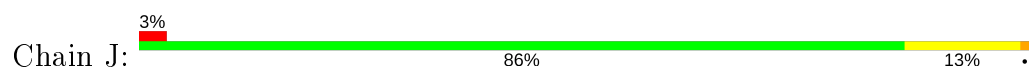


- Molecule 9: Proteasome component PUP3

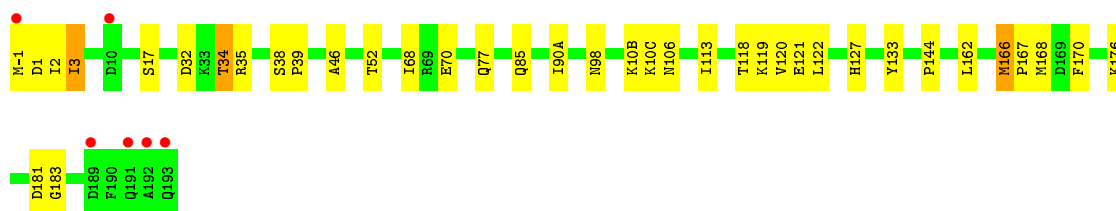
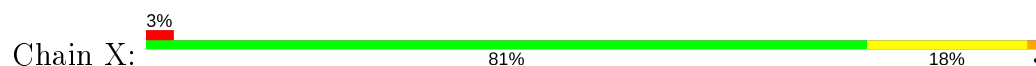




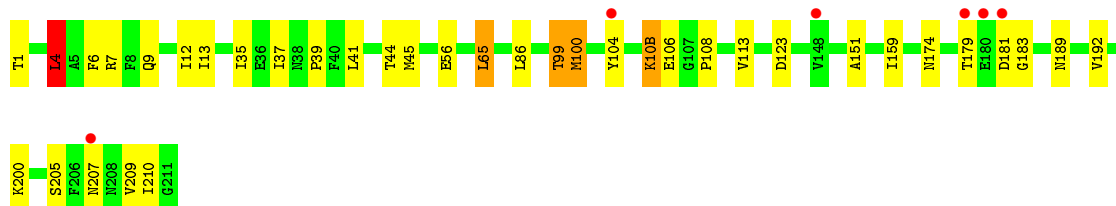
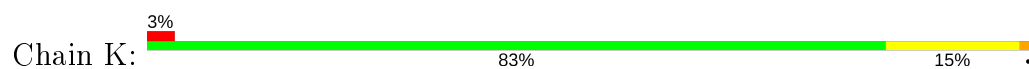
• Molecule 10: Proteasome component C11



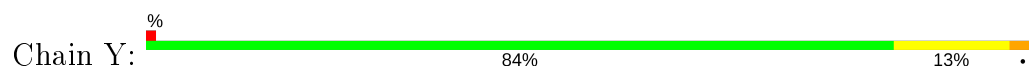
• Molecule 10: Proteasome component C11



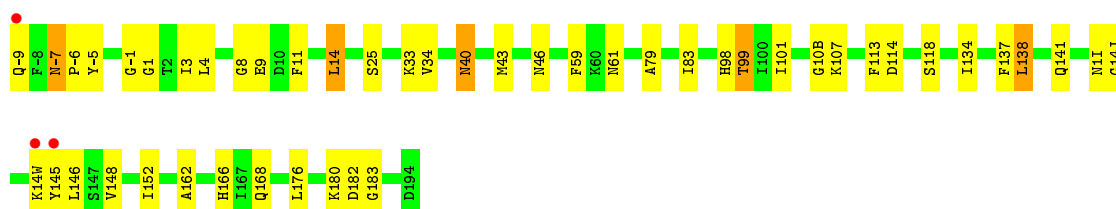
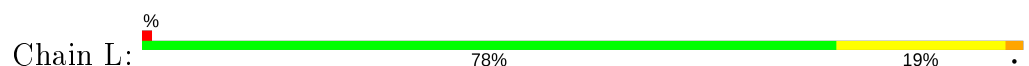
• Molecule 11: Proteasome component PRE2



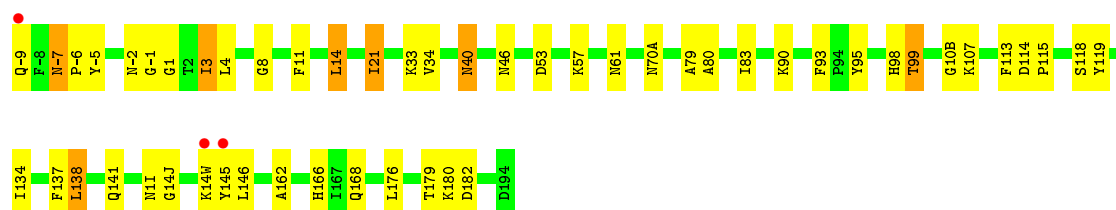
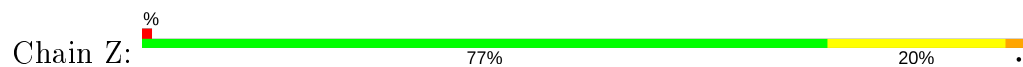
• Molecule 11: Proteasome component PRE2



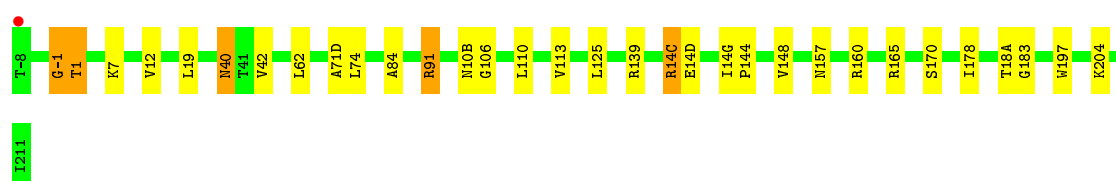
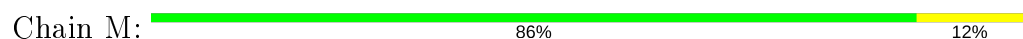
• Molecule 12: Proteasome component C5



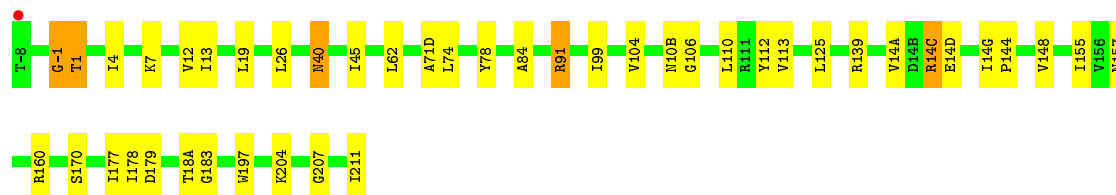
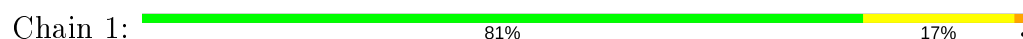
- Molecule 12: Proteasome component C5



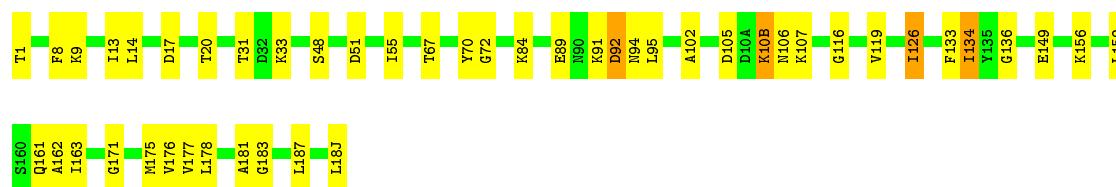
- Molecule 13: Proteasome component PRE4



- Molecule 13: Proteasome component PRE4



- Molecule 14: Proteasome component PRE3



- Molecule 14: Proteasome component PRE3





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.12Å 300.53Å 145.83Å 90.00° 113.16° 90.00°	Depositor
Resolution (Å)	50.00 – 2.68 49.04 – 2.68	Depositor EDS
% Data completeness (in resolution range)	92.0 (50.00-2.68) 92.1 (49.04-2.68)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.226 , 0.253 0.224 , 0.247	Depositor DCC
R_{free} test set	2818 reflections (1.02%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	50753	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BO2

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	0.68	1/1948 (0.1%)	0.55	0/2630
1	O	0.68	1/1948 (0.1%)	0.55	0/2630
2	B	0.41	0/1929	0.58	0/2600
2	P	0.43	0/1929	0.58	0/2600
3	C	0.41	0/1916	0.56	0/2585
3	Q	0.40	0/1916	0.56	0/2585
4	D	0.42	0/1881	0.58	0/2523
4	R	0.41	0/1881	0.58	0/2523
5	E	0.40	0/1819	0.57	1/2451 (0.0%)
5	S	0.41	0/1819	0.55	0/2451
6	F	0.42	0/1933	0.54	0/2602
6	T	0.43	0/1933	0.55	0/2602
7	G	0.45	0/1955	0.55	0/2640
7	U	0.44	0/1955	0.55	0/2640
8	H	0.74	1/1714 (0.1%)	0.55	1/2320 (0.0%)
8	V	0.38	0/1713	0.55	0/2317
9	I	0.72	1/1607 (0.1%)	0.60	2/2162 (0.1%)
9	W	0.65	1/1607 (0.1%)	0.58	1/2162 (0.0%)
10	J	0.41	0/1610	0.56	0/2164
10	X	0.41	0/1610	0.56	0/2164
11	K	0.42	0/1679	0.56	1/2268 (0.0%)
11	Y	0.41	0/1679	0.58	1/2268 (0.0%)
12	L	0.42	0/1790	0.56	0/2405
12	Z	0.42	0/1790	0.58	0/2405
13	1	0.73	1/1851 (0.1%)	0.63	1/2501 (0.0%)
13	M	0.60	1/1851 (0.1%)	0.58	0/2501
14	2	0.66	1/1538 (0.1%)	0.55	0/2078
14	N	0.76	1/1538 (0.1%)	0.56	0/2078
All	All	0.52	9/50339 (0.0%)	0.57	8/67855 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	-1	GLY	C-N	25.93	1.93	1.34
8	H	10(A)	PRO	C-N	25.92	1.93	1.34
14	N	92	ASP	C-N	24.57	1.90	1.34
9	I	36	HIS	C-N	23.90	1.89	1.34
1	O	10(A)	ILE	C-N	23.90	1.89	1.34
1	A	10(A)	ILE	C-N	23.88	1.89	1.34
9	W	36	HIS	C-N	20.15	1.80	1.34
14	2	92	ASP	C-N	20.11	1.80	1.34
13	M	-1	GLY	C-N	18.80	1.77	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	36	HIS	CA-C-N	-6.43	103.05	117.20
11	K	4	LEU	CA-CB-CG	5.82	128.69	115.30
8	H	10(A)	PRO	O-C-N	-5.80	113.41	122.70
9	I	36	HIS	CA-C-N	-5.50	105.11	117.20
5	E	76	LEU	CA-CB-CG	5.43	127.79	115.30
11	Y	4	LEU	CA-CB-CG	5.13	127.10	115.30
13	1	-1	GLY	C-N-CA	-5.11	108.93	121.70
9	I	36	HIS	O-C-N	-5.10	114.54	122.70

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	1921	27	0
1	O	1915	0	1921	30	0
2	B	1905	0	1895	47	0
2	P	1905	0	1895	45	0
3	C	1891	0	1897	35	0
3	Q	1891	0	1897	42	0
4	D	1862	0	1830	25	0
4	R	1862	0	1830	26	0
5	E	1795	0	1793	50	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	1795	0	1793	32	0
6	F	1897	0	1882	34	0
6	T	1897	0	1882	33	0
7	G	1921	0	1906	37	0
7	U	1921	0	1906	36	0
8	H	1685	0	1685	32	0
8	V	1685	0	1685	28	0
9	I	1581	0	1572	31	0
9	W	1581	0	1572	27	0
10	J	1585	0	1590	26	0
10	X	1585	0	1590	34	0
11	K	1644	0	1593	31	0
11	Y	1644	0	1593	22	0
12	L	1757	0	1709	39	0
12	Z	1757	0	1709	41	0
13	1	1824	0	1831	36	0
13	M	1824	0	1831	29	0
14	2	1512	0	1477	46	0
14	N	1512	0	1477	40	0
15	2	28	0	25	7	0
15	H	28	0	25	0	0
15	K	28	0	25	2	0
15	N	28	0	25	3	0
15	V	28	0	25	2	0
15	Y	28	0	25	3	0
16	1	63	0	0	0	0
16	2	53	0	0	3	0
16	A	49	0	0	1	0
16	B	31	0	0	1	0
16	C	32	0	0	0	0
16	D	25	0	0	0	0
16	E	14	0	0	0	0
16	F	35	0	0	1	0
16	G	46	0	0	0	0
16	H	41	0	0	1	0
16	I	52	0	0	1	0
16	J	45	0	0	2	0
16	K	33	0	0	0	0
16	L	42	0	0	3	0
16	M	53	0	0	0	0
16	N	46	0	0	1	0
16	O	24	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	23	0	0	0	0
16	Q	19	0	0	0	0
16	R	24	0	0	3	0
16	S	17	0	0	0	0
16	T	32	0	0	1	0
16	U	53	0	0	1	0
16	V	35	0	0	1	0
16	W	44	0	0	0	0
16	X	38	0	0	1	0
16	Y	30	0	0	3	0
16	Z	38	0	0	3	0
All	All	50753	0	49312	858	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (858) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:-1:GLY:C	13:M:1:THR:N	1.77	1.36
9:W:36:HIS:C	9:W:38:TYR:N	1.80	1.35
14:2:92:ASP:C	14:2:94:ASN:N	1.80	1.33
13:M:-1:GLY:C	13:M:1:THR:H2	1.34	1.30
1:O:10(A):ILE:C	1:O:103:TYR:N	1.89	1.26
9:I:36:HIS:C	9:I:38:TYR:N	1.89	1.25
1:A:10(A):ILE:C	1:A:103:TYR:N	1.89	1.25
14:N:92:ASP:C	14:N:94:ASN:N	1.90	1.25
8:H:10(A):PRO:C	8:H:106:THR:N	1.93	1.22
13:1:-1:GLY:C	13:1:1:THR:N	1.93	1.21
9:I:-1:GLY:C	9:I:1:GLY:N	2.01	1.13
4:R:20(B):ASN:C	4:R:210:ALA:N	2.02	1.13
9:W:-1:GLY:C	9:W:1:GLY:N	2.02	1.12
14:2:70:TYR:C	14:2:72:GLY:N	2.03	1.12
2:P:21(E):VAL:C	2:P:220:TYR:N	2.03	1.12
8:V:10(A):PRO:C	8:V:106:THR:N	2.03	1.11
10:J:181:ASP:C	10:J:183:GLY:N	2.05	1.10
1:O:14(A):SER:C	1:O:148:LEU:N	2.05	1.10
8:H:187:LEU:C	8:H:189:ARG:N	2.05	1.09
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.15	1.08
7:G:14(A):GLU:C	7:G:144:LEU:N	2.06	1.08
13:M:14(G):ILE:C	13:M:144:PRO:N	2.07	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:200:THR:C	2:P:202:THR:N	2.07	1.07
7:U:96:ALA:HA	7:U:107:MET:HE2	1.36	1.07
9:I:12(A):LYS:C	9:I:123:ASP:N	2.08	1.07
10:J:168:MET:CE	10:X:168:MET:HE3	1.85	1.06
1:A:20(A):THR:C	1:A:210:ILE:N	2.09	1.06
7:U:14(A):GLU:C	7:U:144:LEU:N	2.08	1.06
7:G:96:ALA:HA	7:G:107:MET:HE2	1.38	1.05
4:D:14(A):ASP:C	4:D:145:GLY:N	2.09	1.05
7:G:218:ASP:C	7:G:220:LYS:N	2.09	1.05
13:1:-1:GLY:C	13:1:1:THR:H1	1.54	1.04
4:D:20(B):ASN:C	4:D:210:ALA:N	2.11	1.03
12:L:180:LYS:C	12:L:182:ASP:N	2.13	1.03
2:B:14(A):TYR:C	2:B:145:GLY:N	2.12	1.02
4:R:14(A):ASP:C	4:R:145:GLY:N	2.13	1.02
5:E:60:SER:C	5:E:63:TYR:N	2.13	1.02
3:C:14(B):ASP:C	3:C:145:GLU:N	2.12	1.01
5:S:2(E):ASN:C	5:S:210:LEU:N	2.14	1.01
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.22	1.01
3:C:14(A):ARG:C	3:C:144:ASP:N	2.14	1.01
2:P:14(A):TYR:C	2:P:145:GLY:N	2.15	1.00
8:V:91:GLN:C	8:V:93:GLY:N	2.16	0.99
10:J:168:MET:HE3	10:X:168:MET:CE	1.92	0.99
12:L:10(B):GLY:C	12:L:107:LYS:N	2.16	0.98
9:W:10(C):SER:C	9:W:106:GLY:N	2.16	0.98
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.46	0.98
3:C:163:GLN:HE21	3:C:164:THR:H	1.07	0.98
3:Q:14(B):ASP:C	3:Q:145:GLU:N	2.16	0.98
1:O:15:PHE:H	2:P:23:GLN:HE22	1.07	0.97
1:A:14(A):SER:C	1:A:148:LEU:N	2.17	0.97
10:J:168:MET:HE3	10:X:168:MET:HE3	0.97	0.97
8:H:91:GLN:C	8:H:93:GLY:N	2.18	0.97
7:U:18(D):ILE:C	7:U:184:ASN:N	2.18	0.96
5:S:18(F):ILE:C	5:S:183:ASP:N	2.19	0.96
13:M:10(B):ASN:C	13:M:106:GLY:N	2.19	0.95
9:I:-1:GLY:C	9:I:1:GLY:H1	1.65	0.95
13:1:71(D):ALA:C	13:1:74:LEU:N	2.20	0.95
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.00	0.95
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.15	0.95
8:V:187:LEU:C	8:V:189:ARG:N	2.18	0.95
7:U:218:ASP:C	7:U:220:LYS:N	2.20	0.94
5:E:2(E):ASN:C	5:E:210:LEU:N	2.21	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:202:GLU:C	4:D:205:GLU:N	2.21	0.94
11:Y:10(B):LYS:C	11:Y:106:GLU:N	2.20	0.94
7:G:18(M):SER:C	7:G:186:TRP:N	2.21	0.94
7:U:18(M):SER:C	7:U:186:TRP:N	2.21	0.93
3:Q:70:ILE:HD11	3:Q:76:LEU:HB2	1.50	0.93
9:I:10(C):SER:C	9:I:106:GLY:N	2.21	0.93
14:N:70:TYR:C	14:N:72:GLY:N	2.22	0.93
6:F:18(F):GLY:C	6:F:184:LEU:N	2.22	0.93
13:M:-1:GLY:C	13:M:1:THR:H1	1.59	0.93
13:1:-1:GLY:C	13:1:1:THR:H2	1.70	0.93
9:I:-1:GLY:C	9:I:1:GLY:H3	1.73	0.93
9:I:179:LYS:C	9:I:181:LYS:N	2.23	0.93
13:1:14(G):ILE:C	13:1:144:PRO:N	2.23	0.92
9:W:-1:GLY:C	9:W:1:GLY:H3	1.64	0.92
14:N:181:ALA:C	14:N:183:GLY:N	2.22	0.92
9:W:12(A):LYS:C	9:W:123:ASP:N	2.24	0.91
13:M:71(D):ALA:C	13:M:74:LEU:N	2.24	0.91
9:W:179:LYS:C	9:W:181:LYS:N	2.23	0.91
4:D:233:ILE:C	4:D:235:LYS:N	2.25	0.90
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.37	0.89
5:E:18(F):ILE:C	5:E:183:ASP:N	2.25	0.89
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.35	0.89
6:T:18(F):GLY:C	6:T:184:LEU:N	2.26	0.89
12:L:-1:GLY:C	12:L:1:GLY:N	2.27	0.88
13:M:18(A):THR:C	13:M:183:GLY:N	2.26	0.88
6:F:20(C):LYS:C	6:F:207:ASP:N	2.27	0.88
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.38	0.87
10:X:3:ILE:HD13	10:X:46:ALA:HB2	1.58	0.86
13:1:10(B):ASN:C	13:1:106:GLY:N	2.29	0.85
5:S:60:SER:C	5:S:63:TYR:N	2.30	0.85
9:W:-1:GLY:C	9:W:1:GLY:H1	1.77	0.84
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.89	0.84
13:M:14(C):ARG:HH11	13:M:14(C):ARG:HG3	1.41	0.84
1:A:15:PHE:H	2:B:23:GLN:HE22	1.22	0.84
10:X:181:ASP:C	10:X:183:GLY:N	2.30	0.84
12:Z:134:ILE:HD11	12:Z:162:ALA:HB2	1.60	0.83
4:D:18(E):SER:C	4:D:184:LEU:N	2.31	0.82
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.42	0.82
2:B:124:THR:CG2	3:C:130:ARG:HH21	1.93	0.82
10:X:10(C):LYS:C	10:X:106:ASN:N	2.33	0.82
14:N:10(B):LYS:C	14:N:106:ASN:N	2.33	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:THR:C	2:B:202:THR:N	2.32	0.82
2:B:15:PHE:H	3:C:23:GLN:HE22	1.28	0.81
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.45	0.81
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.28	0.81
10:J:10(C):LYS:C	10:J:106:ASN:N	2.34	0.81
12:Z:180:LYS:C	12:Z:182:ASP:N	2.35	0.81
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.28	0.80
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.29	0.80
3:C:201:VAL:HG21	3:C:210:ILE:HD11	1.63	0.80
11:K:207:ASN:HD21	10:X:144:PRO:HG3	1.47	0.80
8:H:41:ILE:HD12	8:H:76:VAL:HG22	1.64	0.79
4:R:233:ILE:C	4:R:235:LYS:N	2.36	0.79
13:1:18(A):THR:C	13:1:183:GLY:N	2.36	0.79
14:2:10(B):LYS:C	14:2:106:ASN:N	2.36	0.79
6:F:35:THR:HG21	6:F:51:GLU:O	1.82	0.79
4:R:202:GLU:C	4:R:205:GLU:N	2.36	0.79
11:K:10(B):LYS:C	11:K:106:GLU:N	2.36	0.79
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.31	0.79
2:B:108:PRO:HB2	2:B:111:ILE:HD13	1.64	0.79
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.13	0.78
3:C:163:GLN:NE2	3:C:164:THR:H	1.81	0.78
14:2:181:ALA:C	14:2:183:GLY:N	2.37	0.78
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.97	0.78
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.67	0.77
2:P:20(B):ALA:C	2:P:205:LEU:N	2.38	0.77
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.81	0.77
10:J:133:TYR:HD1	16:Y:593:HOH:O	1.68	0.76
6:T:176:LEU:HB3	7:U:58:LEU:HD21	1.67	0.76
12:Z:10(B):GLY:C	12:Z:107:LYS:N	2.38	0.76
12:Z:-1:GLY:C	12:Z:1:GLY:N	2.39	0.76
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.50	0.75
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.34	0.75
12:Z:-1:GLY:C	12:Z:1:GLY:HA3	2.07	0.75
5:E:15:PHE:H	6:F:23:GLN:HE22	1.35	0.75
2:B:21(E):VAL:C	2:B:220:TYR:N	2.40	0.74
12:Z:14(W):LYS:C	12:Z:145:TYR:HA	2.07	0.74
14:2:126:ILE:H	14:2:126:ILE:HD13	1.53	0.74
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.52	0.74
6:F:168:GLY:HA3	6:F:201:ALA:HB1	1.69	0.74
3:C:163:GLN:HE21	3:C:164:THR:N	1.84	0.74
6:F:21(C):ASN:C	6:F:219:GLY:N	2.41	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:-1:GLY:C	12:L:1:GLY:H1	1.91	0.74
12:Z:-1:GLY:C	12:Z:1:GLY:CA	2.56	0.74
12:L:14(W):LYS:O	12:L:145:TYR:HA	1.88	0.73
1:O:20(A):THR:C	1:O:210:ILE:N	2.42	0.73
11:K:181:ASP:C	11:K:183:GLY:N	2.42	0.73
1:O:33:GLN:HA	1:O:33:GLN:HE21	1.53	0.73
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.83	0.73
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.02	0.73
5:E:139:ILE:HD11	5:E:221:PHE:HE2	1.54	0.72
1:A:218:GLY:N	16:A:1147:HOH:O	2.22	0.72
3:Q:14(A):ARG:C	3:Q:144:ASP:N	2.42	0.72
13:1:45:ILE:HG12	13:1:99:ILE:HD12	1.71	0.72
2:B:181:LYS:O	2:B:184:MET:HG3	1.88	0.72
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.71	0.72
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.54	0.72
3:C:85:SER:O	3:C:89:ILE:HD13	1.89	0.71
11:K:207:ASN:ND2	10:X:144:PRO:HG3	2.04	0.71
14:N:161:GLN:NE2	14:2:136:GLY:HA2	1.99	0.71
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.72	0.71
8:H:15:ALA:HB3	8:H:159:ILE:HD11	1.72	0.71
6:T:35:THR:HG21	6:T:51:GLU:O	1.90	0.71
11:Y:1:THR:HG1	15:Y:1403:BO2:C21	2.04	0.70
14:2:52:THR:OG1	16:2:316:HOH:O	2.09	0.70
11:Y:99:THR:HG22	11:Y:113:VAL:HB	1.73	0.70
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.06	0.70
12:Z:179:THR:HG1	12:Z:182:ASP:N	1.89	0.70
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.37	0.69
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.38	0.69
4:R:121:LEU:HB2	16:R:853:HOH:O	1.93	0.69
3:Q:76:LEU:HD22	3:Q:89:ILE:HD11	1.75	0.69
14:N:126:ILE:HD13	14:N:126:ILE:H	1.58	0.69
15:2:1405:BO2:H241	16:2:316:HOH:O	1.92	0.68
5:E:221:PHE:HE1	5:E:223:ILE:HD11	1.59	0.68
3:C:15:PHE:H	4:D:23:GLN:HE22	1.39	0.68
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.38	0.68
11:K:37:ILE:HB	11:K:41:LEU:HB3	1.75	0.68
4:R:18(E):SER:C	4:R:184:LEU:N	2.47	0.68
8:V:52:THR:O	8:V:56:THR:HB	1.93	0.68
9:W:6:MET:HG3	9:W:155:ILE:HD13	1.74	0.68
1:O:218:GLY:N	16:O:1029:HOH:O	2.28	0.67
7:G:18(D):ILE:C	7:G:184:ASN:N	2.48	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:32:ASP:OD2	10:X:34:THR:HG22	1.95	0.67
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.75	0.67
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.77	0.67
6:F:192:GLN:O	6:F:196:ILE:HG12	1.95	0.67
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.76	0.67
14:2:105:ASP:OD2	14:2:106:ASN:N	2.29	0.66
12:Z:3:ILE:HD12	12:Z:46:ASN:HB2	1.78	0.66
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.26	0.66
12:L:134:ILE:HD11	12:L:162:ALA:HB2	1.76	0.66
3:C:57:LYS:O	3:C:58:LEU:HB2	1.95	0.66
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.77	0.66
2:B:215:ILE:HD12	2:B:221:GLN:HG2	1.78	0.66
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.43	0.65
7:U:121:GLN:O	7:U:124:THR:HB	1.96	0.65
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.77	0.65
14:N:105:ASP:OD2	14:N:106:ASN:N	2.30	0.65
5:S:207:LEU:HD23	5:S:207:LEU:H	1.62	0.65
1:O:177:GLU:HG2	2:P:58:LEU:HD21	1.79	0.65
10:J:32:ASP:OD2	10:J:34:THR:HG22	1.96	0.65
11:Y:181:ASP:C	11:Y:183:GLY:N	2.50	0.65
3:C:18(D):GLU:C	3:C:182:PRO:N	2.51	0.65
8:H:52:THR:O	8:H:56:THR:HB	1.97	0.65
2:P:121:GLN:O	2:P:124:THR:HB	1.96	0.65
12:Z:-1:GLY:O	12:Z:1:GLY:HA3	1.97	0.65
2:P:6:ARG:HB2	5:S:127:TYR:OH	1.97	0.64
6:T:21(C):ASN:C	6:T:219:GLY:N	2.51	0.64
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.78	0.64
6:F:199:LEU:C	6:F:201:ALA:N	2.51	0.64
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.80	0.64
5:S:12:THR:HG21	5:S:124:THR:HA	1.80	0.64
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.44	0.64
5:E:12:THR:HG21	5:E:124:THR:HA	1.80	0.64
14:N:181:ALA:C	14:N:183:GLY:CA	2.66	0.64
6:T:192:GLN:O	6:T:196:ILE:HG12	1.97	0.64
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.95	0.64
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.63	0.64
6:T:49:ALA:HB1	6:T:197:ILE:CD1	2.27	0.64
1:O:112:LEU:O	1:O:116:VAL:HG23	1.98	0.63
7:U:96:ALA:HA	7:U:107:MET:CE	2.22	0.63
13:1:14(D):GLU:O	13:1:14(G):ILE:HG12	1.98	0.63
10:J:181:ASP:C	10:J:183:GLY:CA	2.66	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.45	0.63
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.26	0.63
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.81	0.63
10:J:24:ILE:O	10:X:133:TYR:OH	2.17	0.63
6:T:49:ALA:HB3	6:T:197:ILE:HD11	1.78	0.63
6:T:49:ALA:CB	6:T:197:ILE:HD11	2.29	0.63
12:Z:114:ASP:HB2	12:Z:118:SER:HB3	1.81	0.63
5:E:123:ASN:N	5:E:123:ASN:HD22	1.96	0.63
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.80	0.63
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.32	0.63
16:L:200:HOH:O	9:W:192:ARG:HG3	1.99	0.63
5:E:28:LEU:HA	5:E:31:ILE:HD13	1.80	0.63
5:S:15:PHE:H	6:T:23:GLN:HE22	1.46	0.62
14:2:3:ILE:HD12	14:2:46:SER:HB3	1.81	0.62
9:W:36:HIS:CA	9:W:38:TYR:N	2.61	0.62
10:X:181:ASP:C	10:X:183:GLY:CA	2.68	0.62
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.05	0.62
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.92	0.62
6:T:199:LEU:C	6:T:201:ALA:N	2.52	0.62
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.79	0.62
12:L:14(W):LYS:C	12:L:145:TYR:HA	2.20	0.62
1:A:200:SER:C	1:A:202:VAL:N	2.53	0.62
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.82	0.62
9:I:7:THR:CG2	9:I:110:ILE:HD12	2.29	0.62
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.29	0.62
2:B:6:ARG:HB2	5:E:127:TYR:OH	2.00	0.62
2:P:69:LYS:HG3	2:P:221:GLN:OE1	2.00	0.62
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.90	0.62
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.46	0.61
4:D:192:LEU:O	4:D:196:ILE:HD13	1.99	0.61
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.81	0.61
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.46	0.61
13:M:40:ASN:H	13:M:40:ASN:HD22	1.47	0.61
1:A:33:GLN:HE21	1:A:33:GLN:HA	1.64	0.61
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.47	0.61
12:L:-1:GLY:C	12:L:1:GLY:CA	2.69	0.61
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.82	0.61
11:K:99:THR:HG22	11:K:113:VAL:HB	1.83	0.61
1:A:121:GLN:O	1:A:124:THR:HB	1.99	0.61
2:B:202:THR:HG22	2:B:204:SER:H	1.65	0.61
14:N:1:THR:HG1	15:N:1404:BO2:C21	2.13	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.82	0.61
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.64	0.60
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.82	0.60
7:G:96:ALA:HA	7:G:107:MET:CE	2.25	0.60
5:E:132:TYR:O	5:E:153:PRO:HB3	2.01	0.60
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.82	0.60
10:J:144:PRO:HG3	11:Y:207:ASN:ND2	2.16	0.60
2:P:160:TRP:CE2	2:P:163:ILE:HD12	2.36	0.60
14:N:13:ILE:CD1	14:N:177:VAL:HG13	2.32	0.60
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.83	0.59
3:C:41:LYS:HG2	3:C:161:SER:O	2.01	0.59
5:E:204:GLU:C	5:E:206:SER:N	2.55	0.59
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.15	0.59
6:F:127:ASN:HD22	6:F:127:ASN:C	2.06	0.59
1:O:121:GLN:O	1:O:124:THR:HB	2.02	0.59
1:A:112:LEU:O	1:A:116:VAL:HG23	2.02	0.59
5:E:139:ILE:HD11	5:E:221:PHE:CE2	2.36	0.59
8:H:114:HIS:CE1	15:N:1404:BO2:H5	2.38	0.59
10:X:181:ASP:C	10:X:183:GLY:HA3	2.22	0.59
10:X:-1:MET:HG2	10:X:1:ASP:N	2.17	0.59
12:L:4:LEU:HD13	12:L:138:LEU:HD21	1.83	0.59
6:T:49:ALA:HB1	6:T:197:ILE:HD13	1.83	0.59
2:B:160:TRP:CE2	2:B:163:ILE:HD12	2.38	0.59
6:F:35:THR:CG2	6:F:51:GLU:O	2.50	0.59
1:O:177:GLU:HG2	2:P:58:LEU:CD2	2.33	0.59
9:I:110:ILE:HD11	9:I:122:ALA:O	2.03	0.58
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.84	0.58
6:T:49:ALA:CB	6:T:197:ILE:CD1	2.81	0.58
13:1:40:ASN:HD22	13:1:40:ASN:H	1.49	0.58
14:N:159:LEU:O	14:N:163:ILE:HD13	2.02	0.58
8:H:6:VAL:O	8:H:13:VAL:HG12	2.03	0.58
4:R:85:ALA:O	4:R:89:ILE:HG12	2.04	0.58
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.38	0.58
8:H:15:ALA:CB	8:H:159:ILE:HD11	2.34	0.58
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.85	0.58
10:X:-1:MET:HG2	10:X:1:ASP:H2	1.68	0.58
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.85	0.58
9:I:33:LYS:O	9:I:44:GLY:HA2	2.04	0.58
12:L:166:HIS:HD2	12:L:168:GLN:H	1.51	0.57
3:C:35:THR:HB	3:C:51:GLU:HG3	1.85	0.57
2:P:202:THR:HG22	2:P:204:SER:H	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.84	0.57
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.86	0.57
14:2:20:THR:HG22	15:2:1405:BO2:H252	1.87	0.57
5:E:60:SER:C	5:E:63:TYR:CA	2.72	0.57
8:H:15:ALA:HB3	8:H:159:ILE:CD1	2.34	0.57
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG12	1.86	0.57
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.34	0.57
11:K:7:ARG:HD2	11:K:108:PRO:O	2.05	0.57
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.70	0.57
14:N:10(B):LYS:HD3	14:N:10(B):LYS:C	2.25	0.57
5:E:210:LEU:HB3	5:E:229:VAL:HG21	1.86	0.56
11:K:7:ARG:HG3	11:K:12:ILE:HD13	1.87	0.56
14:N:181:ALA:C	14:N:183:GLY:HA3	2.26	0.56
3:Q:197:LEU:HD13	3:Q:210:ILE:HD12	1.87	0.56
13:1:14(C):ARG:CG	13:1:14(C):ARG:HH11	2.13	0.56
13:M:165:ARG:O	14:2:26:ILE:HG12	2.05	0.56
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.86	0.56
1:O:45:GLY:HA3	1:O:186:LEU:HD13	1.88	0.56
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	1.87	0.56
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.05	0.56
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.21	0.56
4:D:38:ILE:HD12	4:D:197:LEU:HG	1.87	0.56
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.71	0.56
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.87	0.56
2:B:121:GLN:O	2:B:124:THR:HB	2.06	0.56
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.87	0.56
13:1:7:LYS:HG3	13:1:14(G):ILE:HD12	1.88	0.55
14:2:126:ILE:N	14:2:126:ILE:HD13	2.20	0.55
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.54	0.55
2:B:90:ASN:O	2:B:94:ILE:HD13	2.07	0.55
7:G:121:GLN:O	7:G:124:THR:HB	2.06	0.55
13:M:14(C):ARG:CG	13:M:14(C):ARG:HH11	2.16	0.55
8:H:15:ALA:CB	8:H:159:ILE:CD1	2.84	0.55
3:Q:85:SER:O	3:Q:89:ILE:HD13	2.05	0.55
4:R:38:ILE:HD12	4:R:197:LEU:HG	1.87	0.55
5:E:31:ILE:HD11	5:E:153:PRO:HG2	1.89	0.55
9:I:110:ILE:HD13	9:I:110:ILE:H	1.71	0.55
1:A:21(P):LYS:C	1:A:218:GLY:N	2.59	0.55
5:E:47:VAL:HG23	5:E:189:LEU:HD13	1.88	0.55
6:T:20(C):LYS:C	6:T:207:ASP:N	2.60	0.55
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.17	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:71:THR:OG1	1:O:74:ILE:HD12	2.07	0.55
13:M:-1:GLY:C	13:M:1:THR:CA	2.69	0.55
14:N:156:LYS:HG2	14:N:18(J):LEU:HD11	1.87	0.55
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.42	0.55
5:E:48:LEU:HG	5:E:139:ILE:HD12	1.89	0.55
6:F:38:ILE:HG12	6:F:197:ILE:HD11	1.87	0.55
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.89	0.54
10:J:133:TYR:HE1	16:X:876:HOH:O	1.90	0.54
5:E:97:ASN:ND2	12:L:61:ASN:HD21	2.04	0.54
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.37	0.54
2:B:190:ILE:CG2	2:B:232:ILE:HD11	2.37	0.54
8:H:91:GLN:C	8:H:93:GLY:CA	2.74	0.54
12:L:98:HIS:HD2	16:L:199:HOH:O	1.89	0.54
1:O:150:GLN:O	1:O:157:TYR:HA	2.07	0.54
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.89	0.54
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.89	0.54
11:K:39:PRO:O	11:K:183:GLY:HA2	2.06	0.54
2:B:163:ILE:HG12	2:B:164:SER:N	2.21	0.54
3:C:175:PHE:O	3:C:179:ASN:HB2	2.08	0.54
2:B:107:ILE:HD11	2:B:111:ILE:HG22	1.90	0.54
2:P:159:GLY:HA3	3:Q:62(A):ILE:HD12	1.89	0.54
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.88	0.54
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.90	0.54
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.89	0.54
8:H:35:HIS:CB	8:H:56:THR:HG21	2.37	0.54
7:U:18(A):ILE:HD13	7:U:18(C):HIS:O	2.07	0.54
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.43	0.54
1:O:21(P):LYS:C	1:O:218:GLY:N	2.61	0.54
1:O:33:GLN:CA	1:O:33:GLN:HE21	2.19	0.54
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.43	0.54
1:O:14(A):SER:CA	1:O:148:LEU:N	2.70	0.54
2:P:40:ILE:HD11	2:P:176:LEU:HD22	1.89	0.53
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.44	0.53
5:E:18(E):LYS:O	5:E:183:ASP:N	2.42	0.53
2:B:190:ILE:HG21	2:B:232:ILE:HD11	1.91	0.53
3:Q:52:ARG:HH21	3:Q:211:GLU:HB3	1.74	0.53
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.19	0.53
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.89	0.53
11:K:6:PHE:HA	11:K:123:ASP:O	2.09	0.53
14:N:9:LYS:O	14:N:107:LYS:HD3	2.08	0.53
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.06	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.07	0.53
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.91	0.53
6:T:176:LEU:HB3	7:U:58:LEU:CD2	2.38	0.53
8:V:197:ARG:HH21	9:W:139:GLU:HG3	1.74	0.53
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.90	0.52
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.06	0.52
13:1:13:ILE:HD13	13:1:177:ILE:HG23	1.90	0.52
14:N:14:LEU:O	14:N:175:MET:HA	2.09	0.52
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.91	0.52
13:1:157:ASN:ND2	13:1:160:ARG:HH11	2.04	0.52
14:2:3:ILE:CD1	14:2:46:SER:HB3	2.39	0.52
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.91	0.52
2:P:163:ILE:HG12	2:P:164:SER:N	2.24	0.52
13:M:40:ASN:HD22	13:M:40:ASN:N	2.07	0.52
2:P:142:ASP:O	2:P:145:GLY:N	2.43	0.52
10:X:181:ASP:O	10:X:183:GLY:HA3	2.10	0.52
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.75	0.52
13:1:4:ILE:HD11	13:1:155:ILE:HG23	1.92	0.52
2:B:215:ILE:CD1	2:B:221:GLN:HG2	2.39	0.52
9:I:123:ASP:OD1	9:I:123:ASP:N	2.42	0.52
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.92	0.52
7:U:87:ASN:HD22	7:U:87:ASN:C	2.13	0.52
9:W:-2:ASN:HA	9:W:21:GLY:O	2.10	0.52
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.92	0.52
1:O:173:LYS:O	1:O:177:GLU:HG3	2.10	0.52
11:Y:39:PRO:O	11:Y:183:GLY:HA2	2.10	0.52
10:J:133:TYR:CD1	16:Y:593:HOH:O	2.53	0.52
14:N:134:ILE:CD1	14:N:162:ALA:HB2	2.40	0.52
5:S:73:HIS:HE1	5:S:107:LEU:O	1.91	0.52
8:V:159:ILE:HG22	8:V:163:ILE:CD1	2.39	0.52
5:S:123:ASN:N	5:S:123:ASN:HD22	2.08	0.51
7:U:96:ALA:CA	7:U:107:MET:HE2	2.25	0.51
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.92	0.51
2:P:141:TYR:CE2	2:P:145:GLY:HA2	2.45	0.51
10:X:10(B):LYS:NZ	10:X:10(B):LYS:HB2	2.25	0.51
13:1:-1:GLY:C	13:1:1:THR:CA	2.76	0.51
2:B:163:ILE:HG12	2:B:164:SER:H	1.76	0.51
6:F:127:ASN:HD22	6:F:128:SER:N	2.07	0.51
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.58	0.51
14:2:20:THR:CG2	15:2:1405:BO2:H252	2.40	0.51
3:C:152:GLU:HB2	3:C:153:PRO:HD2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:110:ILE:HG12	9:I:125:ILE:HD13	1.93	0.51
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.58	0.51
8:V:114:HIS:CE1	15:2:1405:BO2:H5	2.46	0.51
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.93	0.51
8:V:148:LYS:O	8:V:152:ILE:HG12	2.10	0.51
8:V:84:LYS:HG3	8:V:85:GLN:N	2.26	0.51
2:B:61:GLN:OE1	2:B:208:ASP:HA	2.11	0.51
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.26	0.51
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.76	0.51
7:U:40:VAL:HB	7:U:18(D):ILE:HD13	1.93	0.51
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	2.09	0.51
13:1:14(C):ARG:HG3	13:1:14(C):ARG:NH1	2.17	0.51
12:L:148:VAL:O	12:L:152:ILE:HG12	2.11	0.51
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.47	0.50
4:R:179:GLU:HB3	4:R:192:LEU:HD21	1.91	0.50
2:P:85:ALA:O	2:P:89:ILE:HG12	2.10	0.50
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.93	0.50
7:G:49:ILE:HG13	7:G:212:VAL:HG22	1.93	0.50
4:R:67:ILE:HD12	4:R:211:GLN:HE21	1.75	0.50
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.93	0.50
5:S:227:GLU:CD	5:S:227:GLU:H	2.15	0.50
8:V:91:GLN:O	8:V:93:GLY:HA3	2.11	0.50
9:W:33:LYS:O	9:W:44:GLY:HA2	2.11	0.50
7:U:109:CYS:HB3	16:U:1330:HOH:O	2.11	0.50
2:B:27:ALA:O	2:B:31:ILE:HG12	2.12	0.50
12:L:-1:GLY:C	12:L:1:GLY:H3	2.11	0.50
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.75	0.50
4:R:52:LYS:HB2	4:R:20(B):ASN:C	2.32	0.50
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.58	0.50
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.39	0.50
12:L:-1:GLY:C	12:L:1:GLY:HA3	2.33	0.50
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.76	0.50
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.42	0.50
3:C:201:VAL:HG21	3:C:210:ILE:CD1	2.39	0.49
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.93	0.49
2:P:181:LYS:O	2:P:184:MET:HG3	2.12	0.49
6:T:203:GLU:O	6:T:206:LYS:HD2	2.11	0.49
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.42	0.49
6:F:69:VAL:HG12	16:F:319:HOH:O	2.12	0.49
12:L:9:GLU:O	12:L:107:LYS:HA	2.11	0.49
3:Q:70:ILE:HD13	3:Q:112:LEU:HD11	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:13:ILE:HD12	14:N:177:VAL:HG22	1.94	0.49
3:Q:18(D):GLU:C	3:Q:182:PRO:N	2.66	0.49
3:C:197:LEU:HD13	3:C:210:ILE:HD12	1.94	0.49
5:E:73:HIS:HE1	5:E:107:LEU:O	1.95	0.49
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.93	0.49
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.26	0.49
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.76	0.49
10:J:143:ARG:HB2	10:J:146:MET:HG3	1.94	0.49
3:C:57:LYS:HD2	3:C:58:LEU:N	2.28	0.49
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.26	0.49
14:N:17:ASP:HB3	14:N:163:ILE:HD11	1.94	0.49
5:S:45:HIS:CD2	5:S:214:ILE:HD11	2.46	0.49
9:W:-1:GLY:C	9:W:1:GLY:CA	2.80	0.49
5:E:67:ILE:HD13	5:E:77:SER:HB3	1.94	0.49
6:F:54:ILE:HD11	6:F:209:GLU:HB2	1.94	0.49
4:D:85:ALA:O	4:D:89:ILE:HG12	2.12	0.49
13:M:7:LYS:HB3	13:M:12:VAL:HG12	1.95	0.49
2:P:173:GLN:HG2	3:Q:56:LEU:HD12	1.95	0.49
11:Y:33:LYS:HE2	15:Y:1403:BO2:H221	1.95	0.49
8:H:84:LYS:HG3	8:H:85:GLN:N	2.27	0.49
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.60	0.49
11:Y:179:THR:O	11:Y:183:GLY:N	2.45	0.49
14:2:20:THR:HG22	15:2:1405:BO2:H221	1.95	0.49
14:2:70:TYR:C	14:2:72:GLY:CA	2.81	0.49
1:A:67:VAL:HG11	1:A:213:ALA:HB3	1.94	0.49
14:N:70:TYR:C	14:N:72:GLY:CA	2.81	0.48
8:V:91:GLN:C	8:V:93:GLY:CA	2.80	0.48
9:W:113:PHE:HA	9:W:118:CYS:O	2.13	0.48
12:Z:-1:GLY:C	12:Z:1:GLY:H3	2.13	0.48
7:G:225:SER:O	7:G:229:ILE:HG12	2.14	0.48
10:J:168:MET:CE	10:X:168:MET:CE	2.69	0.48
3:Q:169:SER:HA	3:Q:172:VAL:HG13	1.95	0.48
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.95	0.48
11:Y:1:THR:OG1	15:Y:1403:BO2:C21	2.60	0.48
1:A:10(A):ILE:C	1:A:103:TYR:CA	2.77	0.48
5:E:160:LEU:HD13	5:E:163:THR:HB	1.95	0.48
8:H:91:GLN:O	8:H:93:GLY:HA3	2.13	0.48
9:I:36:HIS:CA	9:I:38:TYR:N	2.71	0.48
8:V:34:LEU:HB2	16:V:578:HOH:O	2.12	0.48
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.48	0.48
5:E:97:ASN:HD21	12:L:61:ASN:ND2	2.05	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:1(I):ASN:C	12:Z:14(J):GLY:N	2.67	0.48
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.42	0.48
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.96	0.48
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.78	0.48
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.27	0.48
7:G:60:ASP:OD2	7:G:62:THR:OG1	2.32	0.48
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.43	0.48
9:I:-1:GLY:C	9:I:1:GLY:CA	2.82	0.48
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.95	0.48
13:M:14(C):ARG:NH1	13:M:14(C):ARG:HG3	2.21	0.48
11:K:200:LYS:NZ	11:K:209:VAL:O	2.42	0.48
7:U:139:VAL:HG12	7:U:148:ILE:HG13	1.96	0.48
7:G:9:ASP:HA	7:G:14:ILE:HD11	1.96	0.48
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.49	0.48
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.96	0.48
5:S:198:SER:HA	5:S:201:LEU:HG	1.96	0.48
14:2:19:ARG:HG3	14:2:26:ILE:HG23	1.96	0.47
3:C:76:LEU:HD22	3:C:89:ILE:HD11	1.96	0.47
2:P:14(A):TYR:C	2:P:145:GLY:CA	2.83	0.47
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.94	0.47
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.96	0.47
2:P:45:GLY:HA2	2:P:146:TYR:CE1	2.49	0.47
7:U:49:ILE:HG13	7:U:212:VAL:HG22	1.96	0.47
14:2:4:MET:HB3	14:2:126:ILE:HG22	1.96	0.47
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.96	0.47
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.96	0.47
14:2:15:GLY:HA2	14:2:174:ARG:O	2.15	0.47
9:I:110:ILE:HG12	9:I:125:ILE:CD1	2.44	0.47
11:K:35:ILE:HD12	11:K:56:GLU:HB2	1.96	0.47
9:W:12:VAL:HG13	9:W:108:PRO:HB3	1.96	0.47
10:X:113:ILE:HA	10:X:118:THR:O	2.15	0.47
12:Z:114:ASP:OD2	12:Z:115:PRO:HD2	2.13	0.47
8:H:187:LEU:O	8:H:189:ARG:N	2.45	0.47
12:L:59:PHE:CD1	12:L:83:ILE:HD11	2.50	0.47
11:Y:104:TYR:CE2	11:Y:108:PRO:HG3	2.49	0.47
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.23	0.47
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.49	0.47
2:B:14(A):TYR:C	2:B:145:GLY:CA	2.83	0.47
7:G:158:VAL:HG22	7:G:159:GLY:N	2.30	0.47
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.49	0.47
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:172:VAL:HG21	14:2:18(A):ILE:HD11	1.97	0.47
1:A:117:ALA:HB1	1:A:155:GLY:O	2.15	0.47
3:C:53:ARG:HD2	3:C:55:THR:OG1	2.15	0.47
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.96	0.47
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.50	0.47
14:N:161:GLN:HE22	14:2:139:ASP:HB3	1.79	0.47
11:Y:66:HIS:HA	16:Y:1210:HOH:O	2.13	0.47
12:Z:14(W):LYS:O	12:Z:145:TYR:HA	2.14	0.47
13:1:40:ASN:HD22	13:1:40:ASN:N	2.11	0.47
5:E:226:GLY:O	5:E:229:VAL:HG22	2.15	0.47
6:T:54:ILE:HD11	6:T:209:GLU:HB2	1.97	0.47
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.50	0.46
2:B:191:GLU:O	2:B:195:LYS:HG2	2.14	0.46
8:V:30:ASN:O	8:V:189:ARG:NH2	2.46	0.46
1:A:150:GLN:O	1:A:157:TYR:HA	2.15	0.46
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.98	0.46
9:I:105:ASN:O	9:I:106:GLY:N	2.49	0.46
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.12	0.46
10:J:113:ILE:HA	10:J:118:THR:O	2.16	0.46
11:K:35:ILE:HD11	11:K:45:MET:SD	2.56	0.46
8:V:128:GLY:O	8:V:131:SER:HB2	2.15	0.46
8:H:165:ASN:ND2	13:1:139:ARG:HH11	2.12	0.46
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.98	0.46
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.16	0.46
5:S:134:VAL:O	5:S:153:PRO:HG3	2.15	0.46
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.96	0.46
13:1:14(A):VAL:O	13:1:14(A):VAL:HG23	2.15	0.46
11:K:200:LYS:HG3	11:K:205:SER:O	2.16	0.46
5:S:207:LEU:H	5:S:207:LEU:CD2	2.27	0.46
13:1:179:ASP:O	13:1:183:GLY:N	2.48	0.46
11:K:7:ARG:HG3	11:K:12:ILE:CD1	2.45	0.46
11:K:179:THR:O	11:K:183:GLY:N	2.48	0.46
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:H	1.80	0.46
10:J:35:ARG:NH2	16:J:875:HOH:O	2.49	0.46
3:Q:152:GLU:HB2	3:Q:153:PRO:HD2	1.98	0.46
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.51	0.46
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.97	0.46
10:X:162:LEU:O	10:X:166:MET:HB2	2.15	0.46
6:F:199:LEU:HD12	6:F:240:ILE:HD12	1.98	0.46
5:S:45:HIS:HD2	5:S:214:ILE:HD11	1.81	0.46
6:T:127:ASN:HD22	6:T:127:ASN:C	2.19	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:95:GLU:HG2	6:T:115:ARG:CB	2.31	0.46
2:B:150:THR:O	2:B:157:TYR:HA	2.16	0.45
10:J:133:TYR:CZ	10:J:166:MET:HG2	2.52	0.45
1:O:52:LYS:HB2	1:O:20(A):THR:C	2.37	0.45
8:V:34:LEU:HD22	8:V:174:ASP:HB3	1.99	0.45
7:G:96:ALA:CA	7:G:107:MET:HE2	2.27	0.45
8:H:15:ALA:HB1	8:H:159:ILE:HD13	1.98	0.45
10:J:181:ASP:C	10:J:183:GLY:HA3	2.36	0.45
1:O:110:LYS:HG2	16:O:376:HOH:O	2.15	0.45
4:R:86:ARG:HD3	4:R:86:ARG:HA	1.88	0.45
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.31	0.45
2:B:149:TYR:CZ	3:C:62(A):ILE:HD12	2.52	0.45
5:E:15:PHE:H	6:F:23:GLN:NE2	2.10	0.45
11:K:4:LEU:HD13	11:K:159:ILE:HD11	1.97	0.45
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.43	0.45
13:M:42:VAL:HG23	13:M:178:ILE:HD11	1.97	0.45
5:S:60:SER:C	5:S:63:TYR:CA	2.85	0.45
7:U:87:ASN:ND2	7:U:87:ASN:C	2.69	0.45
12:Z:40:ASN:ND2	16:Z:799:HOH:O	2.37	0.45
11:K:1:THR:OG1	15:K:1402:BO2:C21	2.65	0.45
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.99	0.45
3:Q:71:ASP:HA	10:X:68:ILE:HD13	1.99	0.45
11:Y:83:LEU:HD23	11:Y:101:ILE:HD11	1.99	0.45
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.32	0.45
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.81	0.45
12:Z:99:THR:CG2	16:Z:231:HOH:O	2.64	0.45
4:D:81:LEU:O	4:D:84:ASP:HB2	2.17	0.45
7:G:59:LEU:O	7:G:61:PRO:HD3	2.17	0.45
9:I:-2:ASN:HA	9:I:21:GLY:O	2.17	0.45
9:W:55:LEU:HD11	9:W:97:VAL:HG21	1.97	0.45
7:U:18(A):ILE:CD1	7:U:18(C):HIS:O	2.65	0.45
1:A:188:ASP:O	1:A:192:ILE:HG12	2.16	0.45
7:G:186:TRP:O	7:G:190:VAL:HG23	2.17	0.45
8:V:35:HIS:CB	8:V:56:THR:HG21	2.46	0.45
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.98	0.45
2:B:142:ASP:O	2:B:145:GLY:N	2.50	0.45
11:K:1:THR:HG1	15:K:1402:BO2:C21	2.30	0.45
14:N:134:ILE:HD12	14:N:162:ALA:HB2	1.98	0.45
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.99	0.45
2:P:101:LYS:HZ1	10:X:85:GLN:NE2	2.15	0.45
14:2:46:SER:HA	15:2:1405:BO2:H243	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:134:VAL:O	5:E:153:PRO:HG3	2.17	0.45
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.99	0.45
8:H:105:ASP:OD2	8:H:106:THR:N	2.50	0.44
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.99	0.44
12:Z:145:TYR:CG	12:Z:146:LEU:N	2.84	0.44
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.52	0.44
12:L:34:VAL:HG12	12:L:176:LEU:HD22	1.99	0.44
10:X:120:VAL:HG13	10:X:122:LEU:HG	1.99	0.44
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.99	0.44
10:X:98:ASN:HB3	10:X:127:HIS:CD2	2.52	0.44
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.99	0.44
2:B:38:ILE:HD13	2:B:164:SER:HB3	1.99	0.44
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.98	0.44
8:H:172:ASN:HD22	8:H:193:THR:HA	1.81	0.44
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	2.30	0.44
14:N:1:THR:OG1	14:N:33:LYS:NZ	2.44	0.44
7:U:168:LYS:HD2	7:U:201:LEU:HD22	1.99	0.44
14:N:133:PHE:HA	14:2:132:THR:O	2.18	0.44
10:J:181:ASP:O	10:J:183:GLY:HA3	2.17	0.44
2:P:163:ILE:HG12	2:P:164:SER:H	1.81	0.44
6:T:127:ASN:HD22	6:T:128:SER:N	2.15	0.44
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.99	0.44
14:2:55:ILE:O	14:2:59:VAL:HG23	2.18	0.44
11:K:13:ILE:HG13	11:K:151:ALA:HB1	1.98	0.44
6:T:196:ILE:O	6:T:201:ALA:N	2.50	0.44
9:W:110:ILE:HD12	9:W:125:ILE:HG12	1.98	0.44
12:Z:80:ALA:HA	12:Z:113:PHE:HZ	1.81	0.44
13:M:165:ARG:C	14:2:26:ILE:HG12	2.37	0.44
6:F:67:ILE:HB	6:F:223:PHE:CE2	2.53	0.44
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.48	0.44
5:S:139:ILE:HD12	5:S:215:VAL:HG12	1.99	0.44
14:2:175:MET:HB2	14:2:187:LEU:HB2	2.00	0.44
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.99	0.44
6:F:109:ILE:HD12	6:F:109:ILE:N	2.33	0.44
6:F:158:TRP:CZ3	7:G:64:VAL:HA	2.53	0.44
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.81	0.44
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.99	0.44
13:1:7:LYS:HB3	13:1:12:VAL:HG12	2.00	0.44
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.83	0.44
12:Z:99:THR:HG23	16:Z:231:HOH:O	2.18	0.44
2:B:146:TYR:OH	2:B:21(A):LYS:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.53	0.44
4:R:46:VAL:HG23	4:R:146:TYR:HB3	1.99	0.44
4:R:72:ARG:HG3	16:R:1302:HOH:O	2.18	0.44
5:S:230:ALA:HA	5:S:233:ILE:HD12	1.99	0.44
11:K:192:VAL:HG11	9:W:194:ASP:HB3	2.00	0.44
11:Y:44:THR:OG1	11:Y:100:MET:HB2	2.18	0.44
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.99	0.43
13:M:14(D):GLU:O	13:M:14(G):ILE:HG12	2.18	0.43
7:U:34:THR:HB	7:U:35:ILE:HD12	2.00	0.43
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	2.00	0.43
11:K:99:THR:HG22	11:K:113:VAL:O	2.17	0.43
14:N:91:LYS:HE2	14:N:116:GLY:O	2.19	0.43
8:H:90:TYR:O	8:H:91:GLN:C	2.56	0.43
9:I:87:LEU:HD11	9:I:99:PRO:HG2	2.00	0.43
13:M:14(C):ARG:CG	13:M:14(C):ARG:NH1	2.80	0.43
9:I:7:THR:HG23	9:I:110:ILE:HD12	2.00	0.43
9:I:110:ILE:CD1	9:I:122:ALA:O	2.65	0.43
6:T:18:ASP:N	6:T:18:ASP:OD2	2.39	0.43
14:2:14:LEU:O	14:2:175:MET:HA	2.17	0.43
8:H:197:ARG:NH2	9:I:139:GLU:O	2.51	0.43
7:U:107:MET:HE1	7:U:112:LEU:HD13	2.00	0.43
14:2:45:ARG:NH1	16:2:316:HOH:O	2.51	0.43
12:L:1(I):ASN:C	12:L:14(J):GLY:N	2.72	0.43
8:V:1:THR:HG1	15:V:1401:BO2:C21	2.32	0.43
4:D:162:ALA:HB3	5:E:58:LEU:HD23	2.00	0.43
6:F:18(F):GLY:O	6:F:184:LEU:N	2.48	0.43
5:S:180:LEU:HA	5:S:18(C):PHE:CE2	2.54	0.43
7:U:38:LEU:HD23	7:U:197:MET:HE3	2.00	0.43
5:S:103:PHE:O	13:1:78:TYR:HA	2.18	0.43
1:O:200:SER:C	1:O:202:VAL:N	2.72	0.43
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.54	0.43
5:E:221:PHE:CE1	5:E:223:ILE:HD11	2.46	0.43
6:F:67:ILE:HB	6:F:223:PHE:HE2	1.84	0.43
1:O:15:PHE:N	2:P:23:GLN:HE22	1.91	0.43
5:S:160:LEU:HD13	5:S:163:THR:HB	2.01	0.43
4:D:13:SER:HB2	5:E:130:ARG:HD3	2.01	0.43
4:D:159:ARG:HB3	5:E:60:SER:HB3	2.00	0.43
6:F:38:ILE:HD12	6:F:40:ILE:HD11	2.01	0.43
3:Q:168:ASN:O	3:Q:172:VAL:HG12	2.19	0.43
13:1:14(C):ARG:CG	13:1:14(C):ARG:NH1	2.79	0.42
3:C:185:THR:HG22	3:C:187:GLU:H	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:213:SER:HB2	4:D:222:LYS:O	2.19	0.42
1:A:14(A):SER:CA	1:A:148:LEU:N	2.82	0.42
2:B:199:LYS:HE2	2:B:199:LYS:HB3	1.84	0.42
5:E:123:ASN:N	5:E:123:ASN:ND2	2.66	0.42
5:E:185:ASN:HA	5:E:186:PRO:HD2	1.94	0.42
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.53	0.42
7:U:143:GLU:HA	7:U:217:LYS:NZ	2.34	0.42
14:2:65:LEU:HG	14:2:69:GLN:HE21	1.84	0.42
9:I:25:LEU:HD11	10:J:135:PHE:HD2	1.84	0.42
11:K:44:THR:OG1	11:K:100:MET:HB2	2.19	0.42
14:N:13:ILE:HD12	14:N:177:VAL:HG13	2.01	0.42
3:Q:160:TRP:CZ2	4:R:59:LEU:HD23	2.53	0.42
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.84	0.42
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.15	0.42
2:P:87:ILE:O	2:P:91:THR:HG23	2.19	0.42
8:V:3:ILE:HG22	8:V:16:ALA:HB2	2.02	0.42
12:Z:3:ILE:HD12	12:Z:46:ASN:CB	2.47	0.42
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.54	0.42
6:T:193:ALA:O	6:T:197:ILE:HD12	2.20	0.42
11:Y:174:ASN:ND2	11:Y:189:ASN:HD22	2.17	0.42
14:2:126:ILE:N	14:2:126:ILE:CD1	2.82	0.42
2:B:97:GLN:NE2	16:B:246:HOH:O	2.53	0.42
6:F:175:GLU:HB3	6:F:196:ILE:HD12	2.00	0.42
7:G:192:PHE:CD1	7:G:192:PHE:C	2.93	0.42
12:L:14:LEU:HD13	12:L:34:VAL:HG13	2.01	0.42
13:M:-1:GLY:CA	13:M:1:THR:N	2.73	0.42
14:N:20:THR:HG23	14:N:31:THR:OG1	2.19	0.42
10:J:167:PRO:HB2	10:X:168:MET:HE1	2.02	0.42
14:2:156:LYS:HG2	14:2:18(J):LEU:HD11	2.02	0.42
4:D:179:GLU:HB3	4:D:192:LEU:HD21	2.02	0.42
4:D:52:LYS:HB2	4:D:20(B):ASN:C	2.40	0.42
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.67	0.42
7:G:136:LEU:O	7:G:150:LYS:HA	2.19	0.42
11:K:86:LEU:HD13	11:K:86:LEU:C	2.40	0.42
12:L:-7:ASN:ND2	12:L:-5:TYR:H	2.18	0.42
1:O:33:GLN:CA	1:O:33:GLN:NE2	2.82	0.42
6:T:168:GLY:HA3	6:T:201:ALA:HB1	2.01	0.42
14:2:134:ILE:HG21	14:2:158:SER:O	2.19	0.42
14:2:55:ILE:HD11	14:2:95:LEU:HD13	2.01	0.42
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.54	0.42
5:E:67:ILE:HG21	5:E:213:ALA:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:87:ASN:HD22	7:G:87:ASN:C	2.23	0.42
10:J:144:PRO:HG3	11:Y:207:ASN:HD21	1.85	0.42
2:P:159:GLY:HA3	3:Q:62(A):ILE:CD1	2.50	0.42
9:W:123:ASP:OD1	9:W:123:ASP:N	2.53	0.42
10:J:166:MET:HA	10:J:167:PRO:HD3	1.90	0.42
3:Q:140:GLY:HA2	3:Q:215:VAL:HG21	2.01	0.42
5:S:148:LEU:HD21	5:S:163:THR:HG22	2.00	0.42
10:X:2:ILE:HB	10:X:17:SER:HB3	2.02	0.42
5:E:180:LEU:HA	5:E:18(C):PHE:CE2	2.55	0.42
12:L:145:TYR:CD1	12:L:146:LEU:N	2.88	0.42
6:T:147:HIS:HD2	16:T:242:HOH:O	2.01	0.42
7:U:47:VAL:HG11	7:U:190:VAL:HA	2.01	0.42
5:E:41:ARG:NH1	5:E:42:SER:O	2.53	0.41
12:L:79:ALA:O	12:L:83:ILE:HG12	2.20	0.41
1:O:86:ARG:HE	7:U:118:ASN:ND2	2.17	0.41
2:B:173:GLN:HG2	3:C:56:LEU:HD12	2.01	0.41
5:E:48:LEU:HD13	5:E:77:SER:HB3	2.02	0.41
6:F:196:ILE:O	6:F:201:ALA:N	2.53	0.41
8:H:34:LEU:HB2	16:H:540:HOH:O	2.20	0.41
14:N:20:THR:HG22	15:N:1404:BO2:H252	2.02	0.41
12:Z:53:ASP:O	12:Z:57:LYS:HB2	2.19	0.41
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.31	0.41
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.55	0.41
5:E:48:LEU:CD1	5:E:139:ILE:HD12	2.50	0.41
12:L:-1:GLY:O	12:L:1:GLY:HA3	2.20	0.41
4:R:46:VAL:HG11	4:R:139:ALA:HB1	2.03	0.41
8:V:55:VAL:HG23	8:V:86:HIS:CD2	2.56	0.41
14:2:114:PRO:HD2	14:2:118:SER:O	2.20	0.41
7:G:65:SER:OG	7:G:211:GLU:OE2	2.33	0.41
7:G:80:GLY:HA3	7:G:134:VAL:HG12	2.01	0.41
7:G:9:ASP:HA	7:G:14:ILE:CD1	2.51	0.41
3:Q:76:LEU:HD22	3:Q:89:ILE:CD1	2.48	0.41
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.47	0.41
4:D:86:ARG:HD3	4:D:86:ARG:HA	1.83	0.41
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.02	0.41
9:I:132:ASP:HB2	16:I:914:HOH:O	2.21	0.41
12:L:43:MET:HG3	12:L:101:ILE:HG22	2.03	0.41
14:N:126:ILE:HD13	14:N:126:ILE:N	2.32	0.41
5:S:132:TYR:O	5:S:153:PRO:HB3	2.19	0.41
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.21	0.41
12:Z:79:ALA:O	12:Z:83:ILE:HG12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.24	0.41
16:N:583:HOH:O	13:1:211:ILE:HD11	2.20	0.41
5:E:68:ILE:HB	5:E:76:LEU:CD2	2.51	0.41
11:K:99:THR:CG2	11:K:113:VAL:HB	2.49	0.41
5:S:93:ARG:O	5:S:97:ASN:HB2	2.19	0.41
14:2:1:THR:OG1	15:2:1405:BO2:O28	2.31	0.41
6:F:95:GLU:HG3	6:F:115:ARG:HB3	1.99	0.41
1:O:33:GLN:HA	1:O:33:GLN:NE2	2.29	0.41
3:Q:57:LYS:HG3	3:Q:208:LYS:HZ3	1.86	0.41
7:U:41:ARG:HG3	7:U:148:ILE:CD1	2.50	0.41
9:W:48:LEU:HG	9:W:50:THR:HG22	2.03	0.41
9:W:87:LEU:HD11	9:W:99:PRO:HG2	2.02	0.41
2:P:101:LYS:HZ1	10:X:85:GLN:HE22	1.68	0.41
14:2:91:LYS:HE2	14:2:116:GLY:O	2.20	0.41
2:B:20(B):ALA:C	2:B:205:LEU:N	2.73	0.41
1:O:67:VAL:HG11	1:O:213:ALA:HB3	2.01	0.41
6:T:35:THR:CG2	6:T:36:THR:N	2.83	0.41
3:C:75:VAL:HG13	3:C:221:ILE:HD13	2.03	0.41
5:E:198:SER:HA	5:E:201:LEU:HG	2.02	0.41
2:P:141:TYR:CG	2:P:21(E):VAL:HG21	2.56	0.41
4:R:186:LEU:O	4:R:190:GLU:HG3	2.21	0.41
6:T:204:ASP:N	6:T:204:ASP:OD1	2.54	0.41
8:V:1:THR:OG1	15:V:1401:BO2:C21	2.69	0.41
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.41	0.41
8:H:15:ALA:HB1	8:H:159:ILE:CD1	2.51	0.41
12:L:1:GLY:N	16:L:755:HOH:O	2.53	0.41
3:Q:158:SER:CB	4:R:59:LEU:HD21	2.51	0.41
5:S:97:ASN:HA	5:S:97:ASN:HD22	1.64	0.41
7:U:151:THR:HG22	7:U:157:TYR:HB2	2.02	0.41
10:X:2:ILE:O	10:X:3:ILE:HD12	2.21	0.41
5:E:123:ASN:HB3	5:E:130:ARG:O	2.21	0.40
6:F:127:ASN:ND2	6:F:127:ASN:C	2.73	0.40
14:N:8:PHE:CE2	14:N:13:ILE:HD11	2.56	0.40
6:T:186:ALA:O	6:T:190:VAL:HG23	2.22	0.40
10:X:90(A):ILE:HD12	10:X:90(A):ILE:HA	1.88	0.40
14:2:146:MET:HE1	14:2:154:PHE:HB2	2.03	0.40
3:C:37:ALA:O	3:C:164:THR:HA	2.21	0.40
9:I:27:VAL:HG13	16:J:898:HOH:O	2.20	0.40
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.56	0.40
12:Z:90:LYS:HE3	12:Z:93:PHE:O	2.21	0.40
7:G:47:VAL:HG11	7:G:190:VAL:HA	2.01	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:142:ASP:O	4:R:145:GLY:N	2.55	0.40
9:W:107:LYS:HA	9:W:108:PRO:HD3	1.93	0.40
2:B:46:ILE:HG22	2:B:47:VAL:N	2.36	0.40
7:G:43:LYS:HB2	7:G:18(G):GLU:O	2.21	0.40
4:R:110:GLU:HB2	16:R:828:HOH:O	2.22	0.40
5:S:47:VAL:HG23	5:S:189:LEU:HD13	2.04	0.40
10:X:2:ILE:HD13	10:X:170:PHE:CG	2.57	0.40
6:F:63:LYS:HA	6:F:63:LYS:HD3	1.92	0.40
7:G:74:ILE:HD12	7:G:109:CYS:HA	2.03	0.40
7:G:77:VAL:HG13	7:G:137:THR:HB	2.04	0.40
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.91	0.40
11:K:210:ILE:HA	11:K:210:ILE:HD13	1.90	0.40
14:N:67:THR:O	14:N:72:GLY:N	2.54	0.40
2:P:146:TYR:OH	2:P:21(A):LYS:HB2	2.22	0.40
6:T:82:ILE:HB	6:T:83:PRO:HD3	2.03	0.40
10:J:168:MET:HE1	10:X:167:PRO:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	240/250 (96%)	233 (97%)	6 (2%)	1 (0%)	34	58
1	O	240/250 (96%)	231 (96%)	7 (3%)	2 (1%)	19	40
2	B	230/244 (94%)	222 (96%)	4 (2%)	4 (2%)	9	20
2	P	230/244 (94%)	217 (94%)	10 (4%)	3 (1%)	12	27
3	C	231/241 (96%)	226 (98%)	4 (2%)	1 (0%)	34	58
3	Q	231/241 (96%)	226 (98%)	3 (1%)	2 (1%)	17	37
4	D	228/242 (94%)	221 (97%)	6 (3%)	1 (0%)	34	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	228/242 (94%)	218 (96%)	9 (4%)	1 (0%)	34	58
5	E	223/233 (96%)	210 (94%)	11 (5%)	2 (1%)	17	37
5	S	223/233 (96%)	214 (96%)	7 (3%)	2 (1%)	17	37
6	F	234/244 (96%)	220 (94%)	14 (6%)	0	100	100
6	T	234/244 (96%)	224 (96%)	9 (4%)	1 (0%)	34	58
7	G	233/243 (96%)	222 (95%)	10 (4%)	1 (0%)	34	58
7	U	233/243 (96%)	225 (97%)	7 (3%)	1 (0%)	34	58
8	H	216/222 (97%)	211 (98%)	5 (2%)	0	100	100
8	V	214/222 (96%)	210 (98%)	4 (2%)	0	100	100
9	I	194/204 (95%)	189 (97%)	5 (3%)	0	100	100
9	W	194/204 (95%)	189 (97%)	5 (3%)	0	100	100
10	J	191/198 (96%)	184 (96%)	6 (3%)	1 (0%)	29	52
10	X	191/198 (96%)	183 (96%)	8 (4%)	0	100	100
11	K	206/212 (97%)	200 (97%)	6 (3%)	0	100	100
11	Y	206/212 (97%)	200 (97%)	5 (2%)	1 (0%)	29	52
12	L	210/222 (95%)	204 (97%)	6 (3%)	0	100	100
12	Z	210/222 (95%)	204 (97%)	6 (3%)	0	100	100
13	1	223/233 (96%)	216 (97%)	5 (2%)	2 (1%)	17	37
13	M	223/233 (96%)	214 (96%)	8 (4%)	1 (0%)	34	58
14	2	188/196 (96%)	182 (97%)	6 (3%)	0	100	100
14	N	188/196 (96%)	183 (97%)	5 (3%)	0	100	100
All	All	6092/6368 (96%)	5878 (96%)	187 (3%)	27 (0%)	34	58

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	58	LEU
2	P	20(A)	SER
3	Q	58	LEU
2	B	54	VAL
5	E	217	LYS
7	G	239	GLN
2	P	54	VAL
2	P	21(C)	ASP
4	R	12(F)	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	21(C)	ASP
1	O	5	THR
7	U	239	GLN
1	A	5	THR
2	B	6	ARG
2	B	20(A)	SER
13	M	1	THR
5	S	202	ARG
6	T	206	LYS
5	E	203	ASP
5	S	217	LYS
13	1	1	THR
1	O	53	LYS
4	D	12(F)	GLY
10	J	8	VAL
3	Q	183	PRO
13	1	207	GLY
11	Y	39	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%)	206 (99%)	3 (1%)	67	85
1	O	209/209 (100%)	203 (97%)	6 (3%)	42	69
2	B	203/203 (100%)	189 (93%)	14 (7%)	15	33
2	P	203/203 (100%)	191 (94%)	12 (6%)	19	40
3	C	213/213 (100%)	199 (93%)	14 (7%)	16	35
3	Q	213/213 (100%)	201 (94%)	12 (6%)	21	42
4	D	198/198 (100%)	184 (93%)	14 (7%)	14	31
4	R	198/198 (100%)	188 (95%)	10 (5%)	24	46
5	E	192/192 (100%)	173 (90%)	19 (10%)	8	16
5	S	192/192 (100%)	174 (91%)	18 (9%)	8	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	201/201 (100%)	187 (93%)	14 (7%)	15	32
6	T	201/201 (100%)	184 (92%)	17 (8%)	10	22
7	G	207/207 (100%)	193 (93%)	14 (7%)	16	33
7	U	207/207 (100%)	195 (94%)	12 (6%)	20	41
8	H	181/181 (100%)	173 (96%)	8 (4%)	28	53
8	V	181/181 (100%)	170 (94%)	11 (6%)	18	38
9	I	172/172 (100%)	165 (96%)	7 (4%)	30	56
9	W	172/172 (100%)	168 (98%)	4 (2%)	50	76
10	J	175/175 (100%)	167 (95%)	8 (5%)	27	51
10	X	175/175 (100%)	167 (95%)	8 (5%)	27	51
11	K	169/169 (100%)	162 (96%)	7 (4%)	30	56
11	Y	169/169 (100%)	160 (95%)	9 (5%)	22	45
12	L	185/185 (100%)	177 (96%)	8 (4%)	29	54
12	Z	185/185 (100%)	175 (95%)	10 (5%)	22	44
13	1	199/199 (100%)	192 (96%)	7 (4%)	36	62
13	M	199/199 (100%)	193 (97%)	6 (3%)	41	68
14	2	162/162 (100%)	158 (98%)	4 (2%)	47	74
14	N	162/162 (100%)	155 (96%)	7 (4%)	29	54
All	All	5332/5332 (100%)	5049 (95%)	283 (5%)	22	45

All (283) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	64	LEU
1	A	158	PHE
2	B	14	ILE
2	B	55	THR
2	B	58	LEU
2	B	63	THR
2	B	71	ASN
2	B	94	ILE
2	B	121	GLN
2	B	124	THR
2	B	150	THR
2	B	185	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	192	LEU
2	B	216	ARG
2	B	218	ASN
2	B	232	ILE
3	C	10	ARG
3	C	14	ILE
3	C	25	GLU
3	C	57	LYS
3	C	66	LYS
3	C	106	PRO
3	C	121	GLN
3	C	135	SER
3	C	150	GLN
3	C	163	GLN
3	C	172	VAL
3	C	174	GLU
3	C	178	LYS
3	C	208	LYS
4	D	13	SER
4	D	28	LEU
4	D	48	LEU
4	D	52	LYS
4	D	76	CYS
4	D	110	GLU
4	D	126	ARG
4	D	156	THR
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	196	ILE
4	D	215	ILE
4	D	233	ILE
5	E	11	ASP
5	E	12	THR
5	E	13	VAL
5	E	28	LEU
5	E	32	LYS
5	E	57	GLU
5	E	76	LEU
5	E	97	ASN
5	E	121	GLN
5	E	123	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	139	ILE
5	E	185	ASN
5	E	189	LEU
5	E	199	GLN
5	E	206	SER
5	E	207	LEU
5	E	219	THR
5	E	227	GLU
5	E	231	LYS
6	F	36	THR
6	F	43	ASN
6	F	121	GLN
6	F	127	ASN
6	F	144	ASN
6	F	167	LYS
6	F	176	LEU
6	F	18(E)	GLU
6	F	187	ARG
6	F	203	GLU
6	F	205	ASN
6	F	20(B)	GLU
6	F	214	TRP
6	F	21(C)	ASN
7	G	12	ILE
7	G	14	ILE
7	G	49	ILE
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	174	THR
7	G	197	MET
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	22	GLN
8	H	30	ASN
8	H	34	LEU
8	H	56	THR
8	H	68	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	144	GLN
8	H	197	ARG
8	H	223	ASP
9	I	29	ASN
9	I	110	ILE
9	I	123	ASP
9	I	125	ILE
9	I	159	LEU
9	I	160	LEU
9	I	171	TRP
10	J	35	ARG
10	J	52	THR
10	J	70	GLU
10	J	77	GLN
10	J	90(A)	ILE
10	J	10(B)	LYS
10	J	121	GLU
10	J	166	MET
11	K	4	LEU
11	K	9	GLN
11	K	65	LEU
11	K	99	THR
11	K	100	MET
11	K	104	TYR
11	K	10(B)	LYS
12	L	-9	GLN
12	L	-7	ASN
12	L	3	ILE
12	L	14	LEU
12	L	25	SER
12	L	40	ASN
12	L	99	THR
12	L	138	LEU
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	14(C)	ARG
13	M	148	VAL
13	M	204	LYS
14	N	84	LYS
14	N	89	GLU
14	N	10(B)	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	119	VAL
14	N	126	ILE
14	N	134	ILE
14	N	149	GLU
1	O	33	GLN
1	O	54	SER
1	O	62	GLU
1	O	64	LEU
1	O	124	THR
1	O	158	PHE
2	P	55	THR
2	P	57	THR
2	P	62	ASP
2	P	63	THR
2	P	71	ASN
2	P	91	THR
2	P	121	GLN
2	P	150	THR
2	P	185	LYS
2	P	192	LEU
2	P	202	THR
2	P	212	PHE
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	66	LYS
3	Q	121	GLN
3	Q	135	SER
3	Q	150	GLN
3	Q	163	GLN
3	Q	172	VAL
3	Q	174	GLU
3	Q	208	LYS
3	Q	215	VAL
4	R	12	VAL
4	R	28	LEU
4	R	48	LEU
4	R	76	CYS
4	R	126	ARG
4	R	14(A)	ASP
4	R	177	LEU
4	R	191	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	R	215	ILE
4	R	244	GLU
5	S	11	ASP
5	S	12	THR
5	S	32	LYS
5	S	57	GLU
5	S	76	LEU
5	S	97	ASN
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	18(D)	ILE
5	S	185	ASN
5	S	189	LEU
5	S	198	SER
5	S	207	LEU
5	S	214	ILE
5	S	219	THR
5	S	227	GLU
5	S	231	LYS
6	T	11	SER
6	T	36	THR
6	T	38	ILE
6	T	43	ASN
6	T	121	GLN
6	T	127	ASN
6	T	144	ASN
6	T	167	LYS
6	T	169	ARG
6	T	171	SER
6	T	18(E)	GLU
6	T	187	ARG
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
6	T	207	ASP
6	T	214	TRP
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	157	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	169	GLN
7	U	174	THR
7	U	184	ASN
7	U	197	MET
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	22	GLN
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	56	THR
8	V	63	ILE
8	V	68	LEU
8	V	121	VAL
8	V	163	ILE
8	V	197	ARG
8	V	223	ASP
9	W	29	ASN
9	W	159	LEU
9	W	160	LEU
9	W	171	TRP
10	X	3	ILE
10	X	34	THR
10	X	35	ARG
10	X	52	THR
10	X	70	GLU
10	X	77	GLN
10	X	121	GLU
10	X	166	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	65	LEU
11	Y	87	VAL
11	Y	99	THR
11	Y	100	MET
11	Y	104	TYR
11	Y	10(B)	LYS
11	Y	210	ILE
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	3	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	Z	14	LEU
12	Z	21	ILE
12	Z	40	ASN
12	Z	70(A)	ASN
12	Z	98	HIS
12	Z	99	THR
12	Z	138	LEU
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	112	TYR
13	1	14(C)	ARG
13	1	148	VAL
13	1	204	LYS
14	2	3	ILE
14	2	10(B)	LYS
14	2	126	ILE
14	2	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (177) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
1	A	145	ASN
2	B	23	GLN
2	B	71	ASN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	82	ASN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	161	ASN
4	D	211	GLN
4	D	226	ASN
5	E	33	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
6	F	192	GLN
7	G	11	HIS
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	86	HIS
8	H	91	GLN
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	186	GLN
11	K	9	GLN
11	K	85	ASN
11	K	174	ASN
11	K	207	ASN
11	K	208	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	40	ASN
12	L	46	ASN
12	L	61	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	82	ASN
12	L	85	HIS
12	L	98	HIS
12	L	14(B)	ASN
12	L	1(I)	ASN
12	L	166	HIS
13	M	10	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	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
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	121	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	243	GLN
4	R	23	GLN
4	R	99	HIS
4	R	108	ASN
4	R	161	ASN
4	R	211	GLN
4	R	226	ASN
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	178	ASN
7	U	184	ASN
8	V	30	ASN
8	V	66	HIS
8	V	86	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	81	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	X	54	GLN
10	X	85	GLN
10	X	112	GLN
10	X	141	HIS
10	X	186	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	174	ASN
11	Y	207	ASN
11	Y	208	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70	HIS
12	Z	70(A)	ASN
12	Z	14(B)	ASN
12	Z	1(I)	ASN
12	Z	166	HIS
13	1	-7	GLN
13	1	10	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	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BO2	N	1404	-	25,29,29	0.67	0	32,38,38	1.49	5 (15%)
15	BO2	V	1401	-	25,29,29	0.56	0	32,38,38	1.37	5 (15%)
15	BO2	Y	1403	-	25,29,29	0.55	0	32,38,38	1.19	3 (9%)
15	BO2	2	1405	-	25,29,29	0.69	0	32,38,38	1.36	6 (18%)
15	BO2	K	1402	-	25,29,29	0.57	0	32,38,38	1.44	7 (21%)
15	BO2	H	1400	-	25,29,29	0.53	0	32,38,38	1.28	5 (15%)

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	BO2	N	1404	-	-	7/22/28/28	0/2/2/2
15	BO2	V	1401	-	-	7/22/28/28	0/2/2/2
15	BO2	Y	1403	-	-	3/22/28/28	0/2/2/2
15	BO2	2	1405	-	-	7/22/28/28	0/2/2/2
15	BO2	K	1402	-	-	3/22/28/28	0/2/2/2
15	BO2	H	1400	-	-	5/22/28/28	0/2/2/2

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	1401	BO2	C21-C22-C23	4.06	120.50	115.39
15	N	1404	BO2	C21-C22-C23	3.97	120.38	115.39
15	K	1402	BO2	C6-N1-C2	3.27	121.18	116.93
15	K	1402	BO2	C21-C22-C23	3.27	119.50	115.39
15	H	1400	BO2	C21-C22-C23	3.01	119.18	115.39
15	2	1405	BO2	C21-C22-C23	2.99	119.15	115.39
15	2	1405	BO2	C6-N1-C2	2.96	120.77	116.93
15	N	1404	BO2	C6-N1-C2	2.93	120.73	116.93
15	H	1400	BO2	C7-C2-N1	2.89	120.89	117.48
15	V	1401	BO2	C7-C2-N1	2.81	120.80	117.48
15	Y	1403	BO2	C6-N1-C2	2.76	120.51	116.93
15	V	1401	BO2	C6-N1-C2	2.70	120.43	116.93
15	H	1400	BO2	C6-N1-C2	2.59	120.29	116.93
15	2	1405	BO2	C2-C3-N4	-2.55	118.88	122.05
15	N	1404	BO2	C5-N4-C3	2.54	121.23	116.85
15	N	1404	BO2	C2-C3-N4	-2.54	118.90	122.05
15	K	1402	BO2	C5-N4-C3	2.53	121.22	116.85
15	N	1404	BO2	C21-N20-C18	-2.52	116.25	122.77
15	Y	1403	BO2	C5-N4-C3	2.50	121.17	116.85
15	K	1402	BO2	C18-C10-N9	-2.45	104.49	111.16
15	2	1405	BO2	C18-C10-N9	-2.45	104.50	111.16
15	2	1405	BO2	C5-N4-C3	2.37	120.95	116.85
15	K	1402	BO2	C2-C3-N4	-2.21	119.30	122.05
15	K	1402	BO2	C5-C6-N1	-2.19	119.02	122.17
15	K	1402	BO2	C21-N20-C18	-2.18	117.12	122.77
15	Y	1403	BO2	C2-C3-N4	-2.18	119.34	122.05
15	2	1405	BO2	C5-C6-N1	-2.16	119.07	122.17
15	V	1401	BO2	C5-N4-C3	2.11	120.50	116.85
15	V	1401	BO2	C3-C2-N1	-2.02	119.21	121.61
15	H	1400	BO2	C5-N4-C3	2.01	120.32	116.85
15	H	1400	BO2	C3-C2-N1	-2.00	119.23	121.61

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	N	1404	BO2	N20-C21-C22-C23
15	N	1404	BO2	C21-C22-C23-C24
15	N	1404	BO2	C21-C22-C23-C25
15	V	1401	BO2	C3-C2-C7-O8
15	V	1401	BO2	C3-C2-C7-N9
15	V	1401	BO2	N20-C21-C22-C23
15	V	1401	BO2	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	V	1401	BO2	C21-C22-C23-C25
15	Y	1403	BO2	N20-C21-C22-C23
15	Y	1403	BO2	C21-C22-C23-C24
15	Y	1403	BO2	C21-C22-C23-C25
15	2	1405	BO2	N20-C21-C22-C23
15	2	1405	BO2	C21-C22-C23-C24
15	2	1405	BO2	C21-C22-C23-C25
15	K	1402	BO2	N20-C21-C22-C23
15	K	1402	BO2	C21-C22-C23-C24
15	K	1402	BO2	C21-C22-C23-C25
15	H	1400	BO2	N20-C21-C22-C23
15	H	1400	BO2	C21-C22-C23-C24
15	H	1400	BO2	C21-C22-C23-C25
15	N	1404	BO2	N1-C2-C7-O8
15	N	1404	BO2	N1-C2-C7-N9
15	2	1405	BO2	N1-C2-C7-O8
15	2	1405	BO2	N1-C2-C7-N9
15	N	1404	BO2	C3-C2-C7-O8
15	2	1405	BO2	C3-C2-C7-O8
15	N	1404	BO2	C3-C2-C7-N9
15	2	1405	BO2	C3-C2-C7-N9
15	V	1401	BO2	N1-C2-C7-O8
15	V	1401	BO2	N1-C2-C7-N9
15	H	1400	BO2	C3-C2-C7-N9
15	H	1400	BO2	C3-C2-C7-O8

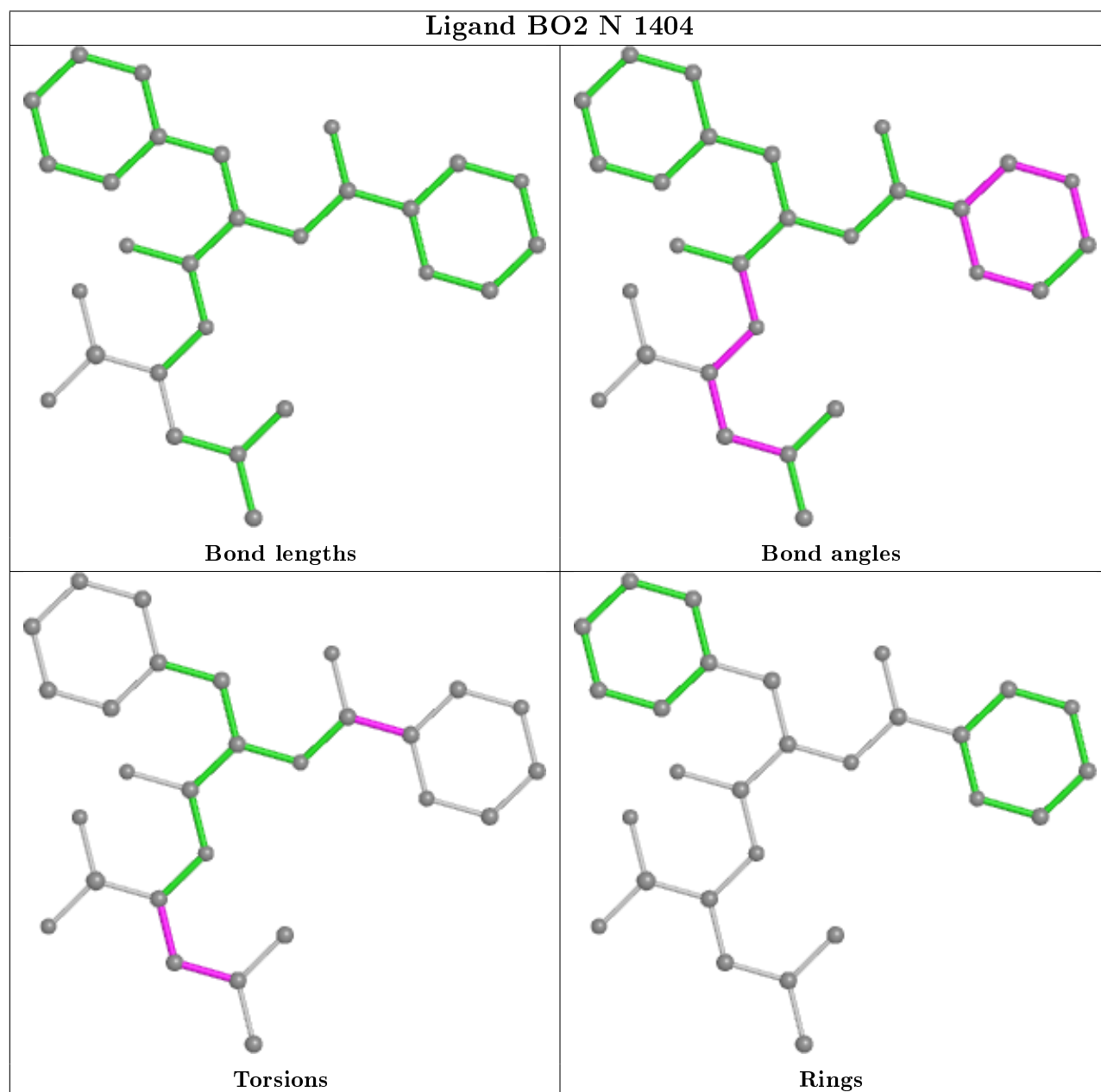
There are no ring outliers.

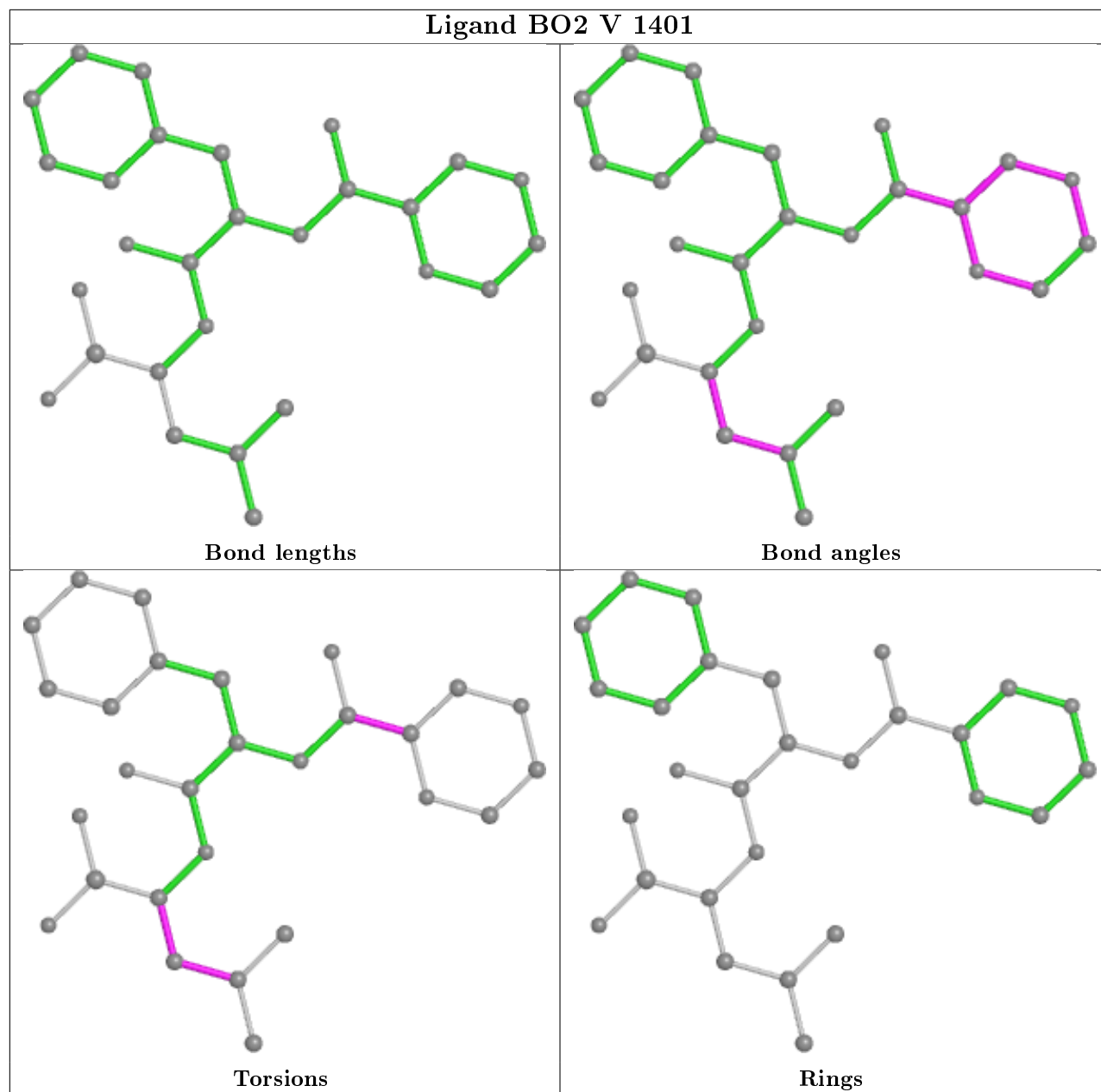
5 monomers are involved in 17 short contacts:

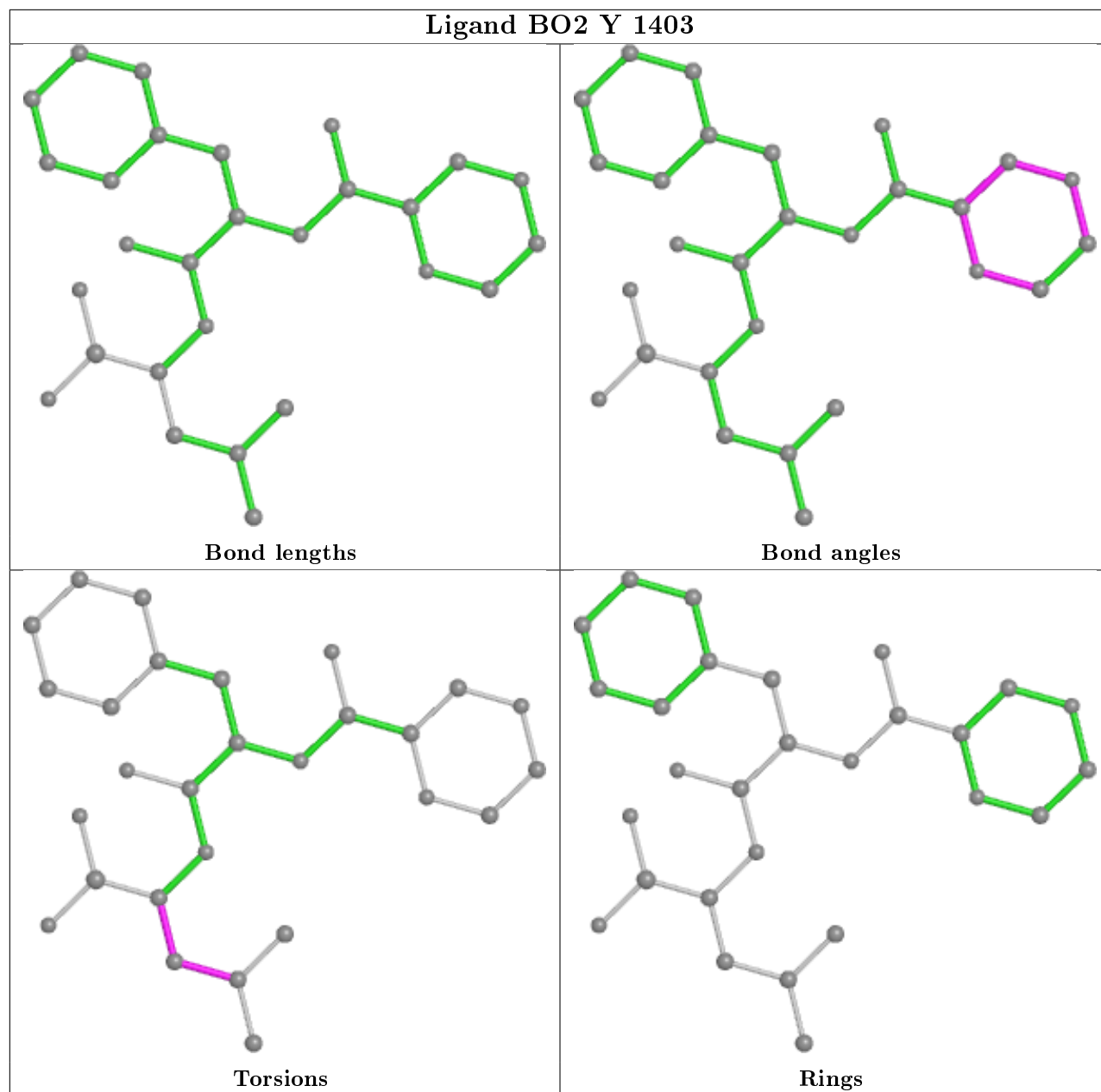
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	N	1404	BO2	3	0
15	V	1401	BO2	2	0
15	Y	1403	BO2	3	0
15	2	1405	BO2	7	0
15	K	1402	BO2	2	0

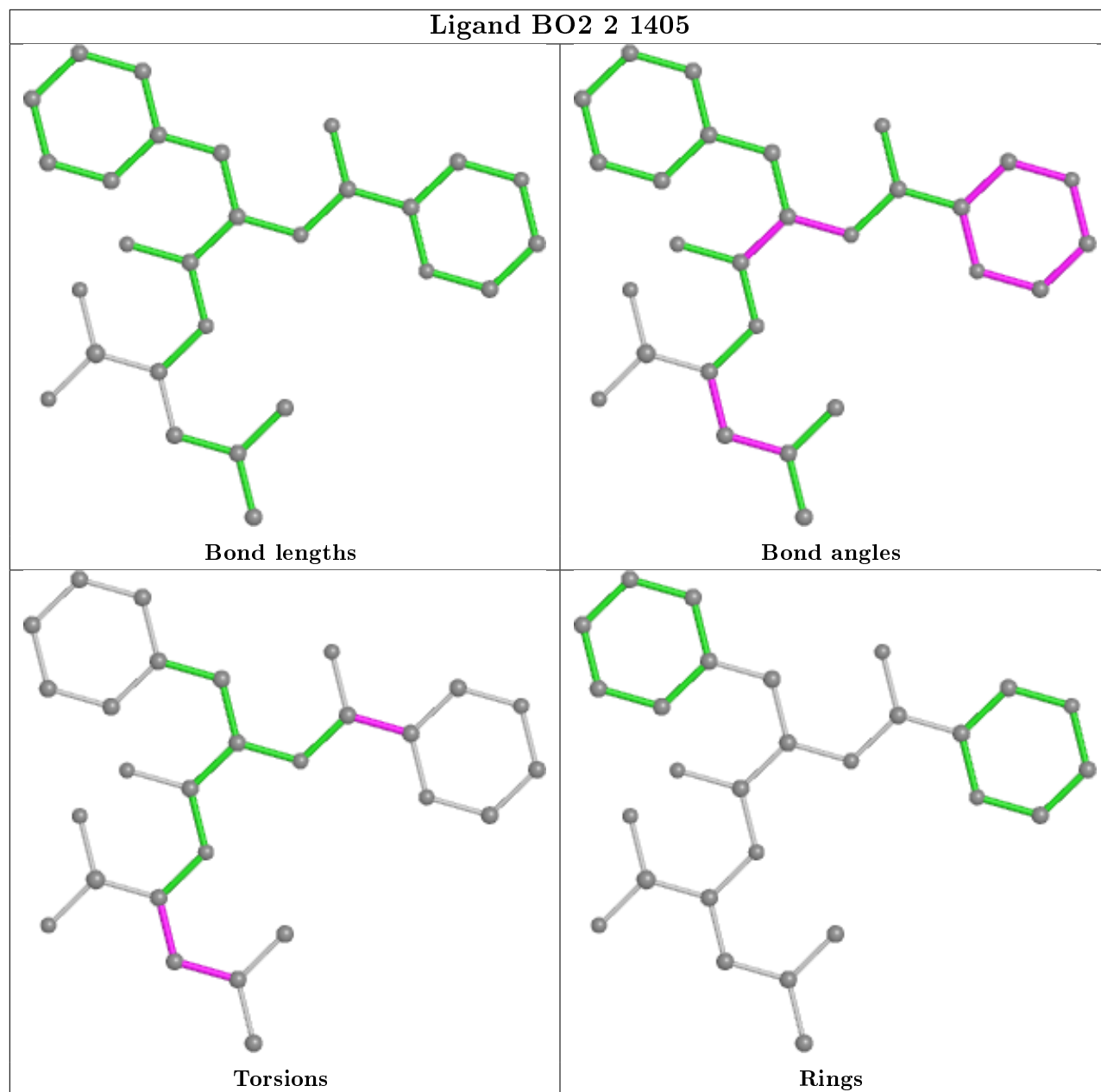
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

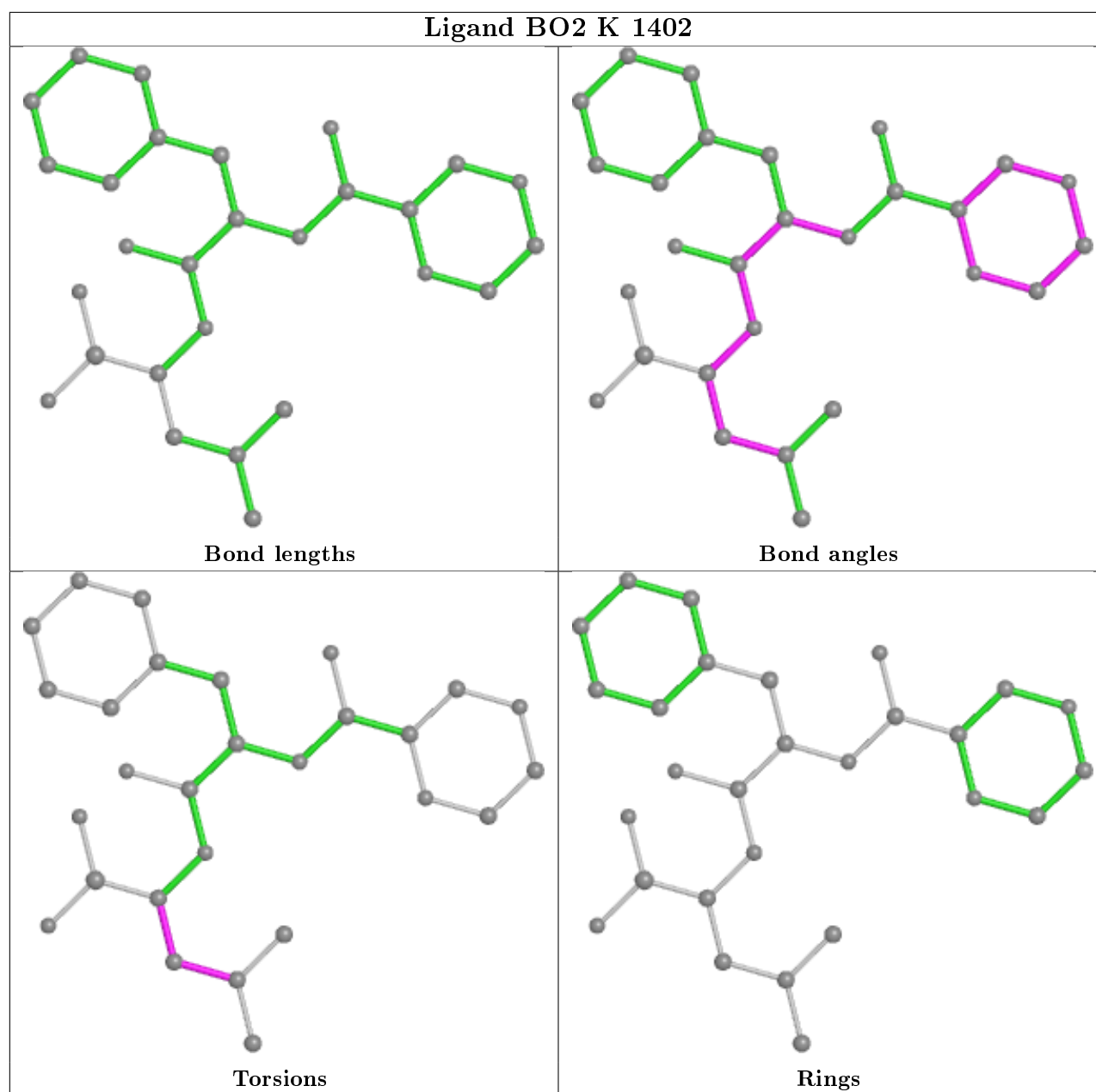
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

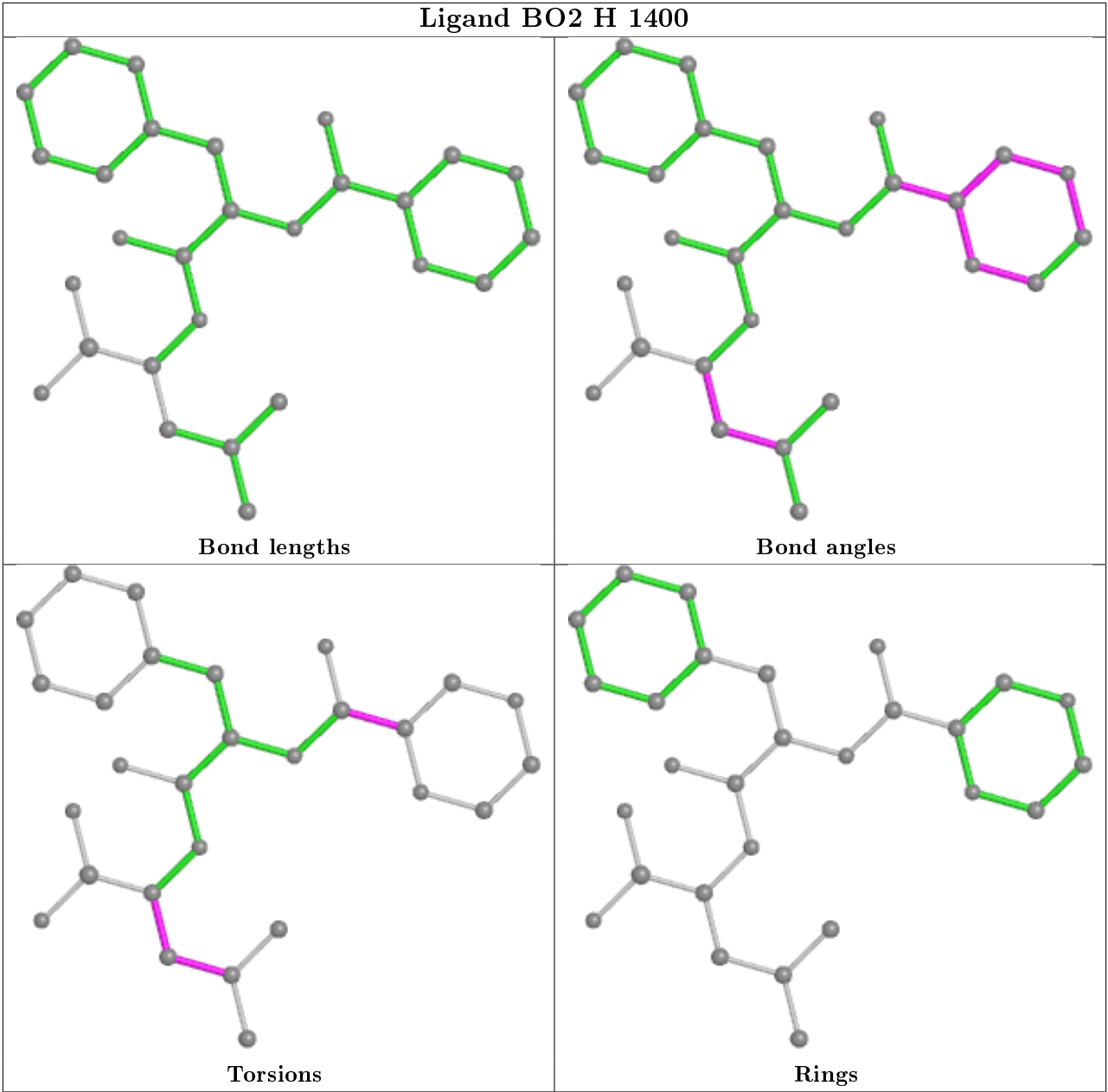












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	P	6

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
2	B	6
4	R	6
4	D	6
9	W	5
1	A	5
13	M	5
13	1	5
9	I	5
12	Z	5
12	L	5
1	O	5
14	N	4
14	2	4
5	S	4
5	E	4
7	U	4
7	G	4
3	Q	4
3	C	4
6	T	4
6	F	4
10	X	3
10	J	3
8	V	3
8	H	3
11	K	2
11	Y	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	21(B):GLY	C	217:ALA	N	3.40
1	P	21(B):GLY	C	217:ALA	N	3.34
1	Z	14(W):LYS	C	145:TYR	N	3.32
1	L	14(W):LYS	C	145:TYR	N	3.28
1	C	203:THR	C	206:GLY	N	3.22
1	P	21(D):GLY	C	219:GLU	N	3.18
1	J	-1:MET	C	1:ASP	N	3.08
1	Q	203:THR	C	206:GLY	N	3.07
1	B	21(D):GLY	C	219:GLU	N	2.99
1	D	12(G):GLU	C	125:GLU	N	2.99
1	X	-1:MET	C	1:ASP	N	2.88
1	R	12(G):GLU	C	125:GLU	N	2.86

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	204:GLU	C	206:SER	N	2.80
1	B	20(B):ALA	C	205:LEU	N	2.73
1	L	1(I):ASN	C	14(J):GLY	N	2.72
1	O	200:SER	C	202:VAL	N	2.72
1	Z	1(I):ASN	C	14(J):GLY	N	2.67
1	Q	18(D):GLU	C	182:PRO	N	2.66
1	O	21(P):LYS	C	218:GLY	N	2.61
1	T	20(C):LYS	C	207:ASP	N	2.60
1	A	21(P):LYS	C	218:GLY	N	2.59
1	E	204:GLU	C	206:SER	N	2.55
1	A	200:SER	C	202:VAL	N	2.53
1	T	199:LEU	C	201:ALA	N	2.52
1	C	18(D):GLU	C	182:PRO	N	2.51
1	F	199:LEU	C	201:ALA	N	2.51
1	T	21(C):ASN	C	219:GLY	N	2.51
1	Y	181:ASP	C	183:GLY	N	2.50
1	G	18(D):ILE	C	184:ASN	N	2.48
1	R	18(E):SER	C	184:LEU	N	2.47
1	K	181:ASP	C	183:GLY	N	2.42
1	O	20(A):THR	C	210:ILE	N	2.42
1	Q	14(A):ARG	C	144:ASP	N	2.42
1	F	21(C):ASN	C	219:GLY	N	2.41
1	B	21(E):VAL	C	220:TYR	N	2.40
1	Z	-1:GLY	C	1:GLY	N	2.39
1	P	20(B):ALA	C	205:LEU	N	2.38
1	Z	10(B):GLY	C	107:LYS	N	2.38
1	2	181:ALA	C	183:GLY	N	2.37
1	K	10(B):LYS	C	106:GLU	N	2.36
1	R	202:GLU	C	205:GLU	N	2.36
1	R	233:ILE	C	235:LYS	N	2.36
1	1	18(A):THR	C	183:GLY	N	2.36
1	2	10(B):LYS	C	106:ASN	N	2.36
1	Z	180:LYS	C	182:ASP	N	2.35
1	J	10(C):LYS	C	106:ASN	N	2.34
1	N	10(B):LYS	C	106:ASN	N	2.33
1	X	10(C):LYS	C	106:ASN	N	2.33
1	B	200:THR	C	202:THR	N	2.32
1	D	18(E):SER	C	184:LEU	N	2.31
1	S	60:SER	C	63:TYR	N	2.30
1	X	181:ASP	C	183:GLY	N	2.30
1	1	10(B):ASN	C	106:GLY	N	2.29
1	F	20(C):LYS	C	207:ASP	N	2.27

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	-1:GLY	C	1:GLY	N	2.27
1	M	18(A):THR	C	183:GLY	N	2.26
1	T	18(F):GLY	C	184:LEU	N	2.26
1	D	233:ILE	C	235:LYS	N	2.25
1	E	18(F):ILE	C	183:ASP	N	2.25
1	M	71(D):ALA	C	74:LEU	N	2.24
1	W	12(A):LYS	C	123:ASP	N	2.24
1	I	179:LYS	C	181:LYS	N	2.23
1	W	179:LYS	C	181:LYS	N	2.23
1	I	14(G):ILE	C	144:PRO	N	2.23
1	F	18(F):GLY	C	184:LEU	N	2.22
1	N	70:TYR	C	72:GLY	N	2.22
1	N	181:ALA	C	183:GLY	N	2.22
1	D	202:GLU	C	205:GLU	N	2.21
1	E	2(E):ASN	C	210:LEU	N	2.21
1	G	18(M):SER	C	186:TRP	N	2.21
1	I	10(C):SER	C	106:GLY	N	2.21
1	U	18(M):SER	C	186:TRP	N	2.21
1	U	218:ASP	C	220:LYS	N	2.20
1	Y	10(B):LYS	C	106:GLU	N	2.20
1	I	71(D):ALA	C	74:LEU	N	2.20
1	M	10(B):ASN	C	106:GLY	N	2.19
1	S	18(F):ILE	C	183:ASP	N	2.19
1	H	91:GLN	C	93:GLY	N	2.18
1	U	18(D):ILE	C	184:ASN	N	2.18
1	V	187:LEU	C	189:ARG	N	2.18
1	A	14(A):SER	C	148:LEU	N	2.17
1	L	10(B):GLY	C	107:LYS	N	2.16
1	Q	14(B):ASP	C	145:GLU	N	2.16
1	V	91:GLN	C	93:GLY	N	2.16
1	W	10(C):SER	C	106:GLY	N	2.16
1	P	14(A):TYR	C	145:GLY	N	2.15
1	C	14(A):ARG	C	144:ASP	N	2.14
1	S	2(E):ASN	C	210:LEU	N	2.14
1	E	60:SER	C	63:TYR	N	2.13
1	L	180:LYS	C	182:ASP	N	2.13
1	R	14(A):ASP	C	145:GLY	N	2.13
1	B	14(A):TYR	C	145:GLY	N	2.12
1	C	14(B):ASP	C	145:GLU	N	2.12
1	D	20(B):ASN	C	210:ALA	N	2.11
1	A	20(A):THR	C	210:ILE	N	2.09
1	D	14(A):ASP	C	145:GLY	N	2.09

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	218:ASP	C	220:LYS	N	2.09
1	I	12(A):LYS	C	123:ASP	N	2.08
1	U	14(A):GLU	C	144:LEU	N	2.08
1	M	14(G):ILE	C	144:PRO	N	2.07
1	P	200:THR	C	202:THR	N	2.07
1	G	14(A):GLU	C	144:LEU	N	2.06
1	H	187:LEU	C	189:ARG	N	2.05
1	J	181:ASP	C	183:GLY	N	2.05
1	O	14(A):SER	C	148:LEU	N	2.05
1	P	21(E):VAL	C	220:TYR	N	2.03
1	V	10(A):PRO	C	106:THR	N	2.03
1	2	70:TYR	C	72:GLY	N	2.03
1	R	20(B):ASN	C	210:ALA	N	2.02
1	W	-1:GLY	C	1:GLY	N	2.02
1	I	-1:GLY	C	1:GLY	N	2.01
1	H	10(A):PRO	C	106:THR	N	1.93
1	1	-1:GLY	C	1:THR	N	1.93
1	N	92:ASP	C	94:ASN	N	1.90
1	A	10(A):ILE	C	103:TYR	N	1.89
1	I	36:HIS	C	38:TYR	N	1.89
1	O	10(A):ILE	C	103:TYR	N	1.89
1	W	36:HIS	C	38:TYR	N	1.80
1	2	92:ASP	C	94:ASN	N	1.80
1	M	-1:GLY	C	1:THR	N	1.77

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.19	5 (2%) 65 65	27, 40, 64, 79	0
1	O	250/250 (100%)	-0.08	7 (2%) 53 52	29, 44, 75, 86	0
2	B	244/244 (100%)	0.02	9 (3%) 41 40	27, 43, 79, 121	0
2	P	244/244 (100%)	0.08	9 (3%) 41 40	27, 44, 75, 123	0
3	C	241/241 (100%)	0.08	14 (5%) 23 21	28, 44, 86, 109	0
3	Q	241/241 (100%)	0.37	26 (10%) 5 4	33, 48, 95, 119	0
4	D	242/242 (100%)	0.05	10 (4%) 37 35	28, 45, 73, 94	0
4	R	242/242 (100%)	0.18	11 (4%) 33 31	30, 49, 73, 101	0
5	E	233/233 (100%)	0.19	14 (6%) 21 20	34, 51, 75, 91	0
5	S	233/233 (100%)	0.21	15 (6%) 19 17	35, 55, 79, 91	0
6	F	244/244 (100%)	-0.04	8 (3%) 46 45	28, 44, 76, 97	0
6	T	244/244 (100%)	0.05	7 (2%) 51 51	26, 45, 80, 89	0
7	G	243/243 (100%)	-0.07	5 (2%) 63 63	26, 40, 70, 91	0
7	U	243/243 (100%)	-0.18	6 (2%) 57 57	26, 39, 64, 83	0
8	H	222/222 (100%)	-0.32	0 100 100	25, 36, 53, 76	0
8	V	222/222 (100%)	-0.37	1 (0%) 91 92	28, 36, 53, 78	0
9	I	204/204 (100%)	-0.35	2 (0%) 82 82	26, 37, 51, 62	0
9	W	204/204 (100%)	-0.23	2 (0%) 82 82	25, 36, 51, 66	0
10	J	198/198 (100%)	-0.19	6 (3%) 50 49	26, 39, 53, 103	0
10	X	198/198 (100%)	-0.12	6 (3%) 50 49	28, 39, 52, 104	0
11	K	212/212 (100%)	-0.19	6 (2%) 53 52	26, 37, 59, 70	0
11	Y	212/212 (100%)	-0.25	3 (1%) 75 76	28, 39, 63, 71	0
12	L	222/222 (100%)	-0.26	3 (1%) 75 76	25, 37, 58, 70	0
12	Z	222/222 (100%)	-0.20	3 (1%) 75 76	28, 38, 60, 71	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	-0.30	1 (0%) 92 93	26, 36, 49, 52	0
13	M	233/233 (100%)	-0.35	1 (0%) 92 93	27, 37, 49, 52	0
14	2	196/196 (100%)	-0.35	0 100 100	23, 34, 51, 63	0
14	N	196/196 (100%)	-0.31	0 100 100	26, 34, 49, 62	0
All	All	6368/6368 (100%)	-0.10	180 (2%) 53 52	23, 41, 73, 123	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	217	ALA	12.8
4	R	12(F)	GLY	12.2
4	R	12(E)	SER	11.2
4	R	12(C)	GLY	9.4
4	R	12(D)	ALA	9.0
5	E	4	PHE	8.6
7	G	240	ASP	8.3
2	B	217	ALA	8.0
4	D	12(C)	GLY	7.7
7	U	240	ASP	7.5
2	P	218	ASN	7.4
2	B	218	ASN	7.4
3	Q	236	ILE	6.8
12	Z	145	TYR	6.6
4	D	12(D)	ALA	6.5
10	J	192	ALA	6.5
13	M	-8	THR	6.5
1	O	236	LEU	6.3
10	X	192	ALA	6.0
4	D	12(E)	SER	5.9
12	L	145	TYR	5.9
10	X	193	GLN	5.6
5	E	203	ASP	5.5
1	A	4	MET	5.5
7	U	6	ALA	5.5
1	O	4	MET	5.5
7	G	6	ALA	5.5
5	S	203	ASP	5.4
3	Q	242	GLU	5.3
3	Q	207	ALA	5.1
10	J	-1	MET	5.1
6	F	5	GLY	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	S	5	ARG	5.1
3	C	55	THR	4.9
3	Q	240	LYS	4.9
3	Q	203	THR	4.8
10	J	193	GLN	4.8
2	P	21(B)	GLY	4.7
5	S	4	PHE	4.7
13	1	-8	THR	4.6
5	E	5	ARG	4.5
4	D	12(F)	GLY	4.5
6	T	5	GLY	4.4
5	E	127	TYR	4.4
3	C	203	THR	4.2
3	C	56	LEU	4.2
10	X	189	ASP	4.1
10	X	-1	MET	4.1
5	S	178	ARG	4.0
4	R	12(B)	GLU	4.0
10	J	191	GLN	4.0
5	S	206	SER	3.9
3	Q	56	LEU	3.9
6	T	240	ILE	3.9
2	B	21(B)	GLY	3.8
4	R	126	ARG	3.8
6	F	240	ILE	3.7
4	D	127	LEU	3.7
7	G	239	GLN	3.6
4	R	12(G)	GLU	3.6
1	O	235	ALA	3.5
1	A	236	LEU	3.5
3	Q	241	GLN	3.5
6	F	201	ALA	3.5
9	W	-8	SER	3.5
5	E	204	GLU	3.4
3	Q	235	GLN	3.4
3	Q	194	VAL	3.4
5	E	233	ILE	3.4
3	Q	238	GLN	3.4
4	R	10	ARG	3.4
5	S	127	TYR	3.3
3	C	240	LYS	3.3
3	Q	232	TYR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	206	SER	3.2
1	O	21(P)	LYS	3.2
3	C	187	GLU	3.1
5	S	201	LEU	3.1
3	Q	184	ALA	3.1
3	Q	191	LYS	3.1
12	L	14(W)	LYS	3.1
3	Q	202	GLN	3.0
6	T	6	THR	3.0
4	D	12(G)	GLU	3.0
9	W	181	LYS	2.9
6	F	184	LEU	2.9
7	G	7	GLY	2.9
7	U	7	GLY	2.9
2	B	219	GLU	2.9
5	E	6	ASN	2.9
3	C	234	THR	2.9
5	E	128	GLY	2.8
3	Q	187	GLU	2.8
7	G	8	TYR	2.8
4	D	12(B)	GLU	2.8
5	E	191	LYS	2.8
3	C	236	ILE	2.8
3	Q	18(D)	GLU	2.8
3	C	208	LYS	2.8
2	B	21(A)	LYS	2.7
3	Q	243	GLN	2.7
1	O	5	THR	2.7
11	K	104	TYR	2.7
3	C	237	GLU	2.6
5	S	202	ARG	2.6
5	S	233	ILE	2.6
7	U	218	ASP	2.6
11	K	179	THR	2.5
7	U	239	GLN	2.5
3	Q	234	THR	2.5
4	D	9	ASP	2.5
4	R	9	ASP	2.5
6	F	204	ASP	2.5
6	T	241	ASN	2.5
3	Q	55	THR	2.5
5	E	192	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	202	GLN	2.5
4	R	121	LEU	2.5
5	E	195	GLU	2.4
4	R	127	LEU	2.4
11	Y	104	TYR	2.4
12	Z	14(W)	LYS	2.4
2	P	185	LYS	2.4
10	X	191	GLN	2.4
3	Q	233	VAL	2.4
3	Q	239	GLU	2.4
11	Y	181	ASP	2.4
10	J	92	ARG	2.4
10	X	10	ASP	2.4
1	O	203	GLU	2.3
4	D	126	ARG	2.3
3	Q	174	GLU	2.3
3	Q	237	GLU	2.3
6	F	6	THR	2.3
1	O	7	ARG	2.3
2	B	54	VAL	2.3
6	F	199	LEU	2.3
7	U	8	TYR	2.3
2	P	181	LYS	2.3
2	B	183	ASP	2.2
3	C	238	GLN	2.2
5	S	33	GLN	2.2
2	P	183	ASP	2.2
11	K	148	VAL	2.2
11	Y	10(A)	ARG	2.2
2	B	200	THR	2.2
10	J	189	ASP	2.2
3	Q	195	ARG	2.2
2	P	219	GLU	2.2
5	S	12	THR	2.2
11	K	181	ASP	2.2
12	L	-9	GLN	2.2
6	T	199	LEU	2.2
5	S	18(B)	THR	2.2
3	Q	18(C)	LYS	2.2
8	V	223	ASP	2.2
6	T	232	ALA	2.2
6	F	43	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	S	195	GLU	2.1
2	B	21(E)	VAL	2.1
3	C	241	GLN	2.1
1	A	235	ALA	2.1
2	P	21(A)	LYS	2.1
3	C	242	GLU	2.1
11	K	180	GLU	2.1
5	S	6	ASN	2.1
1	A	234	GLU	2.1
2	P	235	LYS	2.1
3	C	18(D)	GLU	2.1
5	E	189	LEU	2.1
12	Z	-9	GLN	2.1
11	K	207	ASN	2.1
9	I	-8	SER	2.1
5	E	174	THR	2.0
3	Q	198	LEU	2.0
1	A	203	GLU	2.0
6	T	224	VAL	2.0
4	D	41	ALA	2.0
5	S	18(C)	PHE	2.0
9	I	181	LYS	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	BO2	N	1404	28/28	0.93	0.19	30,33,37,37	0

Continued on next page...

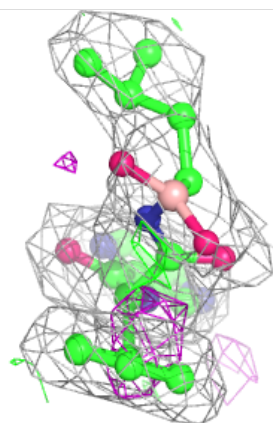
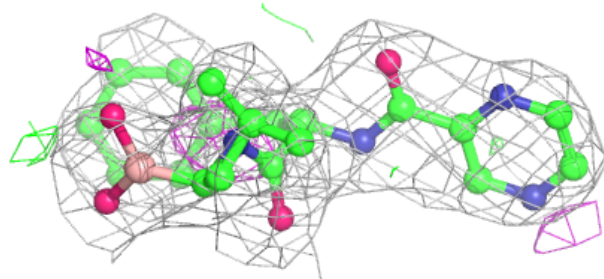
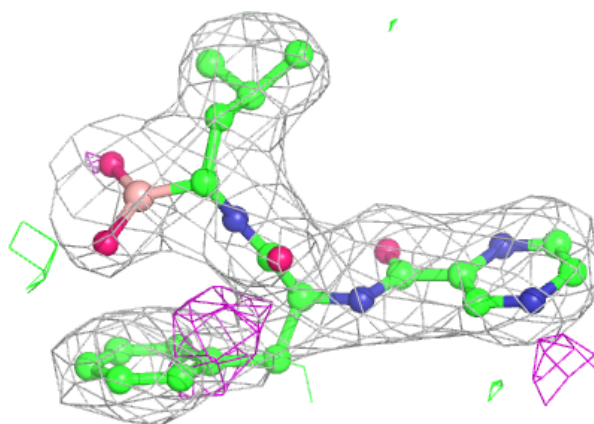
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	BO2	V	1401	28/28	0.94	0.17	40,45,49,49	0
15	BO2	Y	1403	28/28	0.94	0.20	29,38,42,42	0
15	BO2	K	1402	28/28	0.94	0.19	22,35,37,38	0
15	BO2	H	1400	28/28	0.94	0.18	38,41,43,43	0
15	BO2	2	1405	28/28	0.95	0.16	28,33,35,35	0

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

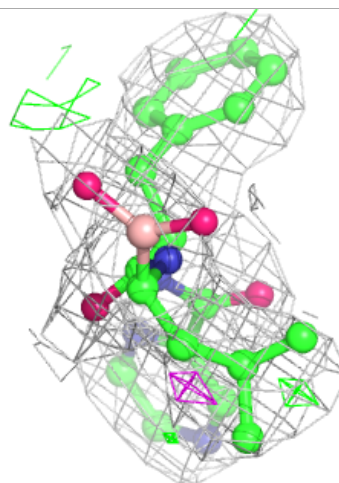
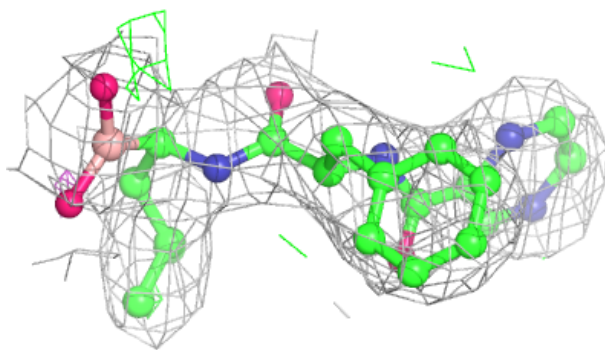
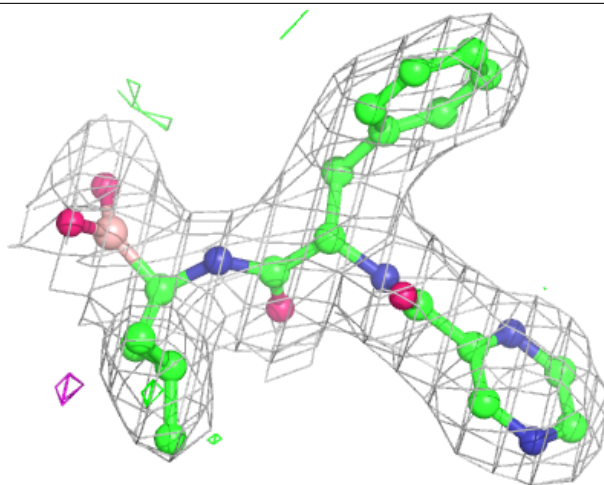
Electron density around BO2 N 1404:

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



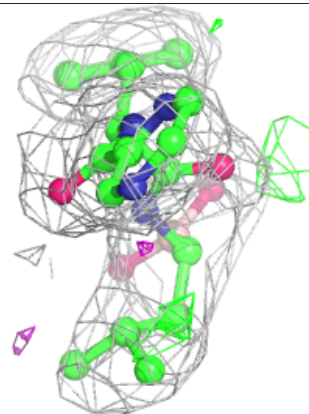
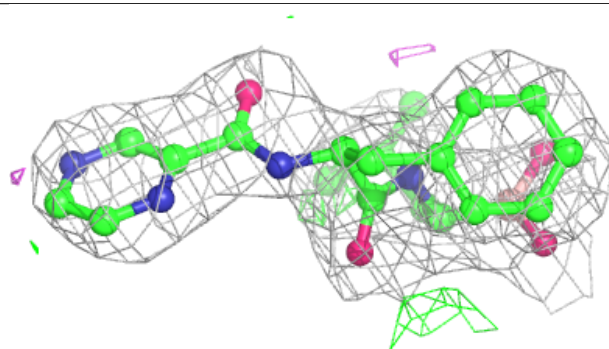
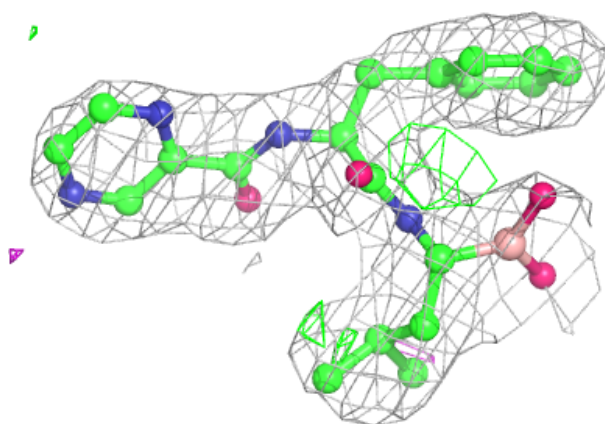
Electron density around BO2 V 1401:

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



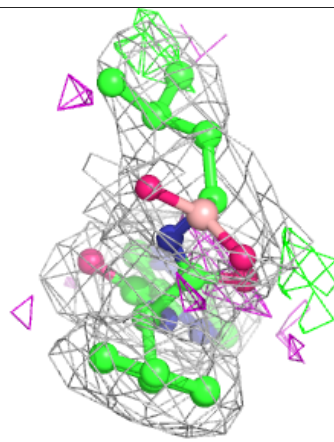
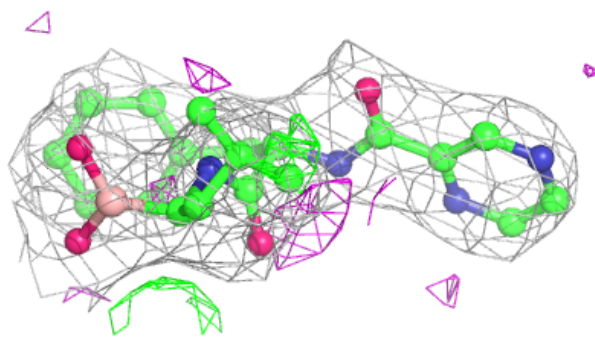
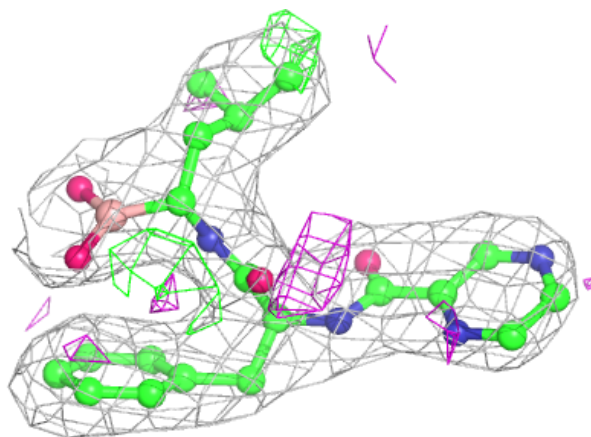
Electron density around BO2 Y 1403:

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



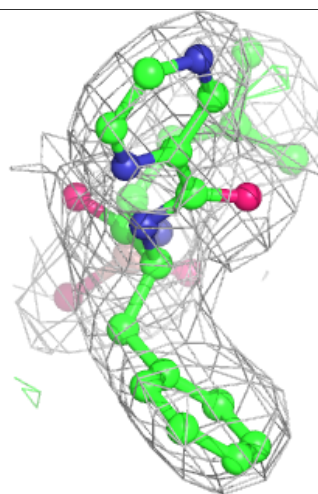
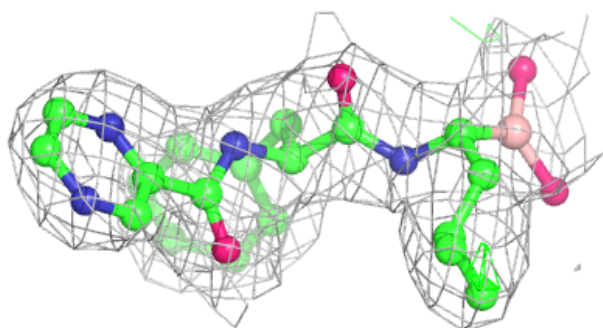
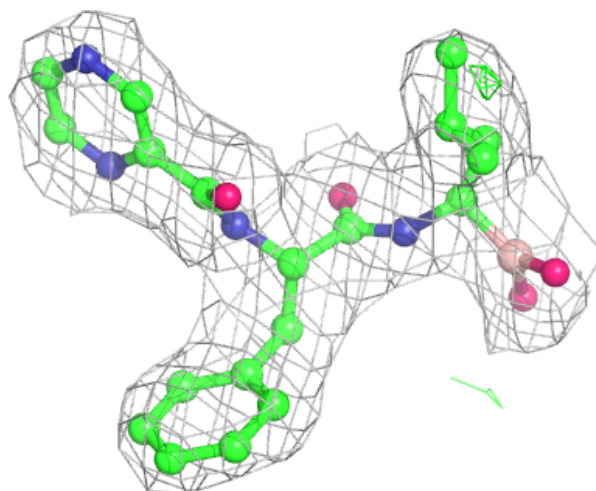
Electron density around BO2 K 1402:

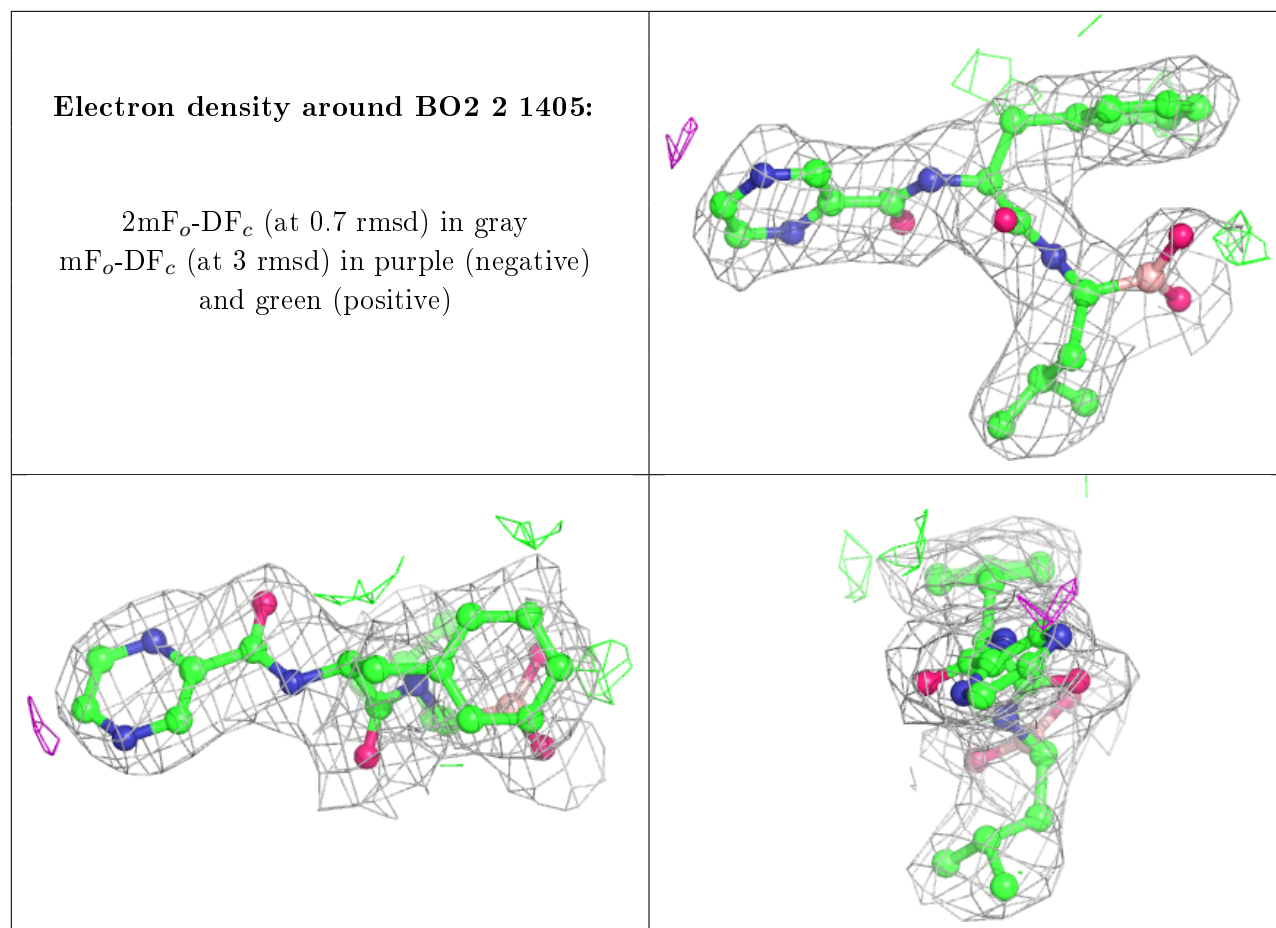
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BO2 H 1400:

$2mF_o-DF_c$ (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.