Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2025 – 01:31 PM EDT

PDB ID	:	9AW6
Title	:	Yeast 20S proteasome soaked with MA9 fraction EF2
Authors	:	Meneghello, R.; Rustiguel, J.K.; Fernandes, A.Z.N.; Trivella, D.B.B.
Deposited on	:	2024-03-05
Resolution	:	3.44 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

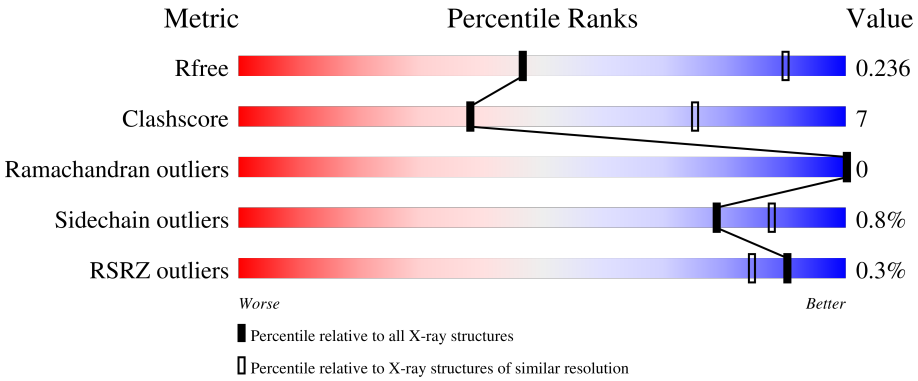
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.44 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}	164625	1587 (3.50-3.38)
Clashscore	180529	1676 (3.50-3.38)
Ramachandran outliers	177936	1665 (3.50-3.38)
Sidechain outliers	177891	1666 (3.50-3.38)
RSRZ outliers	164620	1587 (3.50-3.38)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	85% 14%
1	O	250	82% 18%
2	B	258	76% 18% 6%
2	P	258	% 79% 15% 5%
3	C	254	79% 18% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	254	73% 21% • 5%
4	D	260	% 78% 13% 8%
4	R	260	% 79% 15% 5%
5	E	234	79% 20% •
5	S	234	78% 21% •
6	F	287	70% 15% • 15%
6	T	287	% 70% 15% 15%
7	G	252	77% 19% •
7	U	252	77% 19% •
8	H	232	81% 15% •
8	V	232	76% 20% •
9	I	205	82% 18%
9	W	205	77% 23%
10	J	198	83% 16% •
10	X	198	83% 16% •
11	K	212	82% 17%
11	Y	212	% 84% 16%
12	L	222	83% 16% •
12	Z	222	% 82% 18%
13	M	233	78% 22%
13	a	233	100%
14	N	196	84% 16%
14	b	196	99% •

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 50447 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 subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			
1	O	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1905	1204	321	377	3			
2	P	244	Total	C	N	O	S	0	0	0
			1909	1206	322	378	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1934	1206	339	385	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	239	Total	C	N	O	S	0	0	0
			1854	1161	311	375	7			
4	R	246	Total	C	N	O	S	0	0	0
			1898	1186	318	387	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	232	Total	C	N	O	S	0	0	0
			1784	1120	311	349	4			
5	S	232	Total	C	N	O	S	0	0	0
			1784	1120	311	349	4			

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
6	T	245	Total	C	N	O	S	0	0	0
			1904	1211	331	358	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	242	Total	C	N	O	S	0	0	0
			1916	1218	321	369	8			
7	U	242	Total	C	N	O	S	0	0	0
			1916	1218	321	369	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

- Molecule 9 is a protein called Proteasome subunit beta type-3.

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 subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	0	0
			1570	997	266	301	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

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 subunit beta type-6.

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			

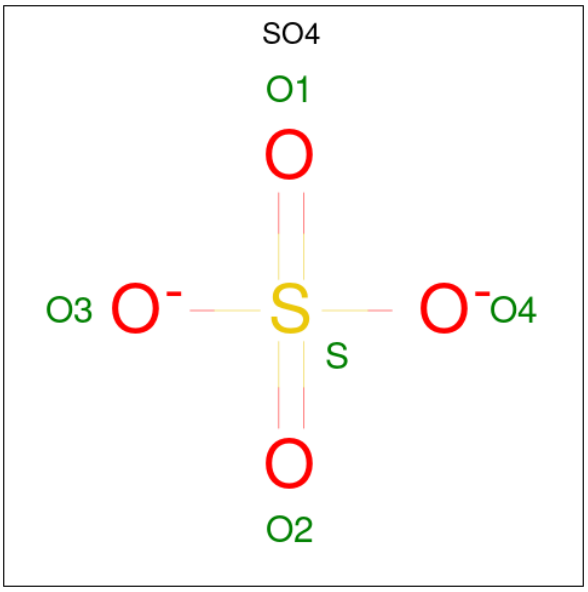
- Molecule 13 is a protein called Proteasome subunit beta type-7.

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

- Molecule 14 is a protein called Proteasome subunit beta type-1.

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

- Molecule 15 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	B	1	Total	O	S		0	0
			5	4	1			
15	C	1	Total	O	S		0	0
			5	4	1			
15	D	1	Total	O	S		0	0
			5	4	1			
15	E	1	Total	O	S		0	0
			5	4	1			
15	E	1	Total	O	S		0	0
			5	4	1			
15	F	1	Total	O	S		0	0
			5	4	1			
15	F	1	Total	O	S		0	0
			5	4	1			
15	G	1	Total	O	S		0	0
			5	4	1			
15	G	1	Total	O	S		0	0
			5	4	1			
15	P	1	Total	O	S		0	0
			5	4	1			
15	Q	1	Total	O	S		0	0
			5	4	1			
15	S	1	Total	O	S		0	0
			5	4	1			
15	S	1	Total	O	S		0	0
			5	4	1			
15	S	1	Total	O	S		0	0
			5	4	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	T	1	Total O S 5 4 1	0	0
15	T	1	Total O S 5 4 1	0	0
15	T	1	Total O S 5 4 1	0	0
15	U	1	Total O S 5 4 1	0	0
15	U	1	Total O S 5 4 1	0	0
15	H	1	Total O S 5 4 1	0	0
15	H	1	Total O S 5 4 1	0	0
15	H	1	Total O S 5 4 1	0	0
15	I	1	Total O S 5 4 1	0	0
15	I	1	Total O S 5 4 1	0	0
15	J	1	Total O S 5 4 1	0	0
15	J	1	Total O S 5 4 1	0	0
15	K	1	Total O S 5 4 1	0	0
15	K	1	Total O S 5 4 1	0	0
15	K	1	Total O S 5 4 1	0	0
15	K	1	Total O S 5 4 1	0	0
15	L	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

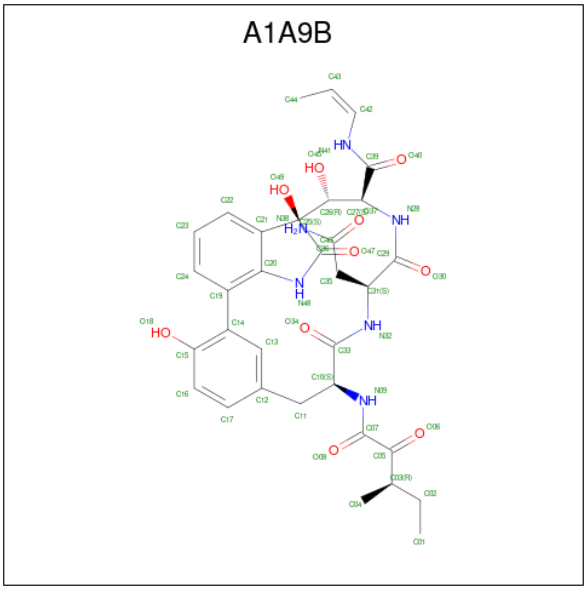
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	N	1	Total O S 5 4 1	0	0
15	V	1	Total O S 5 4 1	0	0
15	V	1	Total O S 5 4 1	0	0
15	W	1	Total O S 5 4 1	0	0
15	X	1	Total O S 5 4 1	0	0
15	Y	1	Total O S 5 4 1	0	0
15	Y	1	Total O S 5 4 1	0	0
15	Y	1	Total O S 5 4 1	0	0
15	Y	1	Total O S 5 4 1	0	0
15	Z	1	Total O S 5 4 1	0	0
15	Z	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	b	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	b	1	Total O S 5 4 1	0	0
15	b	1	Total O S 5 4 1	0	0

- Molecule 16 is (10S,11R,12S,15S,18S)-15-(2-amino-2-oxoethyl)-10,11,23-trihydroxy-18-{[(3R)-3-methyl-2-oxopentanoyl]amino}-9,14,17-trioxo-N-[(1Z)-prop-1-en-1-yl]-8,13,16-triazatetracyclo[18.3.1.0(2,7).0(6,10)]tetracosa-1(24),2,4,6,20,22-hexaene-12-carboxamide (three-letter code: A1A9B) (formula: $C_{33}H_{38}N_6O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	H	1	Total C N O 49 33 6 10	0	0
16	K	1	Total C N O 49 33 6 10	0	0
16	N	1	Total C N O 49 33 6 10	0	0
16	V	1	Total C N O 49 33 6 10	0	0
16	Y	1	Total C N O 49 33 6 10	0	0
16	b	1	Total C N O 49 33 6 10	0	0

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	I	1	Total Mg 1 1	0	0
17	L	1	Total Mg 1 1	0	0
17	W	1	Total Mg 1 1	0	0
17	Y	1	Total Mg 1 1	0	0
17	Z	1	Total Mg 1 1	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	20	Total O 20 20	0	0
18	B	17	Total O 17 17	0	0
18	C	6	Total O 6 6	0	0
18	D	4	Total O 4 4	0	0
18	E	4	Total O 4 4	0	0
18	F	5	Total O 5 5	0	0
18	G	8	Total O 8 8	0	0
18	O	6	Total O 6 6	0	0
18	P	12	Total O 12 12	0	0
18	Q	10	Total O 10 10	0	0
18	R	4	Total O 4 4	0	0
18	S	3	Total O 3 3	0	0
18	T	11	Total O 11 11	0	0
18	U	9	Total O 9 9	0	0
18	H	13	Total O 13 13	0	0

Continued on next page...

Continued from previous page...

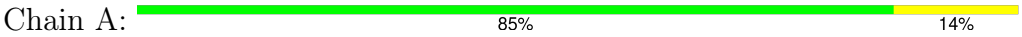
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	I	8	Total O 8 8	0	0
18	J	15	Total O 15 15	0	0
18	K	16	Total O 16 16	0	0
18	L	25	Total O 25 25	0	0
18	M	12	Total O 12 12	0	0
18	N	13	Total O 13 13	0	0
18	V	19	Total O 19 19	0	0
18	W	6	Total O 6 6	0	0
18	X	18	Total O 18 18	0	0
18	Y	8	Total O 8 8	0	0
18	Z	22	Total O 22 22	0	0
18	a	15	Total O 15 15	0	0
18	b	10	Total O 10 10	0	0

3 Residue-property plots (i)

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

• Molecule 1: Proteasome subunit alpha type-2

Chain A:

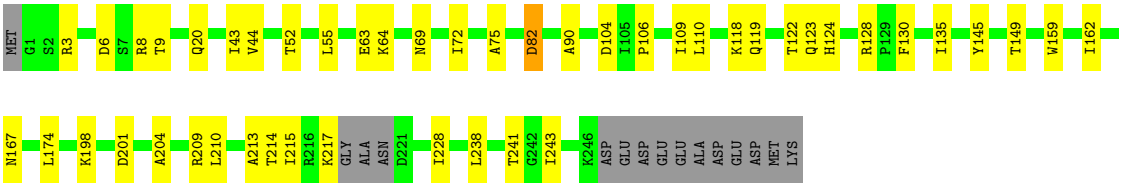


• Molecule 1: Proteasome subunit alpha type-2

Chain O:

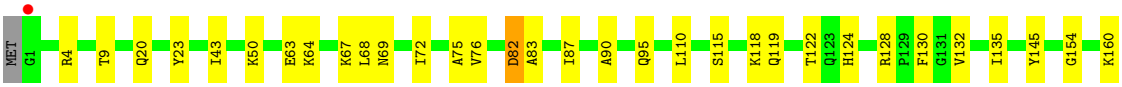
• Molecule 2: Proteasome subunit alpha type-3

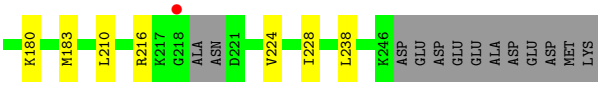
Chain B:



• Molecule 2: Proteasome subunit alpha type-3

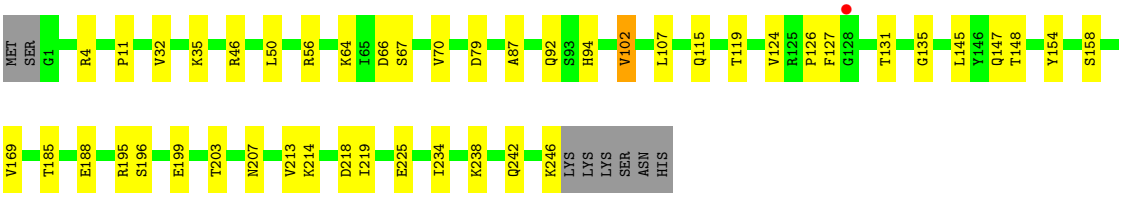
Chain P:





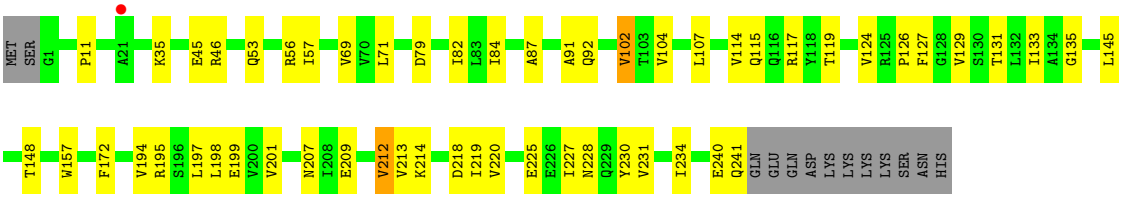
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



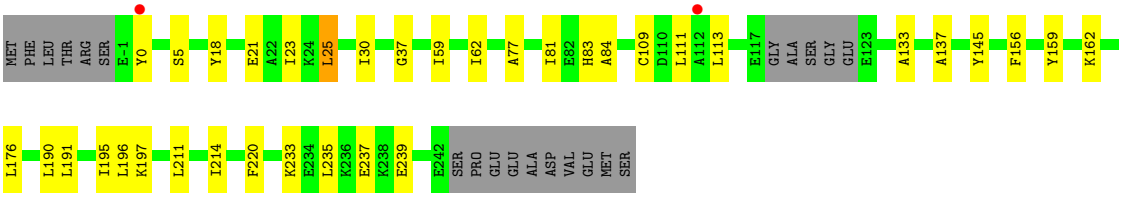
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



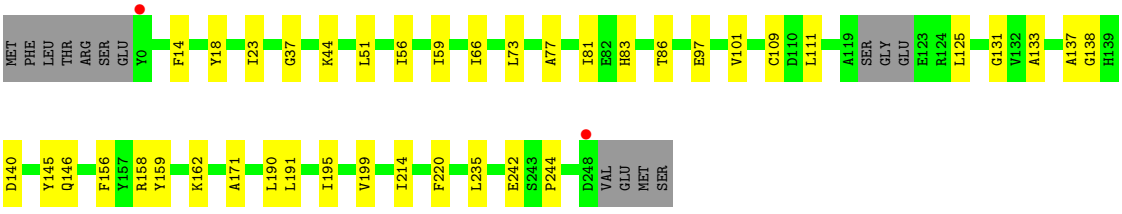
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



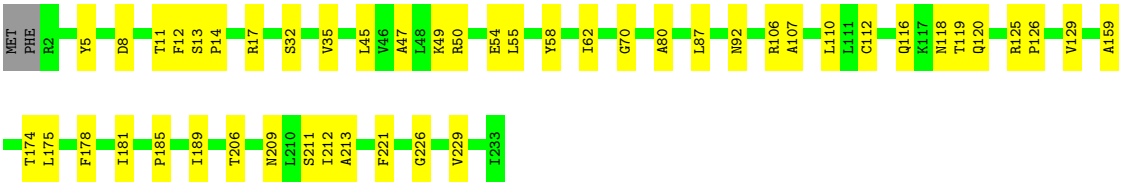
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



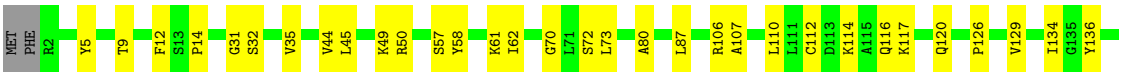
• Molecule 5: Proteasome subunit alpha type-6

Chain E:



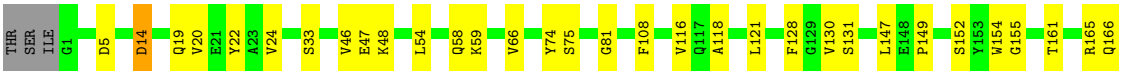
• Molecule 5: Proteasome subunit alpha type-6

Chain S:



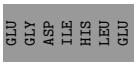
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



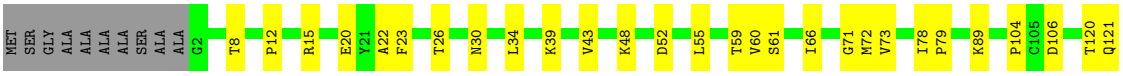
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



• Molecule 7: Proteasome subunit alpha type-1

Chain G:

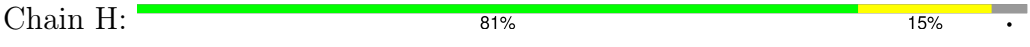


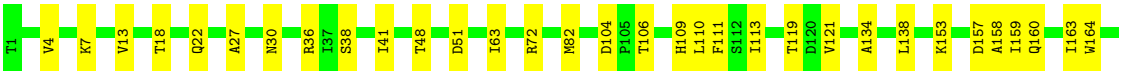
• Molecule 7: Proteasome subunit alpha type-1

Chain U:

• Molecule 8: Proteasome subunit beta type-2

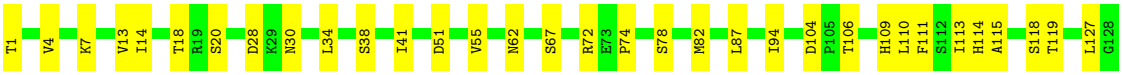
Chain H:





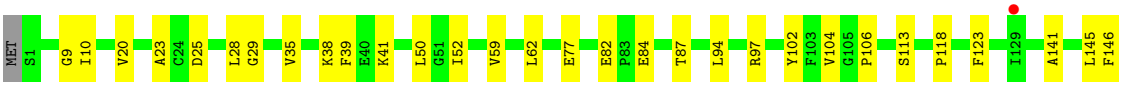
• Molecule 8: Proteasome subunit beta type-2

Chain V:



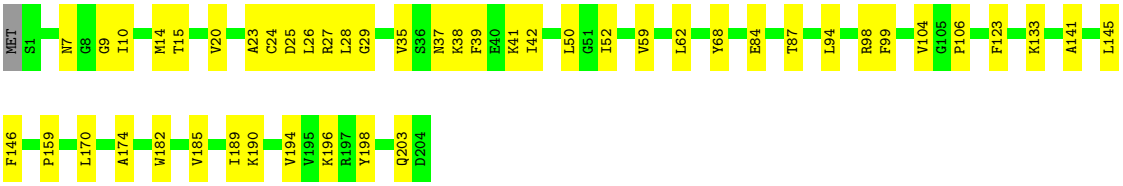
• Molecule 9: Proteasome subunit beta type-3

Chain I:

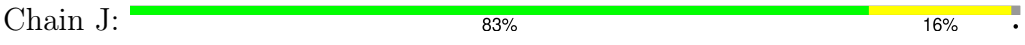


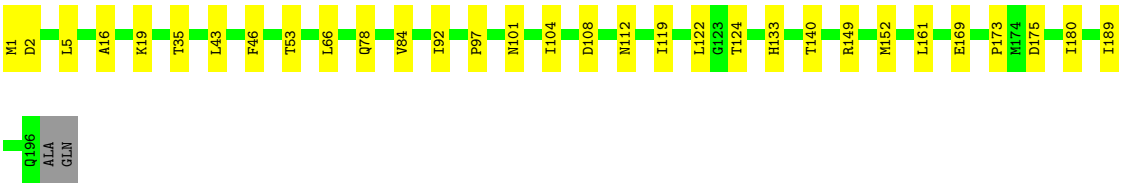
• Molecule 9: Proteasome subunit beta type-3

Chain W:

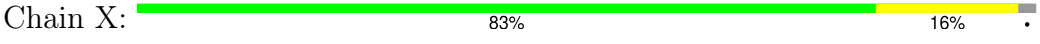


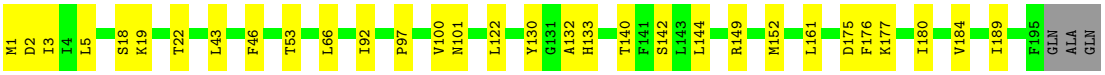
• Molecule 10: Proteasome subunit beta type-4



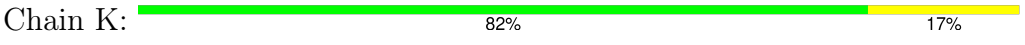


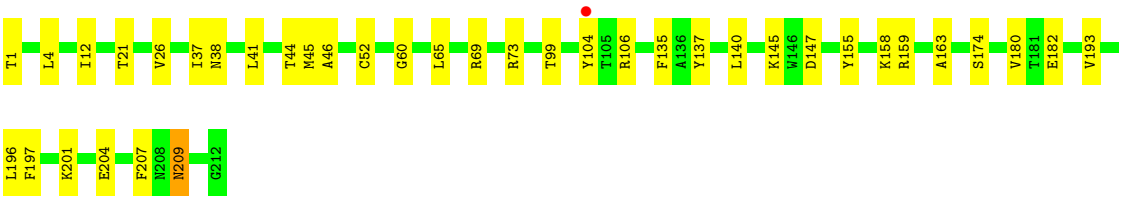
• Molecule 10: Proteasome subunit beta type-4



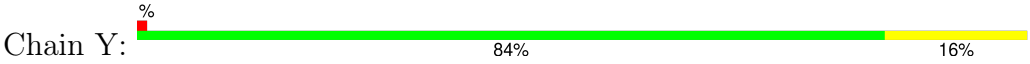


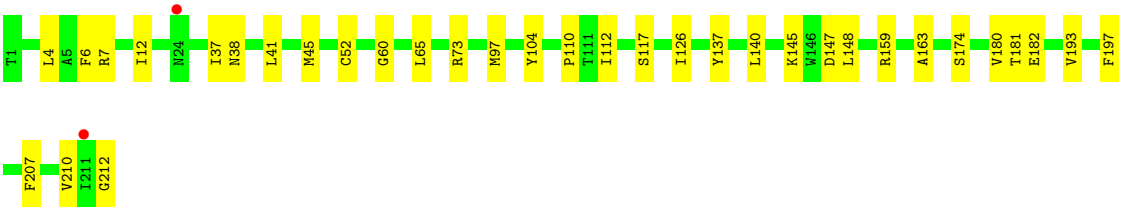
• Molecule 11: Proteasome subunit beta type-5



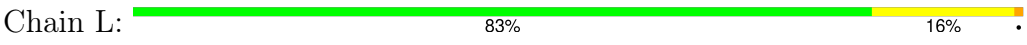


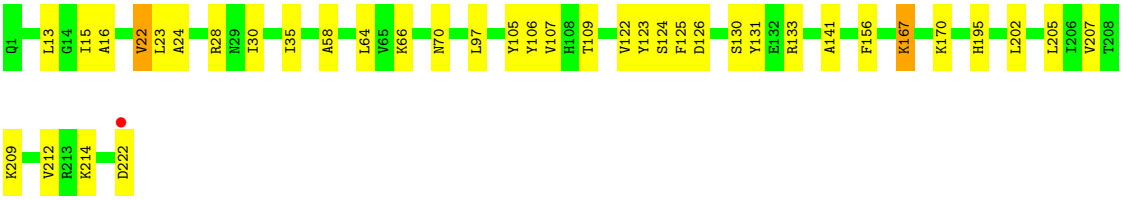
• Molecule 11: Proteasome subunit beta type-5



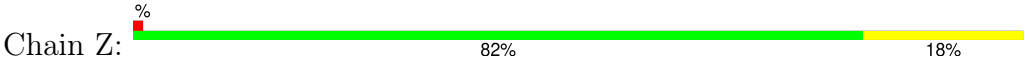


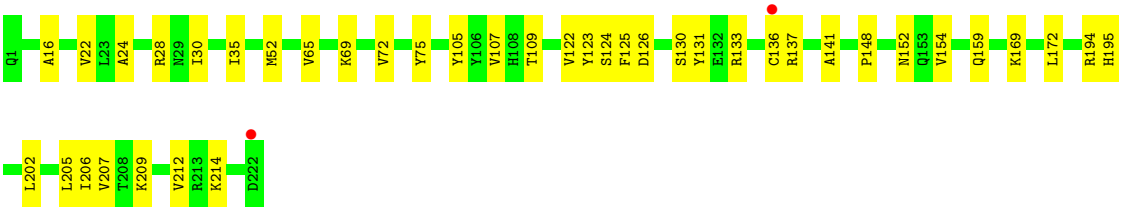
• Molecule 12: Proteasome subunit beta type-6



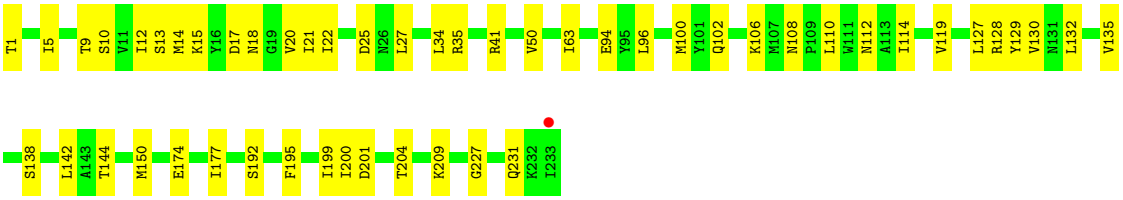


• Molecule 12: Proteasome subunit beta type-6

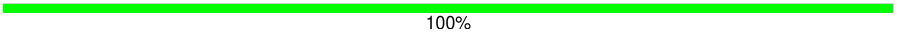




• Molecule 13: Proteasome subunit beta type-7

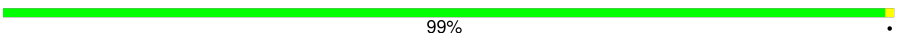


• Molecule 13: Proteasome subunit beta type-7



• Molecule 14: Proteasome subunit beta type-1

• Molecule 14: Proteasome subunit beta type-1




T1
K83
L196

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.37Å 299.67Å 144.66Å 90.00° 112.89° 90.00°	Depositor
Resolution (Å)	48.90 – 3.44 48.90 – 3.44	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.90-3.44) 86.9 (48.90-3.44)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.182 , 0.235 0.182 , 0.236	Depositor DCC
R_{free} test set	6810 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	67.4	Xtriage
Anisotropy	0.892	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 85.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	50447	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, SO4, A1A9B

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	0.25	0/1944	0.47	0/2632
1	O	0.25	0/1944	0.46	0/2632
2	B	0.25	0/1934	0.49	0/2614
2	P	0.25	0/1938	0.48	0/2619
3	C	0.25	0/1963	0.50	0/2656
3	Q	0.25	0/1919	0.50	0/2598
4	D	0.24	0/1879	0.47	0/2531
4	R	0.24	0/1924	0.47	0/2593
5	E	0.25	0/1811	0.49	0/2447
5	S	0.25	0/1811	0.49	0/2447
6	F	0.26	0/1936	0.46	0/2614
6	T	0.25	0/1944	0.47	0/2625
7	G	0.25	0/1954	0.48	0/2645
7	U	0.25	0/1954	0.47	0/2645
8	H	0.24	0/1715	0.47	0/2326
8	V	0.24	0/1715	0.47	0/2326
9	I	0.25	0/1611	0.47	0/2174
9	W	0.25	0/1611	0.48	0/2174
10	J	0.25	0/1598	0.48	0/2154
10	X	0.25	0/1589	0.49	0/2142
11	K	0.25	0/1681	0.48	0/2274
11	Y	0.25	0/1681	0.48	0/2274
12	L	0.25	0/1795	0.49	0/2420
12	Z	0.26	0/1795	0.49	0/2420
13	M	0.25	0/1855	0.50	0/2514
13	a	0.25	0/1855	0.49	0/2514
14	N	0.24	0/1541	0.48	0/2087
14	b	0.25	0/1541	0.48	0/2087
All	All	0.25	0/50438	0.48	0/68184

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1907	0	1917	25	0
1	O	1907	0	1917	29	0
2	B	1905	0	1915	31	0
2	P	1909	0	1918	28	0
3	C	1934	0	1942	31	0
3	Q	1890	0	1903	41	0
4	D	1854	0	1831	24	0
4	R	1898	0	1866	24	0
5	E	1784	0	1788	31	0
5	S	1784	0	1788	30	0
6	F	1896	0	1889	27	0
6	T	1904	0	1900	28	0
7	G	1916	0	1905	34	0
7	U	1916	0	1905	33	0
8	H	1684	0	1688	19	0
8	V	1684	0	1688	26	0
9	I	1581	0	1574	23	0
9	W	1581	0	1574	30	0
10	J	1570	0	1577	19	0
10	X	1561	0	1569	22	0
11	K	1644	0	1595	23	0
11	Y	1644	0	1595	19	0
12	L	1757	0	1711	21	0
12	Z	1757	0	1711	24	0
13	M	1824	0	1832	33	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	20	0
14	b	1512	0	1481	0	0
15	B	5	0	0	0	0
15	C	5	0	0	0	0
15	D	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	E	10	0	0	1	0
15	F	10	0	0	0	0
15	G	10	0	0	0	0
15	H	15	0	0	0	0
15	I	10	0	0	0	0
15	J	10	0	0	0	0
15	K	20	0	0	0	0
15	L	5	0	0	0	0
15	M	40	0	0	0	0
15	N	5	0	0	0	0
15	P	5	0	0	0	0
15	Q	5	0	0	0	0
15	S	15	0	0	0	0
15	T	15	0	0	0	0
15	U	10	0	0	1	0
15	V	10	0	0	0	0
15	W	5	0	0	0	0
15	X	5	0	0	0	0
15	Y	20	0	0	0	0
15	Z	10	0	0	0	0
15	a	25	0	0	0	0
15	b	15	0	0	0	0
16	H	49	0	0	0	0
16	K	49	0	0	1	0
16	N	49	0	0	1	0
16	V	49	0	0	1	0
16	Y	49	0	0	0	0
16	b	49	0	0	0	0
17	I	1	0	0	0	0
17	L	1	0	0	0	0
17	W	1	0	0	0	0
17	Y	1	0	0	0	0
17	Z	1	0	0	0	0
18	A	20	0	0	0	0
18	B	17	0	0	0	0
18	C	6	0	0	0	0
18	D	4	0	0	0	0
18	E	4	0	0	0	0
18	F	5	0	0	0	0
18	G	8	0	0	0	0
18	H	13	0	0	0	0
18	I	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	J	15	0	0	0	0
18	K	16	0	0	0	0
18	L	25	0	0	0	0
18	M	12	0	0	0	0
18	N	13	0	0	0	0
18	O	6	0	0	0	0
18	P	12	0	0	0	0
18	Q	10	0	0	0	0
18	R	4	0	0	0	0
18	S	3	0	0	0	0
18	T	11	0	0	0	0
18	U	9	0	0	2	0
18	V	19	0	0	0	0
18	W	6	0	0	0	0
18	X	18	0	0	0	0
18	Y	8	0	0	0	0
18	Z	22	0	0	0	0
18	a	15	0	0	0	0
18	b	10	0	0	0	0
All	All	50447	0	49292	629	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 7.

All (629) 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)
3:C:131:THR:HG1	3:C:148:THR:HG1	1.28	0.82
8:H:213:LEU:HD13	11:Y:212:GLY:HA2	1.64	0.79
2:P:4:ARG:HH12	6:T:7:SER:HB2	1.50	0.77
2:B:90:ALA:HB1	2:B:110:LEU:HD21	1.66	0.76
13:M:201:ASP:HB3	13:M:204:THR:HG22	1.67	0.76
3:C:64:LYS:HE3	3:C:219:ILE:HD12	1.68	0.74
4:R:242:GLU:HG3	4:R:244:PRO:HD3	1.71	0.73
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.71	0.72
3:Q:212:VAL:HG13	3:Q:220:VAL:HG13	1.72	0.72
2:P:82:ASP:HB3	2:P:130:PHE:HD1	1.56	0.70
3:Q:71:LEU:HD11	3:Q:131:THR:HB	1.73	0.70
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.75	0.69
8:H:38:SER:HB3	8:H:41:ILE:HB	1.73	0.69
7:G:195:GLU:OE2	7:G:235:ARG:NH1	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.74	0.68
3:C:79:ASP:HB3	3:C:127:PHE:HD1	1.59	0.68
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.74	0.68
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.77	0.67
3:Q:79:ASP:HB3	3:Q:127:PHE:HD1	1.59	0.67
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.77	0.66
2:B:135:ILE:HG12	2:B:149:THR:HG22	1.77	0.66
10:J:5:LEU:HD21	10:J:140:THR:HG21	1.78	0.66
2:B:119:GLN:NE2	2:B:123:GLN:OE1	2.29	0.66
5:E:32:SER:HB3	5:E:50:ARG:HG3	1.78	0.66
6:F:14:ASP:OD1	6:F:14:ASP:N	2.28	0.66
12:Z:24:ALA:HB1	12:Z:202:LEU:HD11	1.77	0.65
3:Q:198:LEU:HD11	3:Q:231:VAL:HG12	1.78	0.65
11:K:4:LEU:HD13	11:K:140:LEU:HD11	1.79	0.65
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.79	0.65
13:M:13:SER:HB3	13:M:22:ILE:HG13	1.78	0.65
5:E:62:ILE:HG21	5:E:213:ALA:HB2	1.79	0.65
8:V:38:SER:HB3	8:V:41:ILE:HB	1.78	0.65
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.77	0.64
2:B:63:GLU:HG3	2:B:64:LYS:HG2	1.79	0.64
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.77	0.64
5:S:116:GLN:NE2	5:S:120:GLN:OE1	2.30	0.64
7:U:125:MET:O	18:U:401:HOH:O	2.15	0.64
13:M:21:ILE:HG12	13:M:199:ILE:HG23	1.80	0.64
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.80	0.64
7:U:31:ILE:HG23	7:U:47:GLN:HB2	1.80	0.63
2:P:90:ALA:HB1	2:P:110:LEU:HD21	1.79	0.63
2:B:44:VAL:HG22	2:B:214:THR:HG22	1.80	0.63
4:D:176:LEU:HD12	5:E:55:LEU:HG	1.81	0.63
10:J:173:PRO:HB3	10:X:22:THR:HG21	1.81	0.63
6:T:175:LEU:HD23	6:T:183:LEU:HD11	1.81	0.62
12:L:207:VAL:HG22	12:L:212:VAL:HG22	1.81	0.62
12:Z:207:VAL:HG22	12:Z:212:VAL:HG22	1.81	0.62
3:Q:214:LYS:HB2	3:Q:218:ASP:HB3	1.81	0.62
1:O:118:MET:O	1:O:122:THR:HG23	2.00	0.62
12:Z:30:ILE:HG22	12:Z:35:ILE:HA	1.80	0.62
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.65	0.61
3:C:35:LYS:HE3	3:C:145:LEU:HB3	1.82	0.61
13:M:9:THR:OG1	13:M:10:SER:N	2.34	0.61
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.81	0.61
3:C:35:LYS:HD2	3:C:158:SER:HA	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:119:THR:HG22	5:E:126:PRO:HB3	1.82	0.61
10:J:92:ILE:HG21	10:J:122:LEU:HA	1.83	0.61
10:X:18:SER:HB2	10:X:176:PHE:HB2	1.83	0.61
2:P:63:GLU:HG3	2:P:64:LYS:HG2	1.82	0.61
2:P:145:TYR:O	3:Q:56:ARG:NH2	2.34	0.61
13:M:129:TYR:HE2	13:M:144:THR:HG22	1.64	0.61
2:B:204:ALA:O	2:B:209:ARG:NH2	2.35	0.60
1:O:222:LEU:HG	1:O:232:GLY:HA2	1.83	0.60
11:Y:147:ASP:OD1	11:Y:147:ASP:N	2.33	0.60
7:U:122:ARG:O	18:U:401:HOH:O	2.16	0.60
7:G:66:ILE:HD11	7:G:72:MET:HE1	1.83	0.60
7:U:66:ILE:HD11	7:U:72:MET:HE2	1.84	0.60
9:I:189:ILE:HG23	9:I:194:VAL:HG22	1.83	0.60
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.83	0.60
9:W:189:ILE:HG23	9:W:194:VAL:HG22	1.83	0.60
4:R:66:ILE:HD13	4:R:138:GLY:HA3	1.84	0.59
7:U:148:THR:HG22	7:U:154:TYR:HB2	1.84	0.59
7:G:135:VAL:HG12	7:G:145:ILE:HG12	1.85	0.59
7:G:148:THR:HG22	7:G:154:TYR:HB2	1.85	0.59
11:Y:145:LYS:HG2	11:Y:148:LEU:HG	1.84	0.59
3:C:87:ALA:HB1	3:C:107:LEU:HD21	1.84	0.59
4:R:23:ILE:HD13	4:R:133:ALA:HB2	1.84	0.59
8:V:134:ALA:HB1	8:V:158:ALA:HB1	1.85	0.59
9:W:27:ARG:HB2	9:W:182:TRP:HB2	1.84	0.59
12:Z:52:MET:HE1	12:Z:65:VAL:HA	1.83	0.59
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.68	0.58
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.85	0.58
7:G:138:ASP:OD2	8:H:72:ARG:NH2	2.36	0.58
8:V:18:THR:HB	8:V:30:ASN:HA	1.84	0.58
1:O:119:GLN:NE2	1:O:123:GLN:OE1	2.34	0.58
11:K:21:THR:HG22	11:K:26:VAL:HG12	1.85	0.58
12:L:24:ALA:HB1	12:L:202:LEU:HD11	1.86	0.58
2:P:160:LYS:NZ	3:Q:53:GLN:O	2.36	0.58
11:K:45:MET:HB3	11:K:52:CYS:HB3	1.86	0.58
3:C:214:LYS:HB2	3:C:218:ASP:HB3	1.85	0.58
3:Q:56:ARG:HG3	3:Q:57:ILE:HG23	1.85	0.58
11:K:209:ASN:O	9:W:38:LYS:NZ	2.32	0.58
13:M:1:THR:N	13:M:108:ASN:OD1	2.36	0.58
1:O:111:VAL:HG22	1:O:136:ILE:HD12	1.86	0.57
3:Q:46:ARG:HB3	3:Q:207:ASN:HA	1.85	0.57
9:I:52:ILE:HB	9:I:59:VAL:HG13	1.84	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:9:THR:HG21	5:S:126:PRO:HD3	1.85	0.57
4:R:190:LEU:HD22	4:R:235:LEU:HB2	1.85	0.57
5:S:5:TYR:OH	6:T:5:ASP:OD2	2.20	0.57
13:M:174:GLU:OE2	13:M:209:LYS:NZ	2.37	0.57
8:H:13:VAL:HG22	8:H:177:VAL:HG13	1.86	0.57
7:U:135:VAL:HG12	7:U:145:ILE:HG12	1.87	0.57
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.86	0.56
6:F:33:SER:HG	6:F:75:SER:HG	1.52	0.56
6:T:185:ALA:HB3	6:T:219:GLU:HG3	1.88	0.56
8:H:18:THR:HB	8:H:30:ASN:HA	1.85	0.56
12:L:109:THR:HB	12:L:125:PHE:HB2	1.86	0.56
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.88	0.56
10:J:175:ASP:HB2	10:X:175:ASP:HB2	1.86	0.56
12:L:66:LYS:NZ	13:M:94:GLU:OE2	2.38	0.56
12:Z:109:THR:HB	12:Z:125:PHE:HB2	1.86	0.56
5:E:116:GLN:NE2	5:E:120:GLN:OE1	2.38	0.56
13:M:12:ILE:HD11	13:M:177:ILE:HG23	1.87	0.56
4:D:233:LYS:NZ	4:D:237:GLU:OE2	2.39	0.55
3:C:70:VAL:HG13	3:C:219:ILE:HD13	1.88	0.55
7:U:89:LYS:NZ	15:U:301:SO4:O4	2.37	0.55
11:K:12:ILE:HB	11:K:180:VAL:HB	1.88	0.55
5:E:178:PHE:HA	5:E:181:ILE:HG13	1.89	0.55
11:K:209:ASN:H	11:K:209:ASN:HD22	1.54	0.55
2:P:68:LEU:HD21	2:P:87:ILE:HD12	1.88	0.55
11:Y:7:ARG:NH1	11:Y:110:PRO:O	2.37	0.55
3:Q:213:VAL:HG22	3:Q:219:ILE:HD12	1.89	0.55
12:L:205:LEU:HD22	12:L:214:LYS:HG2	1.88	0.55
7:U:138:ASP:OD2	8:V:72:ARG:NH2	2.40	0.55
12:Z:22:VAL:HG12	12:Z:206:ILE:HG12	1.89	0.55
6:F:58:GLN:OE1	6:F:228:LYS:NZ	2.40	0.55
1:O:49:LYS:HG2	1:O:58:SER:HB2	1.89	0.55
10:J:19:LYS:HG2	10:J:180:ILE:HG13	1.88	0.55
3:Q:71:LEU:HD13	3:Q:133:ILE:HG12	1.88	0.54
12:L:30:ILE:HG22	12:L:35:ILE:HA	1.89	0.54
10:X:92:ILE:HG21	10:X:122:LEU:HA	1.90	0.54
14:N:65:LEU:HG	14:N:69:GLN:HE21	1.71	0.54
3:Q:114:VAL:HG22	3:Q:117:ARG:HH12	1.72	0.54
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.89	0.54
1:O:99:ARG:NH2	8:V:62:ASN:OD1	2.40	0.54
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.89	0.54
2:B:82:ASP:OD1	2:B:82:ASP:N	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:82:ASP:OD1	2:P:82:ASP:N	2.40	0.54
13:M:96:LEU:O	13:M:100:MET:HG2	2.07	0.54
10:X:1:MET:HG2	10:X:2:ASP:H	1.73	0.54
10:X:19:LYS:HG2	10:X:180:ILE:HG13	1.90	0.54
3:C:185:THR:HG23	3:C:188:GLU:H	1.72	0.53
4:R:83:HIS:CG	4:R:111:LEU:HD11	2.43	0.53
2:P:67:LYS:HE3	2:P:228:ILE:HD13	1.90	0.53
4:R:77:ALA:O	4:R:81:ILE:HG12	2.09	0.53
10:X:5:LEU:HD11	10:X:140:THR:HG21	1.90	0.53
1:O:44:VAL:HG22	1:O:213:ILE:HG22	1.89	0.53
4:R:66:ILE:HD11	4:R:101:VAL:HG22	1.89	0.53
5:S:31:GLY:HA2	5:S:50:ARG:HH22	1.74	0.53
2:B:241:THR:HG23	2:B:243:ILE:HG12	1.90	0.53
5:E:13:SER:HB3	5:E:17:ARG:H	1.74	0.53
9:W:10:ILE:HD11	9:W:174:ALA:HB2	1.91	0.53
5:S:80:ALA:HB2	5:S:129:VAL:HG21	1.91	0.53
9:W:23:ALA:HB1	9:W:170:LEU:HD22	1.91	0.53
2:B:174:LEU:HD11	2:B:198:LYS:HD3	1.91	0.52
6:F:48:LYS:NZ	6:F:59:LYS:O	2.39	0.52
1:A:127:VAL:HG23	7:G:121:GLN:HG2	1.91	0.52
4:D:23:ILE:HD13	4:D:133:ALA:HB2	1.90	0.52
3:Q:69:VAL:HG12	3:Q:104:VAL:HG22	1.91	0.52
7:U:219:ALA:HB2	7:U:224:PHE:HD1	1.73	0.52
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.91	0.52
4:R:109:CYS:SG	4:R:156:PHE:HB3	2.50	0.52
6:F:205:GLU:HG3	6:F:206:LYS:HG2	1.91	0.52
14:N:13:ILE:HG12	14:N:177:VAL:HG13	1.91	0.52
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.91	0.52
11:Y:12:ILE:HB	11:Y:180:VAL:HB	1.90	0.52
5:E:45:LEU:HB2	5:E:213:ALA:HB3	1.92	0.52
5:S:144:LEU:HD22	5:S:152:VAL:HG12	1.90	0.52
6:T:16:ARG:HE	6:T:18:PHE:HE1	1.56	0.52
13:M:128:ARG:HH11	13:M:138:SER:HB2	1.75	0.52
11:Y:45:MET:HB3	11:Y:52:CYS:HB3	1.91	0.52
11:Y:104:TYR:CZ	11:Y:182:GLU:HG2	2.44	0.52
6:F:131:SER:HB2	6:F:161:THR:HG21	1.92	0.51
10:J:92:ILE:HA	10:J:97:PRO:HB3	1.90	0.51
13:M:114:ILE:HB	13:M:130:VAL:HG12	1.91	0.51
11:Y:97:MET:N	11:Y:117:SER:OG	2.43	0.51
10:X:3:ILE:HB	10:X:18:SER:HB3	1.92	0.51
6:T:48:LYS:NZ	6:T:59:LYS:O	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:216:ARG:O	2:P:224:VAL:HA	2.11	0.51
10:J:108:ASP:O	10:J:112:ASN:N	2.43	0.51
10:X:184:VAL:HG22	10:X:189:ILE:HG12	1.92	0.51
4:D:159:TYR:CG	4:D:162:LYS:HB2	2.46	0.51
6:T:9:SER:HB2	7:U:126:ARG:HD3	1.93	0.51
6:T:46:VAL:HB	6:T:73:VAL:HG21	1.92	0.51
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.45	0.51
3:Q:131:THR:HG1	3:Q:148:THR:HG1	1.45	0.51
10:J:84:VAL:HG21	10:J:104:ILE:HD11	1.93	0.51
10:X:92:ILE:HA	10:X:97:PRO:HB3	1.93	0.51
5:E:5:TYR:OH	6:F:5:ASP:OD2	2.22	0.51
6:F:154:TRP:CZ3	7:G:60:VAL:HA	2.46	0.51
7:G:191:GLU:HB3	7:G:235:ARG:NH1	2.26	0.51
3:C:169:VAL:HG13	3:C:196:SER:HB3	1.93	0.50
5:E:80:ALA:HB2	5:E:129:VAL:HG21	1.91	0.50
4:R:73:LEU:HD12	4:R:131:GLY:HA3	1.94	0.50
3:C:92:GLN:HG3	10:J:66:LEU:HB2	1.92	0.50
8:V:109:HIS:HB3	8:V:111:PHE:CE2	2.46	0.50
3:C:213:VAL:HG22	3:C:219:ILE:HG23	1.93	0.50
7:G:52:ASP:HB3	7:G:55:LEU:HG	1.93	0.50
3:Q:71:LEU:HD23	3:Q:84:ILE:HG12	1.92	0.50
12:L:123:TYR:CE2	12:L:133:ARG:HB2	2.46	0.50
4:D:5:SER:O	5:E:125:ARG:HB3	2.11	0.50
8:H:111:PHE:HD1	8:H:121:VAL:HG22	1.76	0.50
3:Q:197:LEU:O	3:Q:201:VAL:HG22	2.10	0.50
7:U:190:TRP:HZ3	7:U:227:LEU:HD11	1.77	0.50
10:X:46:PHE:HD2	10:X:53:THR:HB	1.77	0.50
1:A:200:VAL:HG21	1:A:204:PHE:CD1	2.47	0.50
5:E:92:ASN:ND2	12:L:70:ASN:OD1	2.40	0.50
12:Z:123:TYR:CE2	12:Z:133:ARG:HB2	2.47	0.50
4:R:159:TYR:CE2	4:R:162:LYS:HD3	2.46	0.49
3:C:119:THR:HG22	3:C:126:PRO:HB3	1.94	0.49
5:S:178:PHE:HA	5:S:181:ILE:HG13	1.94	0.49
7:U:195:GLU:HG3	7:U:235:ARG:HD3	1.94	0.49
3:Q:131:THR:OG1	3:Q:148:THR:OG1	2.19	0.49
6:T:74:TYR:HB2	6:T:130:VAL:CG2	2.43	0.49
9:W:15:THR:HG22	9:W:20:VAL:HG12	1.94	0.49
3:C:203:THR:OG1	3:C:207:ASN:ND2	2.41	0.49
4:D:109:CYS:SG	4:D:156:PHE:HB3	2.52	0.49
9:I:62:LEU:HD12	9:I:104:VAL:HG21	1.94	0.49
11:Y:38:ASN:ND2	11:Y:41:LEU:HB2	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:181:THR:OG1	11:Y:182:GLU:N	2.46	0.49
7:U:168:GLU:OE1	7:U:168:GLU:N	2.42	0.49
1:A:123:GLN:HG3	2:B:128:ARG:HG2	1.94	0.49
9:W:52:ILE:HG22	9:W:59:VAL:HG22	1.95	0.49
5:S:49:LYS:HB3	5:S:58:TYR:HB3	1.95	0.49
12:L:124:SER:O	12:L:131:TYR:HA	2.13	0.49
11:Y:4:LEU:HD13	11:Y:140:LEU:HD11	1.94	0.49
2:B:9:THR:HB	2:B:20:GLN:HG3	1.95	0.49
3:Q:87:ALA:HB1	3:Q:107:LEU:HD11	1.94	0.49
14:N:40:LYS:HE2	14:N:182:GLY:HA2	1.95	0.49
2:B:167:ASN:ND2	2:B:201:ASP:OD1	2.45	0.49
14:N:59:VAL:HG22	14:N:81:VAL:HG12	1.94	0.48
9:W:189:ILE:HG12	9:W:194:VAL:HG13	1.95	0.48
10:J:43:LEU:HB2	10:J:189:ILE:HD13	1.95	0.48
1:A:85:LEU:HD23	1:A:134:LEU:HD11	1.94	0.48
6:F:118:ALA:HA	6:F:121:LEU:HD12	1.95	0.48
6:T:5:ASP:HB3	6:T:18:PHE:HD2	1.79	0.48
6:T:171:GLU:HG2	6:T:195:ILE:HG12	1.95	0.48
11:K:65:LEU:HB3	11:K:69:ARG:NH1	2.28	0.48
11:K:201:LYS:NZ	11:K:207:PHE:O	2.40	0.48
12:L:64:LEU:HD21	12:L:97:LEU:HD21	1.94	0.48
12:L:141:ALA:HB1	12:L:195:HIS:NE2	2.28	0.48
14:N:12:VAL:HG21	14:N:100:ALA:HB1	1.95	0.48
10:X:53:THR:HG22	10:X:100:VAL:HG13	1.96	0.48
3:C:46:ARG:HB3	3:C:207:ASN:HA	1.94	0.48
4:R:159:TYR:CG	4:R:162:LYS:HB2	2.48	0.48
5:S:32:SER:HB3	5:S:50:ARG:HB2	1.95	0.48
13:M:129:TYR:HB2	13:M:142:LEU:HD13	1.96	0.48
13:M:25:ASP:HA	13:M:195:PHE:HA	1.96	0.48
13:M:119:VAL:HG23	13:M:200:ILE:HG22	1.95	0.48
6:F:185:ALA:HB3	6:F:219:GLU:HG3	1.96	0.48
1:O:62:SER:OG	1:O:64:VAL:O	2.31	0.48
3:Q:119:THR:HG22	3:Q:126:PRO:HB3	1.96	0.48
12:Z:69:LYS:O	12:Z:72:VAL:HG12	2.13	0.48
3:C:32:VAL:HG11	3:C:169:VAL:HG11	1.95	0.48
7:G:106:ASP:OD1	7:G:106:ASP:N	2.46	0.48
3:Q:228:ASN:HA	3:Q:231:VAL:HG22	1.96	0.48
2:P:83:ALA:O	2:P:87:ILE:HG12	2.13	0.48
4:R:191:LEU:O	4:R:195:ILE:HG12	2.14	0.48
3:C:238:LYS:O	3:C:242:GLN:HG2	2.14	0.47
3:Q:195:ARG:O	3:Q:199:GLU:HG2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:101:ASN:HB3	10:J:133:HIS:CE1	2.48	0.47
13:M:25:ASP:OD1	13:M:41:ARG:NH1	2.37	0.47
12:Z:152:ASN:O	12:Z:159:GLN:NE2	2.47	0.47
2:P:69:ASN:OD1	2:P:72:ILE:N	2.47	0.47
4:R:171:ALA:HB2	4:R:199:VAL:HG11	1.97	0.47
7:U:187:GLU:HG2	7:U:192:LYS:CB	2.44	0.47
4:D:21:GLU:O	4:D:25:LEU:HD13	2.13	0.47
1:O:215:GLY:O	1:O:234:ARG:HD2	2.15	0.47
2:B:118:LYS:O	2:B:122:THR:HG23	2.14	0.47
2:B:210:LEU:HD12	2:B:238:LEU:HD11	1.95	0.47
5:E:175:LEU:HD12	6:F:54:LEU:HD23	1.96	0.47
1:O:21:ILE:HD11	1:O:122:THR:HB	1.97	0.47
2:B:145:TYR:HE1	2:B:215:ILE:HG22	1.79	0.47
3:C:147:GLN:O	3:C:154:TYR:HA	2.14	0.47
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.50	0.47
6:F:186:ARG:O	6:F:190:LYS:HG3	2.15	0.47
1:A:31:GLY:O	1:A:166:LYS:HG3	2.15	0.47
2:B:3:ARG:NH1	5:E:8:ASP:OD1	2.48	0.47
3:C:94:HIS:HB3	3:C:102:VAL:HG12	1.96	0.47
4:D:159:TYR:CE2	4:D:162:LYS:HD3	2.49	0.47
4:D:197:LYS:NZ	4:D:239:GLU:OE1	2.39	0.47
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.50	0.47
2:P:210:LEU:HD12	2:P:238:LEU:HD11	1.96	0.47
7:U:5:ARG:HD3	7:U:17:TYR:CD2	2.49	0.47
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.97	0.47
10:J:1:MET:HG2	10:J:2:ASP:H	1.79	0.47
10:J:46:PHE:HD2	10:J:53:THR:HB	1.79	0.47
13:M:63:ILE:HD13	13:M:114:ILE:HD11	1.97	0.47
8:V:222:ASP:N	8:V:222:ASP:OD1	2.48	0.47
5:E:47:ALA:HB3	5:E:211:SER:OG	2.15	0.47
6:T:74:TYR:HB2	6:T:130:VAL:HG21	1.96	0.47
11:K:159:ARG:NH1	11:K:163:ALA:HB2	2.30	0.47
6:F:155:GLY:HA3	7:G:59:THR:HG21	1.96	0.47
9:W:84:GLU:OE1	9:W:84:GLU:N	2.39	0.47
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.97	0.47
5:S:62:ILE:HG21	5:S:213:ALA:HB2	1.97	0.46
2:B:82:ASP:HB3	2:B:130:PHE:HD1	1.79	0.46
7:G:219:ALA:HB2	7:G:224:PHE:HD1	1.80	0.46
1:O:123:GLN:HG3	2:P:128:ARG:HG2	1.96	0.46
2:P:119:GLN:OE1	3:Q:82:ILE:HG12	2.16	0.46
13:M:15:LYS:HG2	13:M:20:VAL:HG12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:137:ALA:HB3	4:D:214:ILE:HD13	1.97	0.46
6:T:128:PHE:O	6:T:149:PRO:HB3	2.15	0.46
7:U:22:ALA:O	7:U:26:THR:HG23	2.15	0.46
12:Z:105:TYR:O	12:Z:107:VAL:N	2.48	0.46
4:D:176:LEU:HD11	5:E:54:GLU:HB2	1.97	0.46
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.50	0.46
13:M:17:ASP:OD1	13:M:18:ASN:N	2.48	0.46
16:V:301:A1A9B:N28	16:V:301:A1A9B:C46	2.78	0.46
6:F:116:VAL:HG21	6:F:147:LEU:HD21	1.96	0.46
1:O:122:THR:HG22	1:O:129:PRO:HB3	1.97	0.46
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.51	0.46
14:N:172:VAL:HG12	14:N:190:PRO:HD3	1.98	0.46
12:Z:141:ALA:HB1	12:Z:195:HIS:NE2	2.31	0.46
2:B:75:ALA:HB3	2:B:135:ILE:HB	1.98	0.46
3:C:135:GLY:HA2	3:C:213:VAL:HG11	1.97	0.46
5:E:185:PRO:O	5:E:189:ILE:HG12	2.15	0.46
8:H:134:ALA:HB1	8:H:158:ALA:HB1	1.97	0.46
9:I:82:GLU:OE2	9:I:113:SER:OG	2.32	0.46
1:A:66:LEU:HD12	1:A:235:PHE:CD1	2.50	0.46
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.51	0.46
8:H:63:ILE:HG12	8:H:82:MET:HE1	1.97	0.46
12:Z:30:ILE:HG22	12:Z:35:ILE:HG12	1.98	0.46
9:I:10:ILE:HB	9:I:145:LEU:HD11	1.98	0.46
1:A:83:ARG:O	1:A:86:VAL:HG12	2.16	0.46
1:A:149:GLN:O	1:A:156:TYR:HA	2.15	0.46
7:G:39:LYS:HB2	7:G:187:GLU:O	2.16	0.46
7:G:104:PRO:HB3	7:G:138:ASP:OD2	2.16	0.46
12:Z:28:ARG:HG2	12:Z:30:ILE:HG23	1.98	0.46
1:O:66:LEU:HD12	1:O:235:PHE:CD1	2.51	0.45
5:S:45:LEU:HB2	5:S:213:ALA:HB3	1.98	0.45
1:A:49:LYS:NZ	1:A:61:LEU:O	2.49	0.45
3:C:246:LYS:HB2	3:C:246:LYS:HE3	1.68	0.45
7:G:73:VAL:HG13	7:G:133:THR:HB	1.98	0.45
5:S:106:ARG:O	5:S:110:LEU:HG	2.16	0.45
1:A:172:LYS:O	1:A:176:GLU:HG3	2.16	0.45
5:S:49:LYS:CB	5:S:58:TYR:HB3	2.47	0.45
8:H:48:THR:HB	8:H:51:ASP:HB2	1.98	0.45
11:K:197:PHE:CE2	9:W:203:GLN:HG3	2.51	0.45
8:V:7:LYS:HD2	8:V:110:LEU:HB3	1.99	0.45
8:V:67:SER:HB2	8:V:74:PRO:HG3	1.97	0.45
4:D:113:LEU:HD23	5:E:125:ARG:HH21	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:47:GLU:OE2	6:F:203:ASN:ND2	2.44	0.45
7:G:66:ILE:HA	7:G:89:LYS:HG2	1.97	0.45
2:P:118:LYS:O	2:P:122:THR:HG23	2.16	0.45
2:P:180:LYS:O	2:P:183:MET:HG3	2.17	0.45
5:S:44:VAL:HG22	5:S:214:ILE:HD13	1.98	0.45
7:U:73:VAL:HG13	7:U:133:THR:HB	1.99	0.45
8:V:55:VAL:HG11	8:V:94:ILE:HG21	1.98	0.45
9:W:26:LEU:HD21	9:W:185:VAL:HG13	1.99	0.45
12:Z:205:LEU:HD22	12:Z:214:LYS:HG2	1.98	0.45
1:A:97:TYR:OH	9:I:77:GLU:OE2	2.28	0.45
2:P:76:VAL:HG23	2:P:132:VAL:HG13	1.99	0.45
5:S:45:LEU:HD13	5:S:72:SER:HB3	1.97	0.45
6:T:14:ASP:CG	6:T:16:ARG:HD3	2.37	0.45
13:M:127:LEU:O	13:M:138:SER:OG	2.26	0.45
6:F:47:GLU:HG3	6:F:208:PHE:HB2	1.98	0.45
7:G:147:LYS:O	7:G:154:TYR:HA	2.16	0.45
3:Q:92:GLN:HG3	10:X:66:LEU:HB2	1.99	0.45
7:U:66:ILE:HA	7:U:89:LYS:HG2	1.97	0.45
7:G:22:ALA:O	7:G:26:THR:HG23	2.17	0.45
1:O:149:GLN:O	1:O:156:TYR:HA	2.16	0.45
2:P:124:HIS:HB3	3:Q:124:VAL:HG23	1.99	0.45
4:R:97:GLU:OE2	12:Z:75:TYR:OH	2.26	0.45
11:K:1:THR:HG21	11:K:46:ALA:HA	1.98	0.45
4:R:86:THR:HA	11:Y:65:LEU:HD11	1.99	0.45
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.98	0.45
9:W:87:THR:HG23	9:W:123:PHE:CE1	2.52	0.45
6:F:189:VAL:HG13	6:F:212:ILE:HG21	1.98	0.45
7:G:23:PHE:HE2	7:G:151:ALA:HB2	1.82	0.45
11:K:145:LYS:HG2	11:K:147:ASP:H	1.81	0.45
8:V:14:ILE:HD12	8:V:34:LEU:HD22	1.99	0.45
1:A:62:SER:OG	1:A:237:LYS:NZ	2.50	0.44
5:S:31:GLY:HA2	5:S:50:ARG:NH2	2.32	0.44
6:T:189:VAL:HG13	6:T:212:ILE:HG21	1.99	0.44
9:I:29:GLY:HA2	9:I:35:VAL:HG23	1.99	0.44
13:M:27:LEU:HB2	13:M:192:SER:HB2	1.99	0.44
5:E:49:LYS:HB3	5:E:58:TYR:HB3	1.98	0.44
9:I:52:ILE:HG22	9:I:59:VAL:HG22	1.99	0.44
11:K:104:TYR:CD1	11:K:182:GLU:HA	2.51	0.44
8:V:1:THR:O	8:V:129:SER:N	2.50	0.44
7:G:61:SER:HA	7:G:215:GLU:OE2	2.17	0.44
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:13:VAL:HG12	8:V:177:VAL:HG13	1.98	0.44
2:B:159:TRP:HH2	3:C:50:LEU:HD12	1.81	0.44
2:P:9:THR:HB	2:P:20:GLN:HG3	1.98	0.44
3:Q:46:ARG:NH2	3:Q:209:GLU:OE2	2.51	0.44
14:N:3:ILE:HB	14:N:44:CYS:HB3	1.99	0.44
5:E:226:GLY:O	5:E:229:VAL:HG22	2.17	0.44
3:Q:231:VAL:O	3:Q:234:ILE:HG13	2.17	0.44
5:S:226:GLY:O	5:S:229:VAL:HG22	2.17	0.44
10:X:43:LEU:HB2	10:X:189:ILE:HD13	1.99	0.44
6:T:118:ALA:HA	6:T:121:LEU:HD12	1.99	0.44
14:N:14:LEU:HD11	14:N:100:ALA:HB3	2.00	0.44
1:A:10:THR:O	2:B:128:ARG:HD3	2.18	0.44
2:B:43:ILE:HD11	2:B:145:TYR:HB3	1.99	0.44
1:O:10:THR:O	2:P:128:ARG:HD3	2.18	0.44
3:Q:135:GLY:HA2	3:Q:213:VAL:HG11	1.99	0.44
8:H:22:GLN:HG3	8:H:27:ALA:HB2	2.00	0.44
9:I:50:LEU:HD11	9:I:106:PRO:HB3	2.00	0.44
11:K:158:LYS:HD3	11:K:196:LEU:HD11	2.00	0.44
10:X:130:TYR:HB2	10:X:144:LEU:HD13	2.00	0.44
5:S:35:VAL:HG23	5:S:159:ALA:HB2	2.00	0.44
11:K:38:ASN:ND2	11:K:41:LEU:HB2	2.33	0.44
2:B:213:ALA:HB2	2:B:228:ILE:HD13	2.00	0.43
7:G:147:LYS:HB3	7:G:157:TYR:HE1	1.82	0.43
1:O:220:ASP:OD1	1:O:220:ASP:N	2.51	0.43
2:P:115:SER:HB3	2:P:154:GLY:O	2.18	0.43
11:K:174:SER:HA	11:K:193:VAL:HG23	2.00	0.43
3:Q:225:GLU:N	3:Q:225:GLU:OE1	2.52	0.43
6:T:5:ASP:HB3	6:T:18:PHE:CD2	2.53	0.43
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.99	0.43
10:J:46:PHE:CD2	10:J:53:THR:HB	2.54	0.43
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.58	0.43
14:N:59:VAL:HG11	14:N:82:PHE:CE2	2.53	0.43
3:C:102:VAL:HG21	3:C:107:LEU:HB2	2.01	0.43
5:E:106:ARG:O	5:E:110:LEU:HG	2.18	0.43
6:F:66:VAL:HG11	6:F:108:PHE:CE1	2.53	0.43
10:J:149:ARG:HB3	10:J:152:MET:HG3	2.00	0.43
12:L:105:TYR:O	12:L:107:VAL:N	2.48	0.43
13:M:227:GLY:HA3	13:M:231:GLN:HB3	1.99	0.43
4:D:113:LEU:HD23	5:E:125:ARG:NH2	2.33	0.43
1:O:115:ALA:HB1	1:O:154:GLY:O	2.19	0.43
5:S:174:THR:HG22	5:S:177:THR:HB	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:82:PHE:HB3	14:N:113:ILE:HD12	1.99	0.43
9:W:159:PRO:HG2	9:W:190:LYS:HD3	1.99	0.43
4:D:62:ILE:HD12	4:D:84:ALA:HB3	2.01	0.43
6:T:116:VAL:HG21	6:T:147:LEU:HD21	2.00	0.43
13:M:102:GLN:O	13:M:106:LYS:HG2	2.19	0.43
3:C:115:GLN:O	3:C:119:THR:HG23	2.19	0.43
5:S:70:GLY:HA3	5:S:221:PHE:CZ	2.53	0.43
6:T:66:VAL:HG11	6:T:108:PHE:CE1	2.54	0.43
10:X:5:LEU:HD23	10:X:132:ALA:HB2	2.01	0.43
6:F:74:TYR:CD1	6:F:81:GLY:HA3	2.54	0.43
6:F:128:PHE:O	6:F:149:PRO:HB3	2.19	0.43
3:Q:11:PRO:HA	4:R:18:TYR:CE1	2.54	0.43
7:U:106:ASP:OD1	7:U:106:ASP:N	2.45	0.43
8:H:109:HIS:HB3	8:H:111:PHE:CE2	2.52	0.43
9:I:203:GLN:HG3	11:Y:197:PHE:CE2	2.53	0.43
11:K:104:TYR:CZ	11:K:182:GLU:HG2	2.53	0.43
12:Z:126:ASP:OD1	12:Z:130:SER:N	2.51	0.43
2:B:6:ASP:HB3	3:C:4:ARG:HH12	1.83	0.43
13:M:132:LEU:HD23	13:M:132:LEU:H	1.84	0.43
8:V:114:HIS:HB3	8:V:118:SER:OG	2.19	0.43
5:E:14:PRO:HA	6:F:22:TYR:CD1	2.54	0.43
6:F:20:VAL:O	6:F:24:VAL:HG23	2.19	0.43
1:O:71:ILE:HG12	1:O:138:GLY:HA3	2.01	0.43
1:O:160:LYS:HD3	1:O:179:TRP:CH2	2.53	0.43
3:Q:194:VAL:HG21	3:Q:230:TYR:HB3	2.00	0.43
5:S:114:LYS:HA	5:S:117:LYS:HE2	2.00	0.43
12:L:222:ASP:HB3	8:V:194:ASN:ND2	2.34	0.43
13:M:150:MET:HG2	8:V:132:LEU:HB3	1.99	0.43
1:O:74:VAL:HG22	1:O:75:TYR:H	1.83	0.43
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.53	0.43
7:U:195:GLU:HA	7:U:239:ILE:HD11	2.00	0.43
11:K:155:TYR:OH	11:K:204:GLU:OE2	2.34	0.43
9:W:28:LEU:HD22	9:W:39:PHE:CD1	2.53	0.43
3:C:11:PRO:HA	4:D:18:TYR:CD1	2.53	0.42
3:C:195:ARG:O	3:C:199:GLU:HG2	2.19	0.42
7:G:8:THR:HB	7:G:120:THR:O	2.19	0.42
7:G:30:ASN:HA	7:G:164:PRO:HG2	2.01	0.42
3:Q:198:LEU:HD23	3:Q:201:VAL:HG23	2.00	0.42
7:U:177:PHE:O	7:U:181:LYS:N	2.47	0.42
14:N:157:HIS:HE1	14:N:196:LEU:HD22	1.84	0.42
8:V:20:SER:HB3	8:V:28:ASP:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:30:ILE:HD12	4:D:196:LEU:HG	2.01	0.42
4:R:137:ALA:HB3	4:R:214:ILE:HD13	2.00	0.42
7:U:78:ILE:HG22	7:U:79:PRO:HD3	2.00	0.42
9:I:97:ARG:HD3	9:I:102:TYR:CE2	2.53	0.42
8:V:4:VAL:HG22	8:V:159:ILE:HD11	2.01	0.42
10:X:149:ARG:HB3	10:X:152:MET:HG3	2.01	0.42
11:Y:159:ARG:NH1	11:Y:163:ALA:HB2	2.34	0.42
7:G:71:GLY:HA3	7:G:224:PHE:CZ	2.54	0.42
3:Q:227:ILE:O	3:Q:231:VAL:HG13	2.18	0.42
6:T:74:TYR:HE2	6:T:78:ILE:HG23	1.84	0.42
8:V:87:LEU:HD13	8:V:115:ALA:HA	2.01	0.42
11:Y:12:ILE:HG23	11:Y:112:ILE:HD11	2.02	0.42
1:A:205:ASN:O	1:A:209:ILE:HG12	2.18	0.42
4:D:191:LEU:O	4:D:195:ILE:HG12	2.20	0.42
3:Q:79:ASP:HB2	3:Q:129:VAL:HG23	2.00	0.42
5:S:134:ILE:HD11	5:S:221:PHE:HE1	1.84	0.42
6:T:107:ALA:O	6:T:111:ARG:HG2	2.20	0.42
8:H:134:ALA:O	8:H:138:LEU:HG	2.19	0.42
9:W:98:ARG:HG3	9:W:99:PHE:CD1	2.55	0.42
1:A:176:GLU:HG2	2:B:55:LEU:HG	2.00	0.42
2:B:8:ARG:HH12	4:D:0:TYR:HB3	1.84	0.42
1:O:128:ARG:HG3	7:U:121:GLN:HG3	2.01	0.42
7:U:23:PHE:HE2	7:U:151:ALA:HB2	1.84	0.42
9:I:87:THR:HG23	9:I:123:PHE:CZ	2.55	0.42
13:M:35:ARG:NH1	14:N:135:TYR:OH	2.52	0.42
13:M:50:VAL:HG23	13:M:200:ILE:HD11	2.01	0.42
14:N:67:THR:HA	14:N:71:GLY:O	2.19	0.42
9:W:14:MET:HB3	9:W:14:MET:HE2	1.96	0.42
1:A:49:LYS:NZ	1:A:58:SER:O	2.50	0.42
2:B:69:ASN:OD1	2:B:72:ILE:N	2.52	0.42
3:C:195:ARG:HG3	3:C:234:ILE:HD13	2.02	0.42
5:E:35:VAL:HG23	5:E:159:ALA:HB2	2.02	0.42
4:R:140:ASP:OD2	4:R:146:GLN:NE2	2.52	0.42
9:W:50:LEU:HD11	9:W:106:PRO:HB3	2.02	0.42
4:D:190:LEU:HD22	4:D:235:LEU:HB2	2.01	0.42
5:S:61:LYS:NZ	5:S:73:LEU:O	2.51	0.42
6:T:187:GLU:O	6:T:191:GLN:HG2	2.19	0.42
8:H:160:GLN:HG2	8:H:164:TRP:NE1	2.34	0.42
9:I:189:ILE:HG12	9:I:194:VAL:HG13	2.02	0.42
8:V:104:ASP:OD1	8:V:106:THR:OG1	2.22	0.42
12:Z:124:SER:OG	12:Z:137:ARG:NH1	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ASP:OD1	1:A:220:ASP:N	2.52	0.42
6:F:33:SER:OG	6:F:75:SER:OG	2.28	0.42
3:Q:172:PHE:HZ	3:Q:195:ARG:HD2	1.85	0.42
4:R:44:LYS:HB3	4:R:56:ILE:HD12	2.02	0.42
2:B:106:PRO:HD2	2:B:109:ILE:HD12	2.02	0.42
4:D:83:HIS:CG	4:D:111:LEU:HD11	2.54	0.42
5:E:118:ASN:ND2	15:E:302:SO4:O2	2.53	0.42
2:P:95:GLN:HB3	9:W:68:TYR:CD2	2.54	0.42
8:H:7:LYS:HD2	8:H:110:LEU:HB3	2.01	0.42
9:I:23:ALA:HB1	9:I:170:LEU:HD22	2.02	0.42
10:J:35:THR:HB	10:J:43:LEU:HD11	2.02	0.42
5:E:70:GLY:HA3	5:E:221:PHE:CE1	2.55	0.42
7:G:15:ARG:HH21	7:G:20:GLU:CD	2.23	0.42
10:J:169:GLU:O	10:X:177:LYS:NZ	2.53	0.42
11:K:65:LEU:HD13	11:K:69:ARG:HH22	1.85	0.42
12:Z:136:CYS:SG	12:Z:154:VAL:HG11	2.60	0.42
1:A:140:ASP:OD1	1:A:143:ASN:N	2.50	0.41
3:C:225:GLU:OE1	3:C:225:GLU:N	2.50	0.41
5:E:206:THR:OG1	5:E:209:ASN:ND2	2.53	0.41
6:F:165:ARG:HG3	6:F:166:GLN:N	2.35	0.41
1:O:55:LEU:HD12	7:U:170:THR:HG23	2.02	0.41
3:Q:240:GLU:O	3:Q:241:GLN:HG2	2.20	0.41
5:S:14:PRO:HA	6:T:22:TYR:CD1	2.55	0.41
12:L:58:ALA:HB3	13:M:135:VAL:HG13	2.01	0.41
12:L:156:PHE:CG	12:L:170:LYS:HD3	2.55	0.41
13:M:14:MET:HG2	13:M:177:ILE:HD11	2.02	0.41
9:W:10:ILE:HB	9:W:145:LEU:HD11	2.03	0.41
12:Z:124:SER:O	12:Z:131:TYR:HA	2.19	0.41
6:F:152:SER:N	7:G:79:PRO:HG3	2.35	0.41
9:I:84:GLU:OE1	9:I:84:GLU:N	2.44	0.41
16:K:301:A1A9B:C46	16:K:301:A1A9B:N28	2.84	0.41
11:Y:174:SER:HA	11:Y:193:VAL:HG23	2.01	0.41
7:G:223:LYS:HA	7:G:223:LYS:HD2	1.92	0.41
3:Q:115:GLN:O	3:Q:119:THR:HG23	2.20	0.41
6:T:47:GLU:HG3	6:T:208:PHE:HB2	2.03	0.41
14:N:8:PHE:HB2	14:N:146:MET:O	2.20	0.41
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.02	0.41
12:Z:194:ARG:HA	12:Z:194:ARG:HD3	1.89	0.41
1:A:23:TYR:CE1	7:G:12:PRO:HA	2.55	0.41
4:D:211:LEU:HD23	4:D:211:LEU:HA	1.93	0.41
9:I:176:ARG:HG3	12:Z:148:PRO:HG3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:110:LEU:O	13:M:112:ASN:N	2.53	0.41
11:Y:6:PHE:HB2	11:Y:126:ILE:HG12	2.02	0.41
3:C:66:ASP:OD1	3:C:67:SER:N	2.48	0.41
2:P:76:VAL:HG21	2:P:83:ALA:CB	2.50	0.41
3:Q:79:ASP:OD1	3:Q:79:ASP:N	2.54	0.41
9:I:38:LYS:HB3	9:I:38:LYS:HE2	1.80	0.41
11:K:44:THR:O	11:K:99:THR:HA	2.21	0.41
12:L:15:ILE:HB	12:L:22:VAL:HG13	2.01	0.41
2:B:159:TRP:CD2	2:B:162:ILE:HD13	2.55	0.41
5:E:11:THR:HG23	6:F:19:GLN:HE22	1.86	0.41
10:J:119:ILE:HA	10:J:124:THR:O	2.21	0.41
11:K:135:PHE:HB3	10:X:142:SER:HB3	2.02	0.41
8:V:127:LEU:C	8:V:131:SER:HB3	2.41	0.41
1:A:243:ILE:O	1:A:247:LEU:HG	2.20	0.41
1:A:250:LEU:HD23	1:A:250:LEU:HA	1.90	0.41
2:B:104:ASP:OD1	2:B:104:ASP:N	3.49	0.41
3:Q:35:LYS:HD2	3:Q:145:LEU:HB3	2.02	0.41
3:Q:91:ALA:HA	3:Q:102:VAL:HG11	2.02	0.41
16:N:202:A1A9B:N28	16:N:202:A1A9B:C46	2.84	0.41
9:W:9:GLY:HA2	9:W:25:ASP:OD2	2.21	0.41
10:X:101:ASN:HB3	10:X:133:HIS:CE1	2.54	0.41
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.91	0.41
4:R:158:ARG:O	5:S:57:SER:N	2.52	0.41
8:H:153:LYS:NZ	8:H:157:ASP:OD2	2.50	0.41
12:L:13:LEU:O	12:L:23:LEU:HD12	2.21	0.41
12:L:28:ARG:HG2	12:L:30:ILE:HG23	2.02	0.41
12:L:126:ASP:OD1	12:L:130:SER:N	2.51	0.41
8:V:78:SER:O	8:V:82:MET:HG3	2.20	0.41
1:A:23:TYR:CD1	7:G:12:PRO:HA	2.56	0.41
6:F:33:SER:HB3	6:F:46:VAL:HG23	2.02	0.41
1:O:69:PRO:HB3	1:O:233:PRO:HB3	2.02	0.41
1:O:217:GLU:HG3	1:O:234:ARG:NH1	2.36	0.41
4:R:59:ILE:HG22	4:R:220:PHE:HZ	1.86	0.41
6:T:33:SER:HB3	6:T:46:VAL:HG23	2.02	0.41
7:U:71:GLY:HA3	7:U:224:PHE:CZ	2.56	0.41
7:U:147:LYS:HB3	7:U:157:TYR:HE1	1.84	0.41
9:I:28:LEU:HD22	9:I:39:PHE:CD1	2.55	0.41
12:L:167:LYS:HE3	12:L:167:LYS:HB3	1.90	0.41
13:M:5:ILE:HG21	14:N:115:LEU:HB2	2.02	0.41
13:M:128:ARG:HG3	13:M:138:SER:HB2	2.03	0.41
9:W:7:ASN:HA	9:W:29:GLY:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:94:LEU:HD11	9:W:106:PRO:HG2	2.03	0.41
7:G:43:VAL:HG11	7:G:194:VAL:HA	2.03	0.41
7:G:78:ILE:HG22	7:G:79:PRO:HD3	2.02	0.41
1:O:196:LEU:HD12	1:O:196:LEU:HA	1.89	0.41
4:R:14:PHE:HD1	4:R:18:TYR:HH	1.69	0.41
9:W:24:CYS:SG	9:W:42:ILE:HG12	2.61	0.41
9:W:62:LEU:HD12	9:W:104:VAL:HG21	2.03	0.41
10:X:46:PHE:CD2	10:X:53:THR:HB	2.54	0.41
5:E:189:ILE:HD12	5:E:212:ILE:HG21	2.02	0.40
7:U:70:ILE:HG21	7:U:108:LEU:HD23	2.02	0.40
8:V:51:ASP:O	8:V:55:VAL:HG22	2.21	0.40
11:Y:207:PHE:O	11:Y:210:VAL:HG12	2.21	0.40
12:Z:169:LYS:HB3	12:Z:169:LYS:HE2	1.88	0.40
4:D:59:ILE:HG22	4:D:220:PHE:HZ	1.85	0.40
7:G:48:LYS:NZ	7:G:60:VAL:O	2.53	0.40
2:P:43:ILE:HD11	2:P:145:TYR:HB3	2.03	0.40
5:S:136:TYR:CZ	5:S:217:LYS:HB2	2.57	0.40
5:S:185:PRO:O	5:S:189:ILE:HG13	2.21	0.40
7:U:52:ASP:HB3	7:U:55:LEU:HG	2.02	0.40
14:N:8:PHE:CE1	14:N:13:ILE:HG13	2.56	0.40
8:V:160:GLN:HG2	8:V:164:TRP:NE1	2.36	0.40
12:Z:172:LEU:HD12	12:Z:172:LEU:H	1.86	0.40
1:A:61:LEU:HB2	7:G:155:VAL:HG23	2.03	0.40
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.56	0.40
1:O:42:GLY:HA2	1:O:214:ILE:O	2.22	0.40
3:Q:45:GLU:HG3	3:Q:207:ASN:OD1	2.21	0.40
9:I:9:GLY:HA2	9:I:25:ASP:OD2	2.20	0.40
11:K:106:ARG:HD2	11:K:106:ARG:HA	1.89	0.40
10:X:161:LEU:HD23	10:X:161:LEU:HA	1.92	0.40
4:D:77:ALA:O	4:D:81:ILE:HG12	2.22	0.40
2:P:75:ALA:HB3	2:P:135:ILE:HB	2.03	0.40
6:T:23:ALA:O	6:T:27:VAL:HG23	2.21	0.40
8:H:104:ASP:OD1	8:H:106:THR:OG1	2.24	0.40
14:N:32:ASP:CG	14:N:185:ARG:HH22	2.24	0.40
9:W:196:LYS:HE2	9:W:198:TYR:CE1	2.56	0.40
2:B:145:TYR:OH	2:B:217:LYS:HG2	2.21	0.40
3:Q:157:TRP:CZ2	4:R:51:LEU:HD12	2.57	0.40
5:S:197:SER:HA	5:S:200:LEU:HG	2.04	0.40
6:T:16:ARG:NH2	6:T:21:GLU:OE1	2.54	0.40
7:U:61:SER:HA	7:U:215:GLU:OE2	2.22	0.40
9:W:29:GLY:HA2	9:W:35:VAL:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	247/250 (99%)	239 (97%)	8 (3%)	0	100	100
1	O	247/250 (99%)	239 (97%)	8 (3%)	0	100	100
2	B	239/258 (93%)	229 (96%)	10 (4%)	0	100	100
2	P	240/258 (93%)	231 (96%)	9 (4%)	0	100	100
3	C	244/254 (96%)	236 (97%)	8 (3%)	0	100	100
3	Q	239/254 (94%)	229 (96%)	10 (4%)	0	100	100
4	D	235/260 (90%)	225 (96%)	10 (4%)	0	100	100
4	R	242/260 (93%)	230 (95%)	12 (5%)	0	100	100
5	E	230/234 (98%)	217 (94%)	13 (6%)	0	100	100
5	S	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
6	F	242/287 (84%)	234 (97%)	8 (3%)	0	100	100
6	T	243/287 (85%)	235 (97%)	8 (3%)	0	100	100
7	G	240/252 (95%)	233 (97%)	7 (3%)	0	100	100
7	U	240/252 (95%)	233 (97%)	7 (3%)	0	100	100
8	H	220/232 (95%)	212 (96%)	8 (4%)	0	100	100
8	V	220/232 (95%)	212 (96%)	8 (4%)	0	100	100
9	I	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
9	W	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
10	J	194/198 (98%)	188 (97%)	6 (3%)	0	100	100
10	X	193/198 (98%)	186 (96%)	7 (4%)	0	100	100
11	K	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
11	Y	210/212 (99%)	201 (96%)	9 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
12	Z	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
13	M	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
13	a	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6299/6586 (96%)	6052 (96%)	247 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/209 (100%)	207 (100%)	1 (0%)	86	92
1	O	208/209 (100%)	207 (100%)	1 (0%)	86	92
2	B	204/216 (94%)	202 (99%)	2 (1%)	73	84
2	P	204/216 (94%)	203 (100%)	1 (0%)	86	92
3	C	218/226 (96%)	216 (99%)	2 (1%)	75	86
3	Q	213/226 (94%)	211 (99%)	2 (1%)	75	86
4	D	198/215 (92%)	197 (100%)	1 (0%)	86	92
4	R	202/215 (94%)	201 (100%)	1 (0%)	86	92
5	E	191/193 (99%)	188 (98%)	3 (2%)	58	76
5	S	191/193 (99%)	188 (98%)	3 (2%)	58	76
6	F	201/238 (84%)	197 (98%)	4 (2%)	50	72
6	T	202/238 (85%)	199 (98%)	3 (2%)	60	77
7	G	207/210 (99%)	206 (100%)	1 (0%)	86	92
7	U	207/210 (99%)	207 (100%)	0	100	100
8	H	181/190 (95%)	180 (99%)	1 (1%)	84	91

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	V	181/190 (95%)	181 (100%)	0	100 100
9	I	172/173 (99%)	170 (99%)	2 (1%)	67 81
9	W	172/173 (99%)	169 (98%)	3 (2%)	56 75
10	J	174/175 (99%)	173 (99%)	1 (1%)	84 91
10	X	173/175 (99%)	173 (100%)	0	100 100
11	K	169/169 (100%)	166 (98%)	3 (2%)	54 74
11	Y	169/169 (100%)	167 (99%)	2 (1%)	67 81
12	L	185/185 (100%)	181 (98%)	4 (2%)	47 70
12	Z	185/185 (100%)	184 (100%)	1 (0%)	86 92
13	M	199/199 (100%)	199 (100%)	0	100 100
13	a	199/199 (100%)	198 (100%)	1 (0%)	86 92
14	N	162/162 (100%)	161 (99%)	1 (1%)	84 91
14	b	162/162 (100%)	161 (99%)	1 (1%)	84 91
All	All	5337/5520 (97%)	5292 (99%)	45 (1%)	79 88

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	52	THR
2	B	82	ASP
3	C	56	ARG
3	C	102	VAL
4	D	25	LEU
5	E	12	PHE
5	E	112	CYS
5	E	174	THR
6	F	14	ASP
6	F	130	VAL
6	F	208	PHE
6	F	214	TRP
7	G	34	LEU
1	O	2	THR
2	P	82	ASP
3	Q	102	VAL
3	Q	212	VAL
4	R	125	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	S	12	PHE
5	S	112	CYS
5	S	174	THR
6	T	203	ASN
6	T	208	PHE
6	T	214	TRP
8	H	36	ARG
9	I	146	PHE
9	I	182	TRP
10	J	78	GLN
11	K	73	ARG
11	K	137	TYR
11	K	209	ASN
12	L	22	VAL
12	L	106	TYR
12	L	167	LYS
12	L	209	LYS
14	N	83	LYS
9	W	37	ASN
9	W	133	LYS
9	W	146	PHE
11	Y	73	ARG
11	Y	137	TYR
12	Z	209	LYS
13	a	25	ASP
14	b	83	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
9	I	71	ASN
14	b	161	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 69 ligands modelled in this entry, 5 are monoatomic - leaving 64 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	SO4	a	305	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	C	301	-	4,4,4	0.67	0	6,6,6	0.12	0
15	SO4	S	302	-	4,4,4	0.67	0	6,6,6	0.09	0
16	A1A9B	Y	301	-	51,52,52	3.52	19 (37%)	67,76,76	3.33	19 (28%)
15	SO4	T	301	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	S	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	Y	306	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	a	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	H	302	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	I	302	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	a	303	-	4,4,4	0.67	0	6,6,6	0.06	0
15	SO4	b	202	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	B	301	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	Q	301	-	4,4,4	0.67	0	6,6,6	0.07	0
16	A1A9B	N	202	-	51,52,52	3.56	19 (37%)	67,76,76	3.33	16 (23%)
15	SO4	V	302	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	K	303	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	H	304	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	E	302	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	P	301	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	F	302	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	K	305	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	M	304	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	U	301	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	M	305	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	X	201	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	H	303	-	4,4,4	0.67	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	SO4	J	201	-	4,4,4	0.68	0	6,6,6	0.06	0
15	SO4	b	203	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	T	302	-	4,4,4	0.67	0	6,6,6	0.11	0
16	A1A9B	H	301	-	51,52,52	3.54	18 (35%)	67,76,76	3.44	18 (26%)
15	SO4	G	301	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	E	301	-	4,4,4	0.67	0	6,6,6	0.06	0
15	SO4	M	307	-	4,4,4	0.68	0	6,6,6	0.06	0
15	SO4	M	302	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	L	302	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	N	201	-	4,4,4	0.67	0	6,6,6	0.06	0
15	SO4	Y	303	-	4,4,4	0.67	0	6,6,6	0.09	0
16	A1A9B	b	201	-	51,52,52	3.56	19 (37%)	67,76,76	3.35	16 (23%)
16	A1A9B	V	301	-	51,52,52	3.56	19 (37%)	67,76,76	3.44	18 (26%)
15	SO4	W	302	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	a	304	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	K	302	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	K	304	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	F	301	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	S	303	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	Y	304	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	V	303	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	M	306	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	T	303	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	Z	302	-	4,4,4	0.68	0	6,6,6	0.08	0
16	A1A9B	K	301	-	51,52,52	3.56	19 (37%)	67,76,76	3.45	18 (26%)
15	SO4	G	302	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	a	302	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	b	204	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	M	303	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	M	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	J	202	-	4,4,4	0.67	0	6,6,6	0.12	0
15	SO4	I	303	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	D	301	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	M	308	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	U	302	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	Y	305	-	4,4,4	0.69	0	6,6,6	0.08	0
15	SO4	Z	303	-	4,4,4	0.67	0	6,6,6	0.10	0

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
16	A1A9B	Y	301	-	-	11/59/76/76	0/3/4/4
16	A1A9B	H	301	-	-	10/59/76/76	0/3/4/4
16	A1A9B	K	301	-	-	14/59/76/76	0/3/4/4
16	A1A9B	N	202	-	-	11/59/76/76	0/3/4/4
16	A1A9B	b	201	-	-	4/59/76/76	0/3/4/4
16	A1A9B	V	301	-	-	9/59/76/76	0/3/4/4

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	301	A1A9B	C25-C21	11.90	1.66	1.51
16	b	201	A1A9B	C25-C21	11.84	1.66	1.51
16	N	202	A1A9B	C25-C21	11.81	1.66	1.51
16	H	301	A1A9B	C25-C21	11.76	1.66	1.51
16	K	301	A1A9B	C25-C21	11.52	1.66	1.51
16	Y	301	A1A9B	C25-C21	11.50	1.66	1.51
16	K	301	A1A9B	O49-C25	-11.08	1.26	1.42
16	Y	301	A1A9B	O49-C25	-11.05	1.27	1.42
16	H	301	A1A9B	O49-C25	-11.00	1.27	1.42
16	b	201	A1A9B	O49-C25	-10.98	1.27	1.42
16	N	202	A1A9B	O49-C25	-10.96	1.27	1.42
16	V	301	A1A9B	O49-C25	-10.87	1.27	1.42
16	K	301	A1A9B	C39-N41	10.76	1.49	1.34
16	b	201	A1A9B	C39-N41	10.50	1.48	1.34
16	H	301	A1A9B	C39-N41	10.50	1.48	1.34
16	N	202	A1A9B	C39-N41	10.43	1.48	1.34
16	V	301	A1A9B	C39-N41	10.41	1.48	1.34
16	Y	301	A1A9B	C39-N41	10.29	1.48	1.34
16	N	202	A1A9B	C33-N32	7.22	1.49	1.34
16	H	301	A1A9B	C33-N32	7.17	1.49	1.34
16	V	301	A1A9B	C33-N32	7.15	1.49	1.34
16	V	301	A1A9B	C29-N28	7.14	1.49	1.34
16	Y	301	A1A9B	C33-N32	7.11	1.49	1.34
16	Y	301	A1A9B	C29-N28	7.09	1.49	1.34
16	b	201	A1A9B	C33-N32	7.07	1.49	1.34
16	b	201	A1A9B	C29-N28	7.07	1.49	1.34
16	N	202	A1A9B	C29-N28	7.06	1.49	1.34
16	H	301	A1A9B	C29-N28	7.03	1.49	1.34
16	K	301	A1A9B	C33-N32	7.01	1.49	1.34
16	K	301	A1A9B	C29-N28	6.90	1.48	1.34
16	K	301	A1A9B	C07-N09	6.67	1.48	1.34
16	Y	301	A1A9B	C07-N09	6.56	1.47	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	301	A1A9B	C07-N09	6.54	1.47	1.34
16	b	201	A1A9B	C07-N09	6.50	1.47	1.34
16	N	202	A1A9B	C07-N09	6.47	1.47	1.34
16	V	301	A1A9B	C07-N09	6.35	1.47	1.34
16	N	202	A1A9B	C36-N38	4.41	1.47	1.32
16	H	301	A1A9B	C36-N38	4.40	1.47	1.32
16	b	201	A1A9B	C36-N38	4.39	1.47	1.32
16	K	301	A1A9B	C36-N38	4.38	1.47	1.32
16	Y	301	A1A9B	C36-N38	4.37	1.47	1.32
16	V	301	A1A9B	C36-N38	4.37	1.46	1.32
16	N	202	A1A9B	C46-N48	-4.09	1.30	1.35
16	b	201	A1A9B	C46-N48	-4.08	1.30	1.35
16	Y	301	A1A9B	C46-N48	-4.05	1.30	1.35
16	H	301	A1A9B	C46-N48	-3.99	1.30	1.35
16	K	301	A1A9B	C46-N48	-3.98	1.30	1.35
16	V	301	A1A9B	C46-N48	-3.92	1.30	1.35
16	Y	301	A1A9B	C20-N48	-3.65	1.30	1.38
16	K	301	A1A9B	C20-N48	-3.59	1.31	1.38
16	N	202	A1A9B	C20-N48	-3.59	1.31	1.38
16	b	201	A1A9B	C20-N48	-3.59	1.31	1.38
16	H	301	A1A9B	C20-N48	-3.59	1.31	1.38
16	V	301	A1A9B	C20-N48	-3.57	1.31	1.38
16	K	301	A1A9B	C19-C14	2.71	1.55	1.49
16	b	201	A1A9B	C42-N41	2.62	1.47	1.40
16	V	301	A1A9B	C42-N41	2.62	1.47	1.40
16	Y	301	A1A9B	C42-N41	2.60	1.47	1.40
16	N	202	A1A9B	C42-N41	2.60	1.47	1.40
16	N	202	A1A9B	C19-C14	2.59	1.55	1.49
16	K	301	A1A9B	O18-C15	2.57	1.41	1.36
16	N	202	A1A9B	O18-C15	2.55	1.41	1.36
16	b	201	A1A9B	O18-C15	2.53	1.41	1.36
16	b	201	A1A9B	C19-C14	2.53	1.55	1.49
16	V	301	A1A9B	C19-C14	2.52	1.55	1.49
16	K	301	A1A9B	C25-C26	2.52	1.57	1.55
16	H	301	A1A9B	O18-C15	2.49	1.41	1.36
16	K	301	A1A9B	C42-N41	2.49	1.47	1.40
16	V	301	A1A9B	C25-C26	2.49	1.57	1.55
16	V	301	A1A9B	O18-C15	2.49	1.41	1.36
16	Y	301	A1A9B	O18-C15	2.48	1.41	1.36
16	Y	301	A1A9B	C19-C14	2.43	1.54	1.49
16	H	301	A1A9B	C19-C14	2.42	1.54	1.49
16	H	301	A1A9B	C42-N41	2.41	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	301	A1A9B	O08-C07	-2.40	1.19	1.23
16	V	301	A1A9B	O08-C07	-2.34	1.19	1.23
16	K	301	A1A9B	O40-C39	-2.30	1.19	1.23
16	V	301	A1A9B	O40-C39	-2.28	1.19	1.23
16	N	202	A1A9B	O40-C39	-2.27	1.19	1.23
16	b	201	A1A9B	O40-C39	-2.26	1.19	1.23
16	N	202	A1A9B	C25-C26	2.25	1.57	1.55
16	H	301	A1A9B	O08-C07	-2.25	1.19	1.23
16	K	301	A1A9B	O08-C07	-2.25	1.19	1.23
16	Y	301	A1A9B	O40-C39	-2.25	1.19	1.23
16	H	301	A1A9B	O40-C39	-2.24	1.19	1.23
16	N	202	A1A9B	C22-C21	2.24	1.42	1.39
16	N	202	A1A9B	C11-C12	2.23	1.56	1.51
16	N	202	A1A9B	O08-C07	-2.23	1.19	1.23
16	H	301	A1A9B	O30-C29	-2.23	1.19	1.23
16	Y	301	A1A9B	O34-C33	-2.22	1.19	1.23
16	H	301	A1A9B	C22-C21	2.21	1.42	1.39
16	b	201	A1A9B	O08-C07	-2.21	1.19	1.23
16	V	301	A1A9B	C22-C21	2.21	1.42	1.39
16	K	301	A1A9B	O30-C29	-2.21	1.19	1.23
16	b	201	A1A9B	C22-C21	2.20	1.42	1.39
16	K	301	A1A9B	O34-C33	-2.20	1.19	1.23
16	V	301	A1A9B	C11-C12	2.19	1.56	1.51
16	b	201	A1A9B	O34-C33	-2.18	1.19	1.23
16	b	201	A1A9B	C11-C12	2.17	1.56	1.51
16	b	201	A1A9B	O30-C29	-2.17	1.19	1.23
16	V	301	A1A9B	O30-C29	-2.16	1.19	1.23
16	V	301	A1A9B	O34-C33	-2.16	1.19	1.23
16	Y	301	A1A9B	O30-C29	-2.15	1.19	1.23
16	N	202	A1A9B	O30-C29	-2.12	1.19	1.23
16	Y	301	A1A9B	C22-C21	2.12	1.42	1.39
16	H	301	A1A9B	O34-C33	-2.12	1.19	1.23
16	K	301	A1A9B	C22-C21	2.11	1.42	1.39
16	K	301	A1A9B	C11-C12	2.11	1.56	1.51
16	Y	301	A1A9B	C11-C12	2.11	1.56	1.51
16	N	202	A1A9B	O34-C33	-2.09	1.19	1.23
16	b	201	A1A9B	C25-C26	2.05	1.56	1.55
16	H	301	A1A9B	O47-C46	-2.01	1.19	1.22
16	Y	301	A1A9B	O47-C46	-2.00	1.19	1.22

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	301	A1A9B	C20-N48-C46	22.64	129.65	111.26
16	b	201	A1A9B	C20-N48-C46	22.59	129.62	111.26
16	K	301	A1A9B	C20-N48-C46	22.49	129.53	111.26
16	H	301	A1A9B	C20-N48-C46	22.48	129.52	111.26
16	N	202	A1A9B	C20-N48-C46	22.48	129.52	111.26
16	Y	301	A1A9B	C20-N48-C46	22.21	129.31	111.26
16	H	301	A1A9B	C25-C46-N48	-7.68	98.39	108.21
16	K	301	A1A9B	C25-C46-N48	-7.66	98.41	108.21
16	b	201	A1A9B	C25-C46-N48	-7.66	98.42	108.21
16	V	301	A1A9B	C25-C46-N48	-7.63	98.46	108.21
16	Y	301	A1A9B	C25-C46-N48	-7.62	98.47	108.21
16	N	202	A1A9B	C25-C46-N48	-7.60	98.50	108.21
16	K	301	A1A9B	C25-C26-C27	6.31	117.68	112.78
16	H	301	A1A9B	O47-C46-C25	5.08	131.07	125.22
16	Y	301	A1A9B	O47-C46-C25	5.06	131.04	125.22
16	K	301	A1A9B	O47-C46-C25	5.00	130.98	125.22
16	V	301	A1A9B	C31-C35-C36	5.00	122.26	112.21
16	N	202	A1A9B	O47-C46-C25	4.96	130.93	125.22
16	H	301	A1A9B	C25-C26-C27	4.91	116.59	112.78
16	V	301	A1A9B	O47-C46-C25	4.89	130.85	125.22
16	b	201	A1A9B	O47-C46-C25	4.85	130.81	125.22
16	V	301	A1A9B	C21-C20-N48	-4.83	104.76	110.00
16	K	301	A1A9B	C21-C20-N48	-4.75	104.84	110.00
16	b	201	A1A9B	C21-C20-N48	-4.71	104.89	110.00
16	N	202	A1A9B	C21-C20-N48	-4.64	104.97	110.00
16	H	301	A1A9B	C21-C20-N48	-4.61	105.00	110.00
16	Y	301	A1A9B	C21-C20-N48	-4.45	105.17	110.00
16	b	201	A1A9B	O47-C46-N48	4.20	130.73	126.28
16	K	301	A1A9B	O47-C46-N48	4.08	130.61	126.28
16	V	301	A1A9B	O47-C46-N48	4.06	130.59	126.28
16	N	202	A1A9B	O47-C46-N48	4.02	130.54	126.28
16	H	301	A1A9B	O47-C46-N48	4.01	130.53	126.28
16	Y	301	A1A9B	O47-C46-N48	3.97	130.49	126.28
16	K	301	A1A9B	C27-C39-N41	3.79	123.65	116.56
16	H	301	A1A9B	O40-C39-N41	-3.61	118.42	123.47
16	H	301	A1A9B	C43-C42-N41	-3.55	113.18	123.80
16	K	301	A1A9B	O40-C39-N41	-3.44	118.66	123.47
16	V	301	A1A9B	C25-C26-C27	3.43	115.44	112.78
16	H	301	A1A9B	C27-C39-N41	3.41	122.94	116.56
16	K	301	A1A9B	C43-C42-N41	-3.40	113.62	123.80
16	V	301	A1A9B	C43-C42-N41	-3.40	113.64	123.80
16	Y	301	A1A9B	C43-C42-N41	-3.39	113.65	123.80
16	N	202	A1A9B	C43-C42-N41	-3.38	113.68	123.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	b	201	A1A9B	C22-C21-C25	3.36	135.52	130.81
16	H	301	A1A9B	C22-C21-C25	3.35	135.50	130.81
16	Y	301	A1A9B	O40-C39-N41	-3.31	118.84	123.47
16	b	201	A1A9B	C43-C42-N41	-3.31	113.91	123.80
16	N	202	A1A9B	C22-C21-C25	3.25	135.36	130.81
16	H	301	A1A9B	C31-C35-C36	3.22	118.68	112.21
16	V	301	A1A9B	C22-C21-C25	3.18	135.26	130.81
16	Y	301	A1A9B	C12-C11-C10	3.08	121.56	113.36
16	Y	301	A1A9B	C22-C21-C25	3.06	135.09	130.81
16	Y	301	A1A9B	C42-N41-C39	-3.06	117.49	123.65
16	V	301	A1A9B	O40-C39-N41	-3.04	119.22	123.47
16	V	301	A1A9B	C12-C11-C10	3.03	121.41	113.36
16	N	202	A1A9B	O40-C39-N41	-2.97	119.32	123.47
16	b	201	A1A9B	O40-C39-N41	-2.93	119.37	123.47
16	K	301	A1A9B	C22-C21-C25	2.90	134.87	130.81
16	Y	301	A1A9B	C27-C39-N41	2.84	121.87	116.56
16	Y	301	A1A9B	C25-C21-C20	-2.81	105.19	108.47
16	H	301	A1A9B	C25-C21-C20	-2.80	105.20	108.47
16	N	202	A1A9B	C25-C26-C27	2.77	114.93	112.78
16	Y	301	A1A9B	C31-C35-C36	2.75	117.73	112.21
16	N	202	A1A9B	C25-C21-C20	-2.74	105.27	108.47
16	b	201	A1A9B	C25-C21-C20	-2.73	105.28	108.47
16	N	202	A1A9B	C42-N41-C39	-2.73	118.15	123.65
16	b	201	A1A9B	C42-N41-C39	-2.71	118.19	123.65
16	V	301	A1A9B	C42-N41-C39	-2.68	118.26	123.65
16	b	201	A1A9B	C27-C39-N41	2.66	121.54	116.56
16	K	301	A1A9B	C25-C21-C20	-2.65	105.38	108.47
16	V	301	A1A9B	C27-C39-N41	2.64	121.50	116.56
16	b	201	A1A9B	C25-C26-C27	2.63	114.82	112.78
16	V	301	A1A9B	C25-C21-C20	-2.62	105.41	108.47
16	H	301	A1A9B	C39-C27-N28	-2.61	103.24	110.32
16	K	301	A1A9B	C19-C20-N48	2.59	135.06	131.09
16	N	202	A1A9B	C27-C39-N41	2.56	121.36	116.56
16	K	301	A1A9B	C31-C35-C36	2.55	117.34	112.21
16	b	201	A1A9B	C14-C19-C20	-2.55	118.22	124.79
16	b	201	A1A9B	C31-C35-C36	2.54	117.32	112.21
16	K	301	A1A9B	C10-C33-N32	2.52	121.99	116.63
16	N	202	A1A9B	C14-C19-C20	-2.51	118.31	124.79
16	N	202	A1A9B	C31-C35-C36	2.49	117.21	112.21
16	V	301	A1A9B	C19-C20-N48	2.46	134.87	131.09
16	K	301	A1A9B	C26-C27-C39	-2.45	105.98	111.32
16	Y	301	A1A9B	C10-N09-C07	2.42	126.06	122.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	301	A1A9B	C19-C20-N48	2.42	134.80	131.09
16	b	201	A1A9B	C19-C20-N48	2.39	134.76	131.09
16	N	202	A1A9B	C19-C20-N48	2.38	134.73	131.09
16	K	301	A1A9B	O34-C33-N32	-2.35	118.76	122.96
16	H	301	A1A9B	C19-C20-N48	2.34	134.68	131.09
16	Y	301	A1A9B	C13-C14-C15	2.33	120.37	117.63
16	H	301	A1A9B	C14-C19-C20	-2.31	118.85	124.79
16	Y	301	A1A9B	C14-C19-C20	-2.30	118.87	124.79
16	H	301	A1A9B	C10-C33-N32	2.26	121.44	116.63
16	Y	301	A1A9B	C26-C27-C39	-2.18	106.57	111.32
16	H	301	A1A9B	C13-C14-C15	2.17	120.19	117.63
16	K	301	A1A9B	O08-C07-N09	-2.14	119.33	123.09
16	Y	301	A1A9B	C25-C26-C27	2.13	114.43	112.78
16	V	301	A1A9B	O30-C29-N28	-2.10	119.20	122.96
16	H	301	A1A9B	O34-C33-N32	-2.09	119.21	122.96
16	b	201	A1A9B	C13-C14-C15	2.09	120.08	117.63
16	K	301	A1A9B	C14-C19-C20	-2.08	119.43	124.79
16	V	301	A1A9B	C10-C33-N32	2.07	121.03	116.63
16	V	301	A1A9B	C14-C19-C20	-2.06	119.48	124.79
16	N	202	A1A9B	C13-C14-C15	2.02	120.00	117.63

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	H	301	A1A9B	C01-C02-C03-C05
16	H	301	A1A9B	O40-C39-N41-C42
16	K	301	A1A9B	C05-C07-N09-C10
16	K	301	A1A9B	O08-C07-N09-C10
16	K	301	A1A9B	N32-C31-C35-C36
16	K	301	A1A9B	O40-C39-N41-C42
16	N	202	A1A9B	C01-C02-C03-C05
16	N	202	A1A9B	C03-C05-C07-N09
16	N	202	A1A9B	C03-C05-C07-O08
16	N	202	A1A9B	O06-C05-C07-N09
16	N	202	A1A9B	O06-C05-C07-O08
16	V	301	A1A9B	C01-C02-C03-C05
16	V	301	A1A9B	O06-C05-C07-N09
16	H	301	A1A9B	C27-C39-N41-C42
16	K	301	A1A9B	C27-C39-N41-C42
16	K	301	A1A9B	N09-C10-C11-C12
16	K	301	A1A9B	C11-C10-C33-O34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	K	301	A1A9B	C11-C10-C33-N32
16	H	301	A1A9B	C11-C10-C33-O34
16	H	301	A1A9B	C11-C10-C33-N32
16	K	301	A1A9B	C29-C31-C35-C36
16	H	301	A1A9B	C01-C02-C03-C04
16	V	301	A1A9B	C01-C02-C03-C04
16	Y	301	A1A9B	C31-C35-C36-N38
16	Y	301	A1A9B	C31-C35-C36-O37
16	K	301	A1A9B	C33-C10-C11-C12
16	H	301	A1A9B	O06-C05-C07-N09
16	K	301	A1A9B	O06-C05-C07-N09
16	Y	301	A1A9B	O06-C05-C07-N09
16	Y	301	A1A9B	C03-C05-C07-O08
16	V	301	A1A9B	C15-C14-C19-C20
16	Y	301	A1A9B	N28-C27-C39-O40
16	N	202	A1A9B	C02-C03-C05-O06
16	N	202	A1A9B	C02-C03-C05-C07
16	H	301	A1A9B	C03-C05-C07-N09
16	K	301	A1A9B	C03-C05-C07-N09
16	V	301	A1A9B	C03-C05-C07-N09
16	Y	301	A1A9B	C03-C05-C07-N09
16	Y	301	A1A9B	O30-C29-C31-N32
16	Y	301	A1A9B	N28-C27-C39-N41
16	V	301	A1A9B	O30-C29-C31-N32
16	Y	301	A1A9B	N28-C29-C31-N32
16	V	301	A1A9B	O30-C29-C31-C35
16	N	202	A1A9B	C01-C02-C03-C04
16	b	201	A1A9B	O30-C29-C31-N32
16	H	301	A1A9B	N09-C10-C33-O34
16	K	301	A1A9B	C03-C05-C07-O08
16	b	201	A1A9B	C02-C03-C05-O06
16	H	301	A1A9B	N09-C10-C33-N32
16	V	301	A1A9B	N28-C29-C31-N32
16	b	201	A1A9B	N28-C29-C31-N32
16	N	202	A1A9B	O30-C29-C31-N32
16	V	301	A1A9B	N28-C29-C31-C35
16	K	301	A1A9B	C15-C14-C19-C20
16	N	202	A1A9B	C15-C14-C19-C20
16	Y	301	A1A9B	C15-C14-C19-C20
16	b	201	A1A9B	C15-C14-C19-C20
16	Y	301	A1A9B	C11-C10-N09-C07
16	N	202	A1A9B	N09-C10-C33-O34

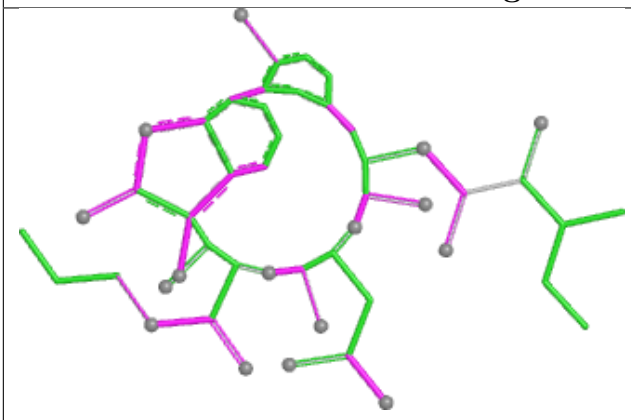
There are no ring outliers.

5 monomers are involved in 5 short contacts:

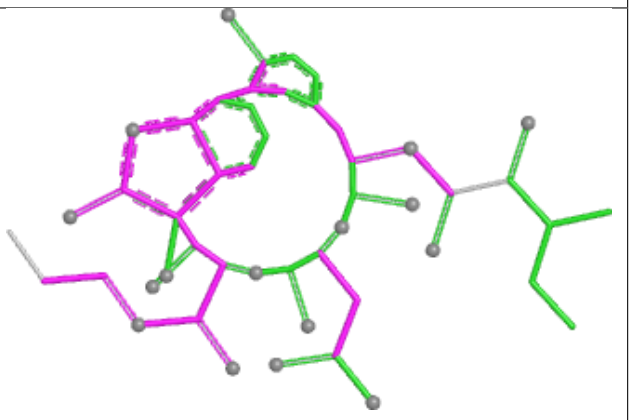
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	N	202	A1A9B	1	0
15	E	302	SO4	1	0
15	U	301	SO4	1	0
16	V	301	A1A9B	1	0
16	K	301	A1A9B	1	0

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 then 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.

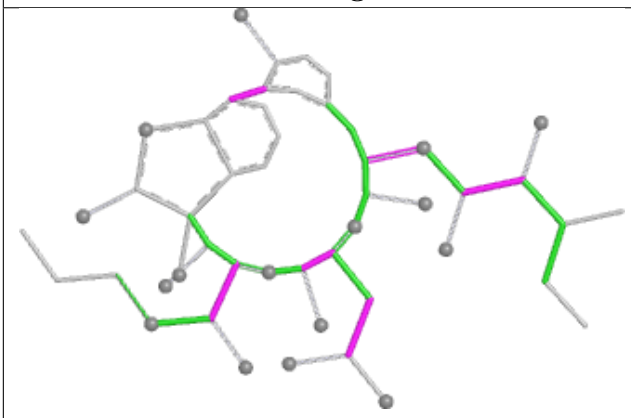
Ligand A1A9B Y 301



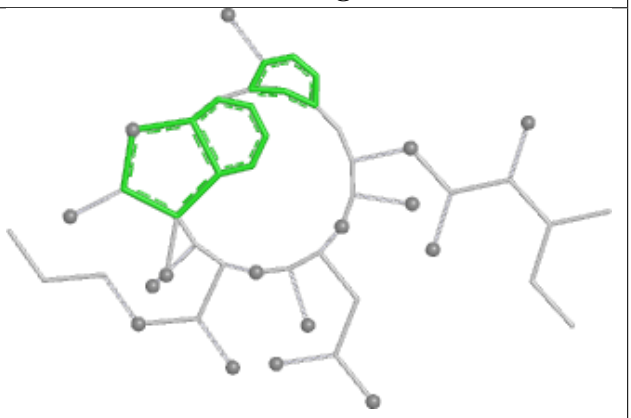
Bond lengths



Bond angles

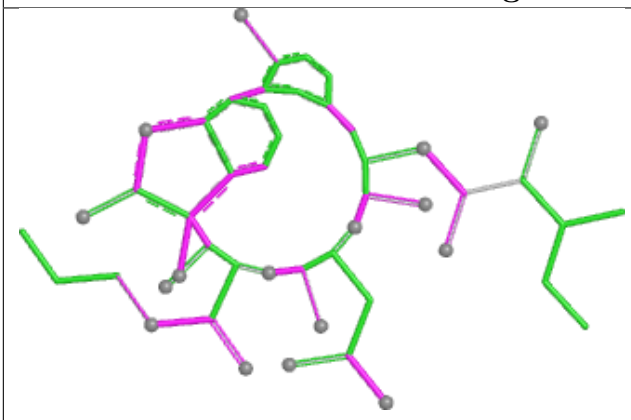


Torsions

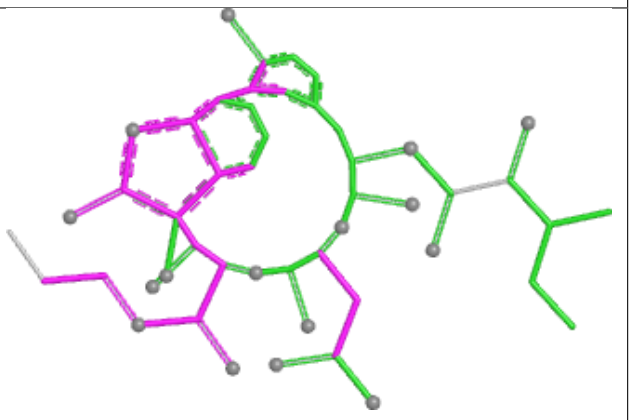


Rings

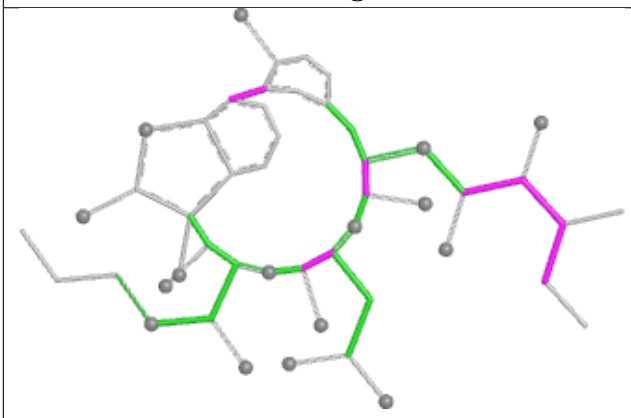
Ligand A1A9B N 202



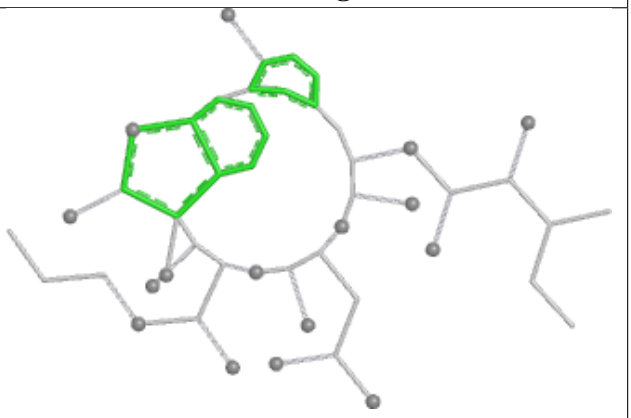
Bond lengths



Bond angles

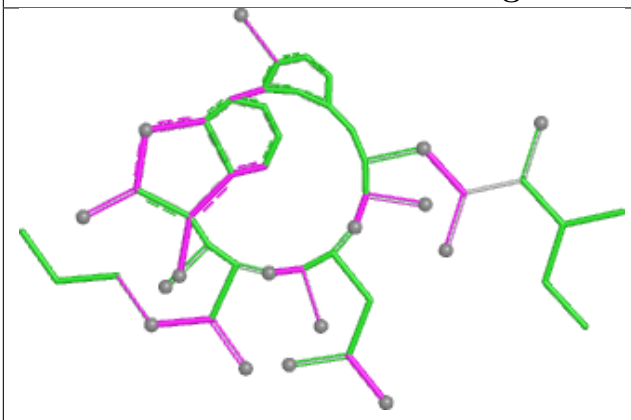


Torsions

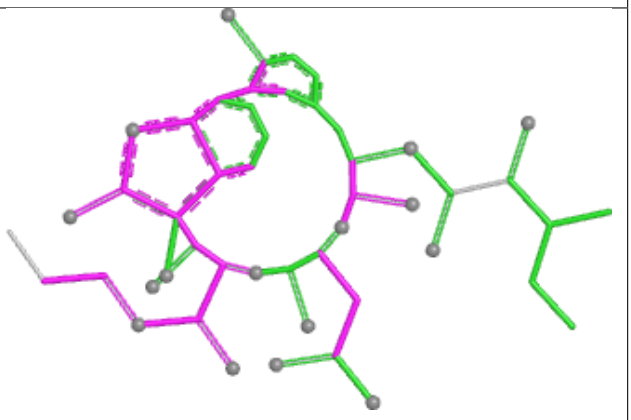


Rings

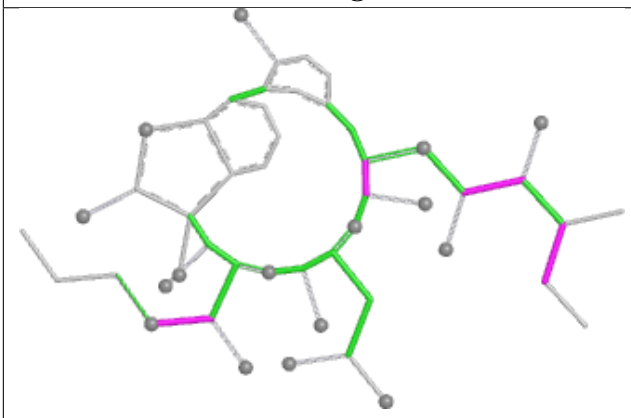
Ligand A1A9B H 301



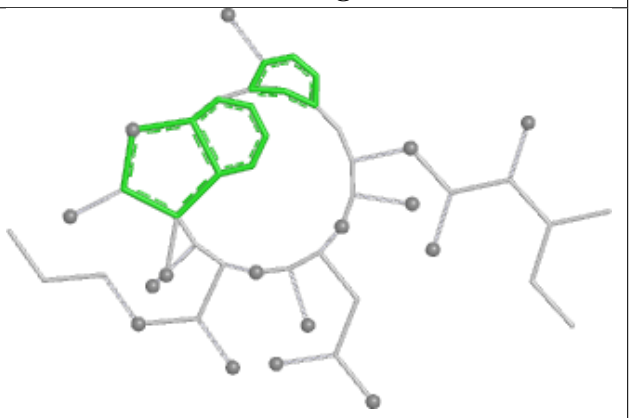
Bond lengths



Bond angles

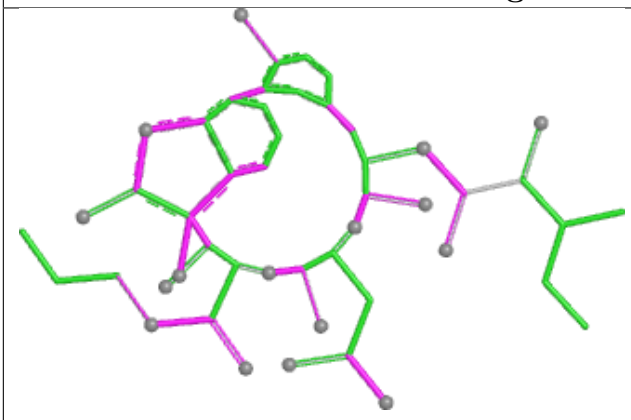


Torsions

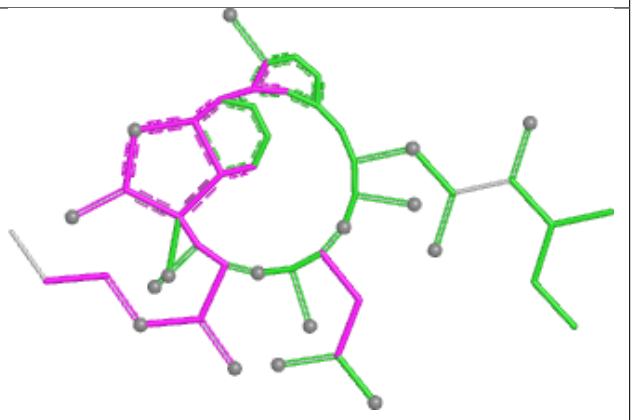


Rings

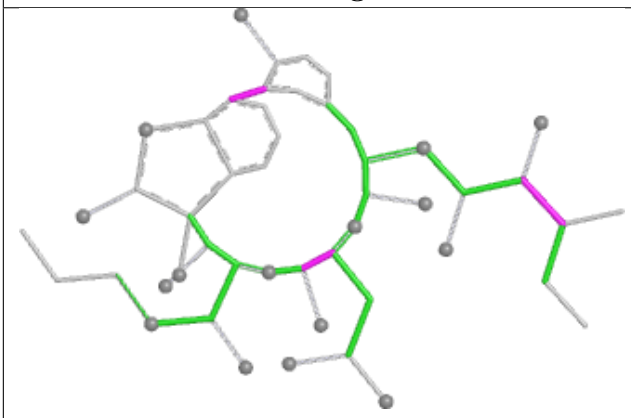
Ligand A1A9B b 201



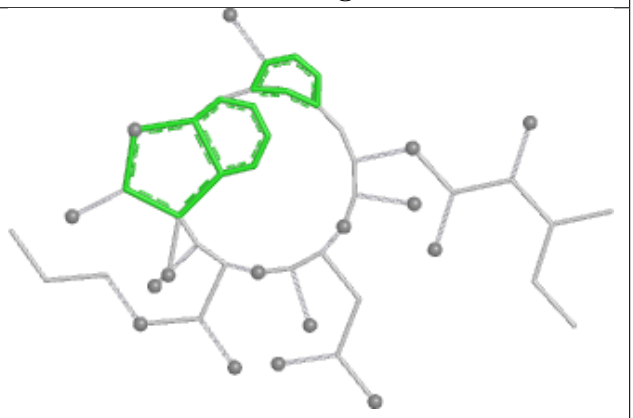
Bond lengths



Bond angles

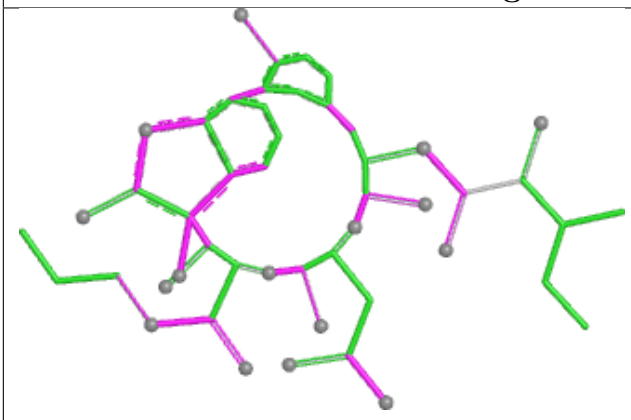


Torsions

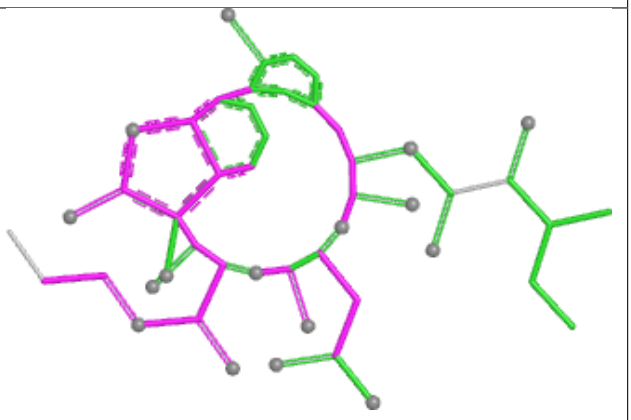


Rings

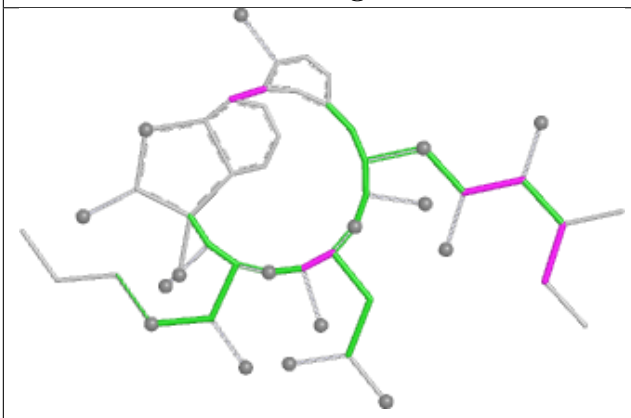
Ligand A1A9B V 301



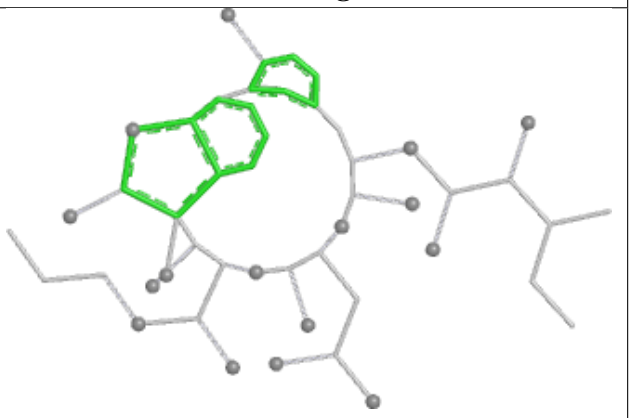
Bond lengths



Bond angles

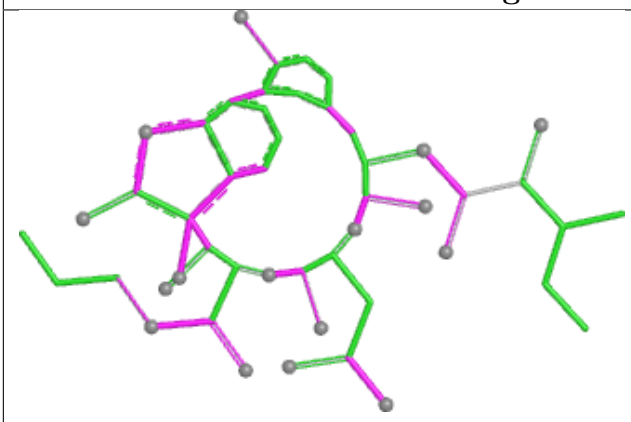


Torsions

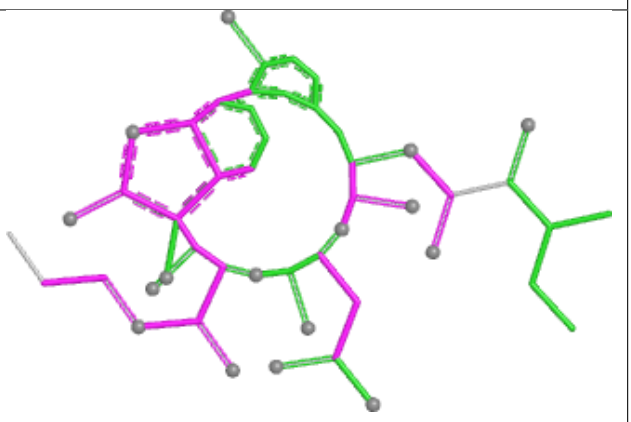


Rings

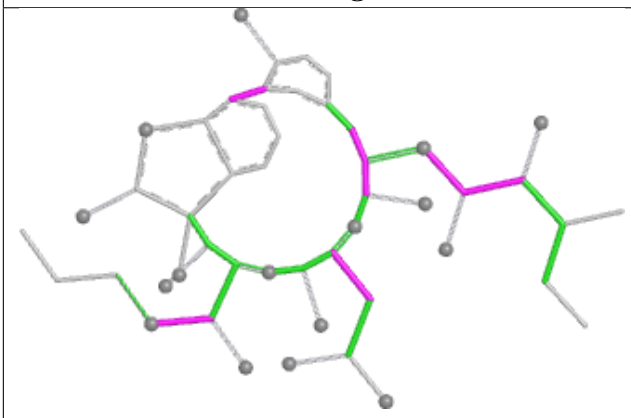
Ligand A1A9B K 301



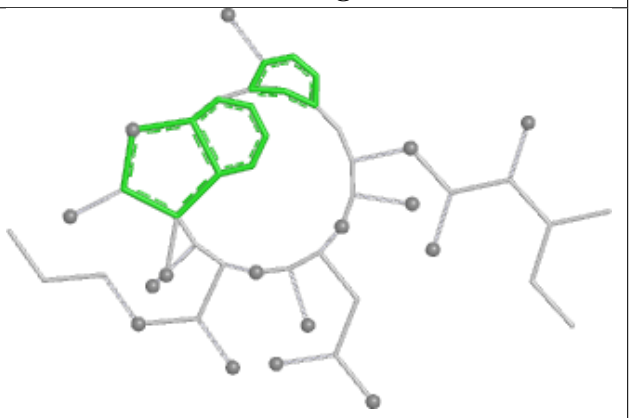
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	249/250 (99%)	-0.25	1 (0%) 89 81	50, 78, 117, 143	0
1	O	249/250 (99%)	-0.16	0 100 100	55, 84, 115, 131	0
2	B	243/258 (94%)	-0.15	0 100 100	56, 83, 116, 143	0
2	P	244/258 (94%)	-0.11	2 (0%) 82 70	52, 82, 120, 146	0
3	C	246/254 (96%)	-0.11	1 (0%) 89 81	54, 89, 142, 189	0
3	Q	241/254 (94%)	-0.06	1 (0%) 89 81	60, 95, 146, 170	0
4	D	239/260 (91%)	-0.12	2 (0%) 82 70	59, 85, 115, 172	0
4	R	246/260 (94%)	-0.16	2 (0%) 82 70	60, 89, 132, 178	0
5	E	232/234 (99%)	-0.08	0 100 100	61, 95, 126, 139	0
5	S	232/234 (99%)	0.08	0 100 100	59, 96, 133, 154	0
6	F	244/287 (85%)	-0.00	0 100 100	59, 87, 124, 151	0
6	T	245/287 (85%)	-0.08	2 (0%) 82 70	57, 86, 122, 137	0
7	G	242/252 (96%)	-0.21	0 100 100	57, 82, 112, 175	0
7	U	242/252 (96%)	-0.15	0 100 100	55, 81, 107, 132	0
8	H	222/232 (95%)	-0.15	0 100 100	56, 79, 100, 156	0
8	V	222/232 (95%)	-0.23	0 100 100	56, 79, 100, 140	0
9	I	204/205 (99%)	-0.18	1 (0%) 87 78	52, 76, 102, 132	0
9	W	204/205 (99%)	-0.15	0 100 100	51, 75, 107, 130	0
10	J	196/198 (98%)	-0.28	0 100 100	54, 76, 105, 138	0
10	X	195/198 (98%)	-0.17	0 100 100	56, 76, 99, 156	0
11	K	212/212 (100%)	-0.28	1 (0%) 87 78	58, 76, 104, 134	0
11	Y	212/212 (100%)	-0.20	2 (0%) 81 67	56, 80, 113, 134	0
12	L	222/222 (100%)	-0.26	1 (0%) 87 78	55, 78, 97, 120	0
12	Z	222/222 (100%)	-0.13	2 (0%) 81 67	59, 78, 107, 121	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/233 (100%)	-0.18	1 (0%) 89 81	58, 79, 105, 141	0
13	a	233/233 (100%)	-0.25	0 100 100	55, 74, 98, 115	0
14	N	196/196 (100%)	-0.22	0 100 100	55, 76, 99, 126	0
14	b	196/196 (100%)	-0.29	0 100 100	58, 75, 99, 120	0
All	All	6363/6586 (96%)	-0.16	19 (0%) 90 84	50, 81, 118, 189	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	248	ASP	3.7
4	D	112	ALA	2.9
4	D	0	TYR	2.5
4	R	0	TYR	2.3
12	Z	222	ASP	2.3
3	Q	21	ALA	2.2
13	M	233	ILE	2.2
6	T	151	GLY	2.2
11	Y	24	ASN	2.2
2	P	1	GLY	2.1
3	C	128	GLY	2.1
6	T	0	ILE	2.1
12	L	222	ASP	2.1
11	Y	211	ILE	2.1
12	Z	136	CYS	2.1
2	P	218	GLY	2.1
9	I	129	ILE	2.0
11	K	104	TYR	2.0
1	A	2	THR	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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	MG	I	301	1/1	0.70	0.32	65,65,65,65	0
15	SO4	B	301	5/5	0.74	0.17	97,119,137,147	5
15	SO4	Y	306	5/5	0.76	0.10	108,111,131,135	5
15	SO4	b	203	5/5	0.77	0.23	75,98,114,128	5
15	SO4	T	303	5/5	0.77	0.13	69,84,95,113	5
15	SO4	F	302	5/5	0.78	0.20	75,76,95,108	5
15	SO4	M	306	5/5	0.81	0.14	91,100,124,129	5
15	SO4	P	301	5/5	0.81	0.21	104,116,142,162	5
15	SO4	M	304	5/5	0.83	0.16	63,88,112,114	5
15	SO4	S	302	5/5	0.84	0.18	73,88,91,114	5
15	SO4	E	302	5/5	0.84	0.14	86,91,100,101	5
15	SO4	Y	304	5/5	0.84	0.21	68,73,88,98	5
15	SO4	H	302	5/5	0.84	0.20	94,94,109,127	5
15	SO4	a	302	5/5	0.84	0.20	86,90,101,116	5
15	SO4	I	303	5/5	0.84	0.16	72,76,107,128	5
15	SO4	J	202	5/5	0.84	0.19	93,107,121,137	5
17	MG	W	301	1/1	0.84	0.39	65,65,65,65	0
15	SO4	a	301	5/5	0.85	0.12	92,105,120,135	5
16	A1A9B	V	301	49/49	0.85	0.16	57,105,128,138	0
15	SO4	M	301	5/5	0.86	0.13	91,96,100,108	5
15	SO4	M	302	5/5	0.86	0.19	73,84,95,111	5
15	SO4	T	301	5/5	0.86	0.24	83,101,130,147	0
15	SO4	K	304	5/5	0.86	0.10	60,60,74,97	5
15	SO4	L	302	5/5	0.87	0.17	88,90,130,139	5
15	SO4	Y	303	5/5	0.87	0.17	94,103,113,123	5
15	SO4	S	303	5/5	0.87	0.13	84,91,102,114	5
15	SO4	a	304	5/5	0.87	0.15	113,121,160,164	0
17	MG	Y	302	1/1	0.87	0.10	87,87,87,87	1
17	MG	Z	301	1/1	0.87	0.09	60,60,60,60	0
15	SO4	a	305	5/5	0.88	0.18	74,90,113,116	5
15	SO4	I	302	5/5	0.88	0.14	75,79,91,97	5
15	SO4	T	302	5/5	0.88	0.18	102,103,141,142	5
15	SO4	S	301	5/5	0.88	0.28	64,75,94,104	5
15	SO4	K	302	5/5	0.88	0.23	52,75,78,84	5
15	SO4	D	301	5/5	0.88	0.20	81,87,90,90	5
15	SO4	V	302	5/5	0.88	0.18	97,98,101,129	5
16	A1A9B	N	202	49/49	0.89	0.13	55,79,103,123	0

Continued on next page...

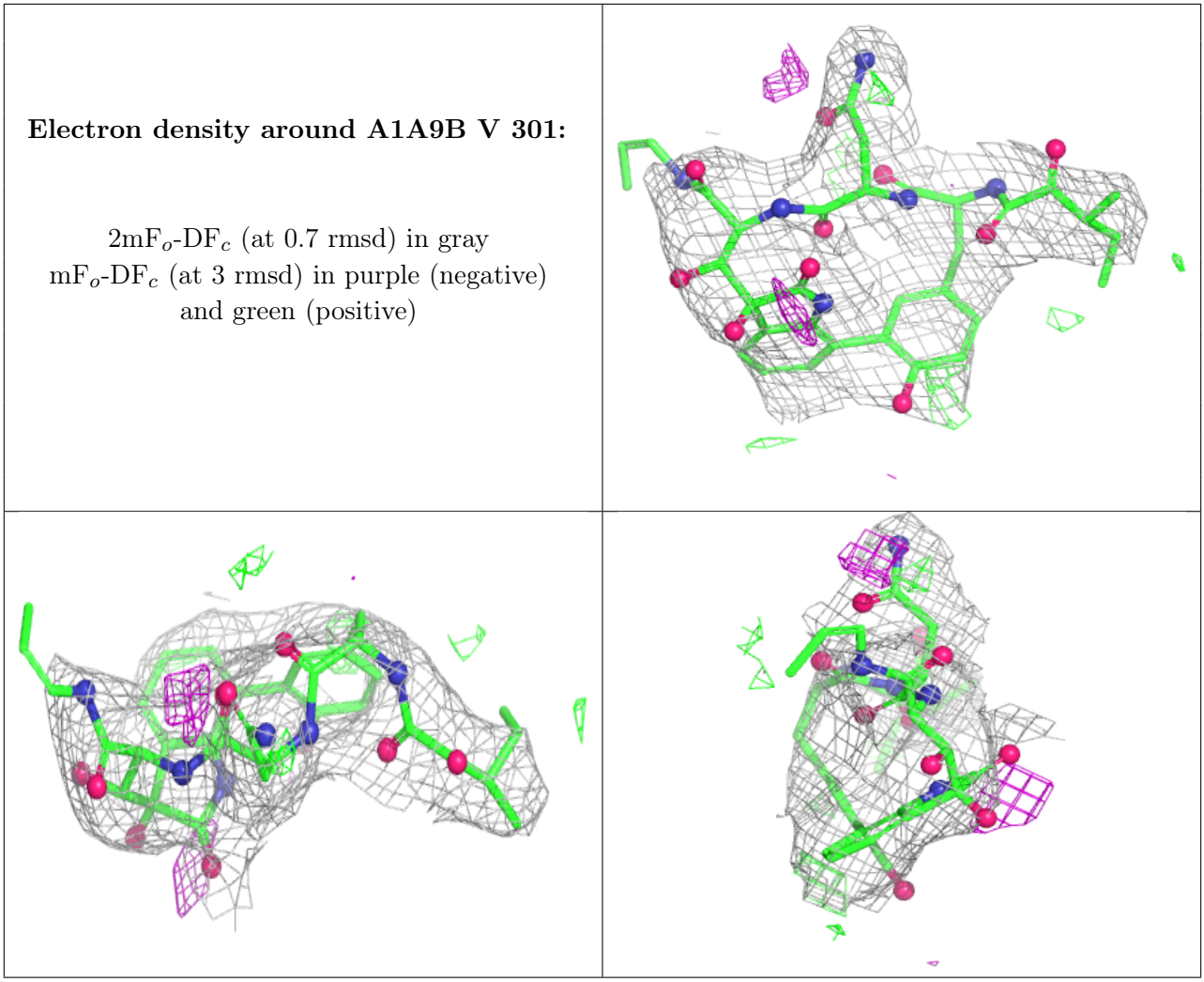
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	SO4	V	303	5/5	0.89	0.11	72,84,105,116	5
16	A1A9B	b	201	49/49	0.89	0.12	55,74,92,103	0
15	SO4	W	302	5/5	0.89	0.19	74,79,100,108	5
15	SO4	E	301	5/5	0.89	0.11	86,95,99,120	5
15	SO4	N	201	5/5	0.89	0.18	78,81,98,102	5
15	SO4	K	305	5/5	0.89	0.18	95,96,119,136	5
16	A1A9B	H	301	49/49	0.90	0.12	64,90,125,148	0
15	SO4	K	303	5/5	0.90	0.09	69,84,93,95	5
15	SO4	H	304	5/5	0.90	0.17	77,82,108,112	5
15	SO4	Y	305	5/5	0.90	0.11	66,77,95,117	5
15	SO4	a	303	5/5	0.91	0.15	67,69,87,98	5
15	SO4	b	204	5/5	0.91	0.14	70,72,77,83	5
15	SO4	F	301	5/5	0.91	0.19	72,80,91,101	5
15	SO4	U	302	5/5	0.91	0.17	68,81,90,104	5
15	SO4	b	202	5/5	0.91	0.14	64,70,85,87	5
15	SO4	Z	302	5/5	0.92	0.20	65,75,86,89	5
15	SO4	Z	303	5/5	0.92	0.12	63,83,107,108	5
15	SO4	M	303	5/5	0.92	0.22	70,98,109,133	5
15	SO4	H	303	5/5	0.92	0.13	75,75,79,93	5
15	SO4	Q	301	5/5	0.92	0.17	77,78,95,97	5
15	SO4	M	308	5/5	0.92	0.13	94,104,112,130	5
16	A1A9B	K	301	49/49	0.93	0.12	52,74,103,108	0
15	SO4	G	301	5/5	0.93	0.17	83,87,99,119	5
15	SO4	G	302	5/5	0.94	0.12	79,80,92,114	5
17	MG	L	301	1/1	0.94	0.09	53,53,53,53	0
15	SO4	X	201	5/5	0.94	0.15	76,77,83,108	5
16	A1A9B	Y	301	49/49	0.94	0.10	51,73,93,99	0
15	SO4	C	301	5/5	0.94	0.15	55,62,91,98	5
15	SO4	M	307	5/5	0.95	0.15	51,63,72,78	5
15	SO4	J	201	5/5	0.95	0.15	47,63,78,86	5
15	SO4	M	305	5/5	0.96	0.14	63,67,77,80	5
15	SO4	U	301	5/5	0.96	0.15	81,96,103,118	5

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.

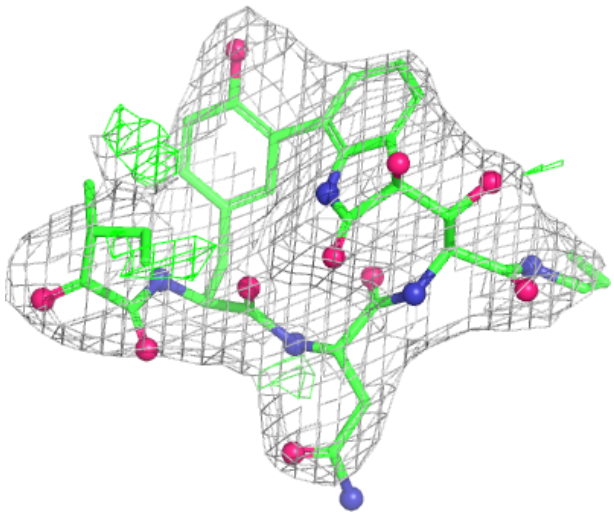
Electron density around A1A9B V 301:

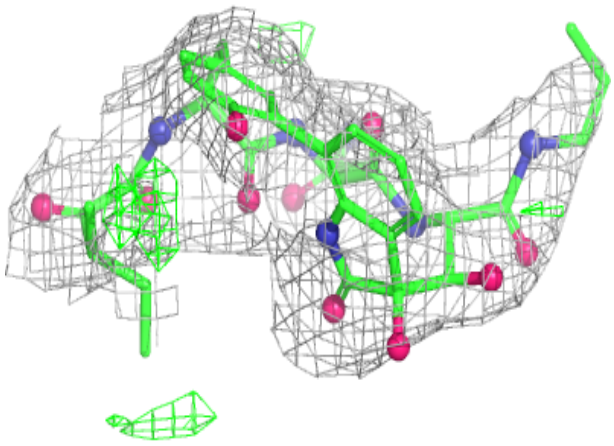
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

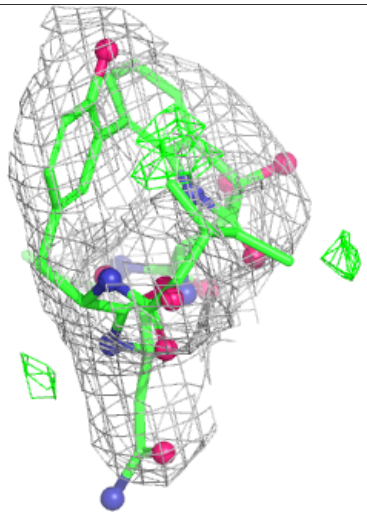


Electron density around A1A9B N 202:

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

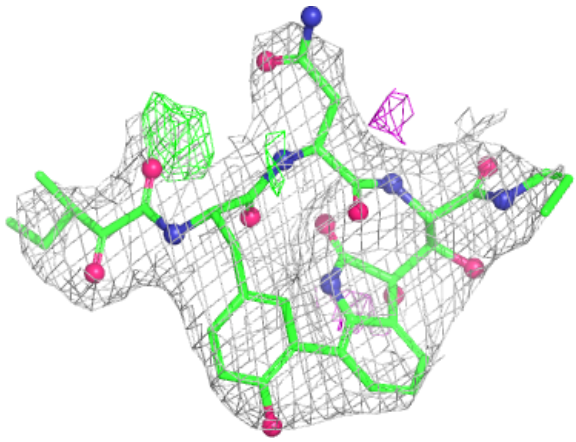


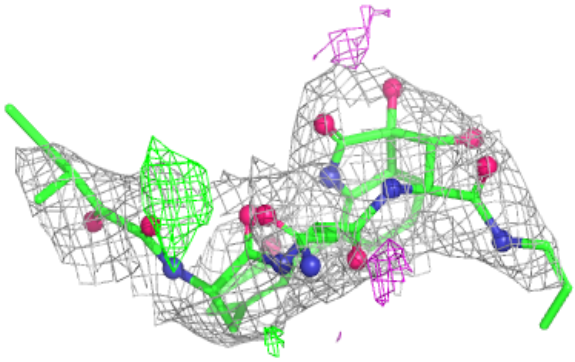


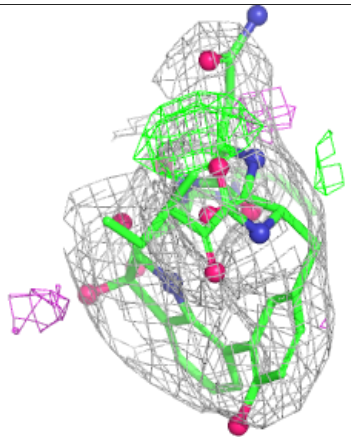


Electron density around A1A9B b 201:

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

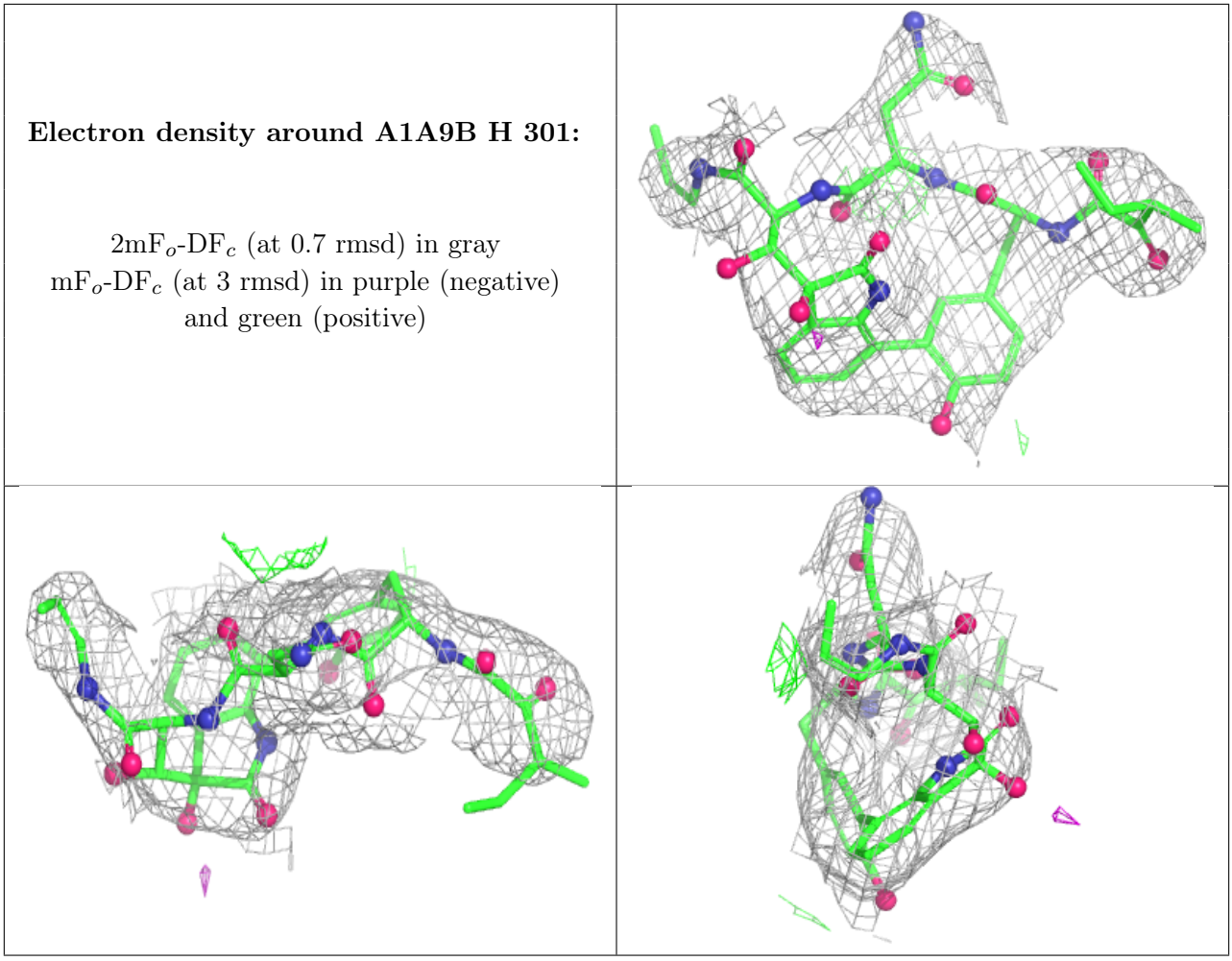






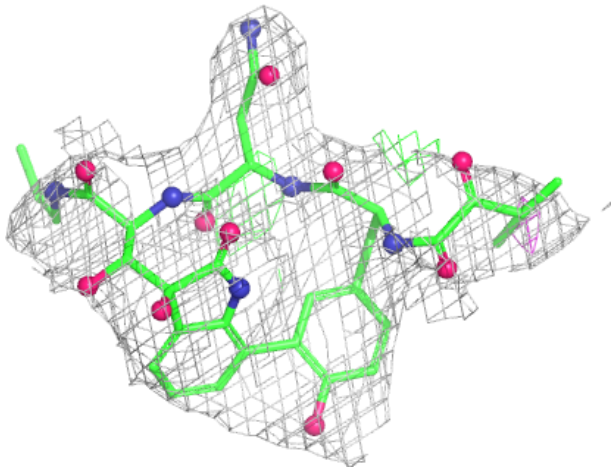
Electron density around A1A9B H 301:

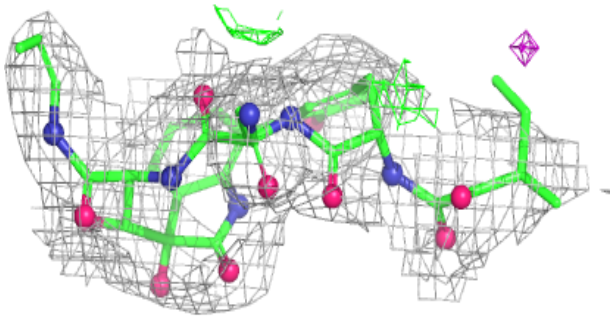
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

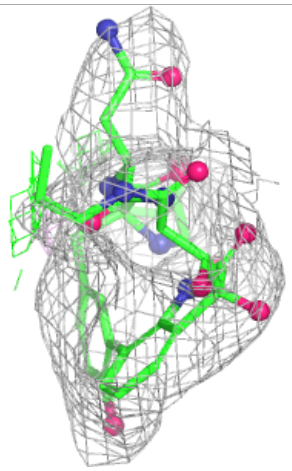


Electron density around A1A9B K 301:

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

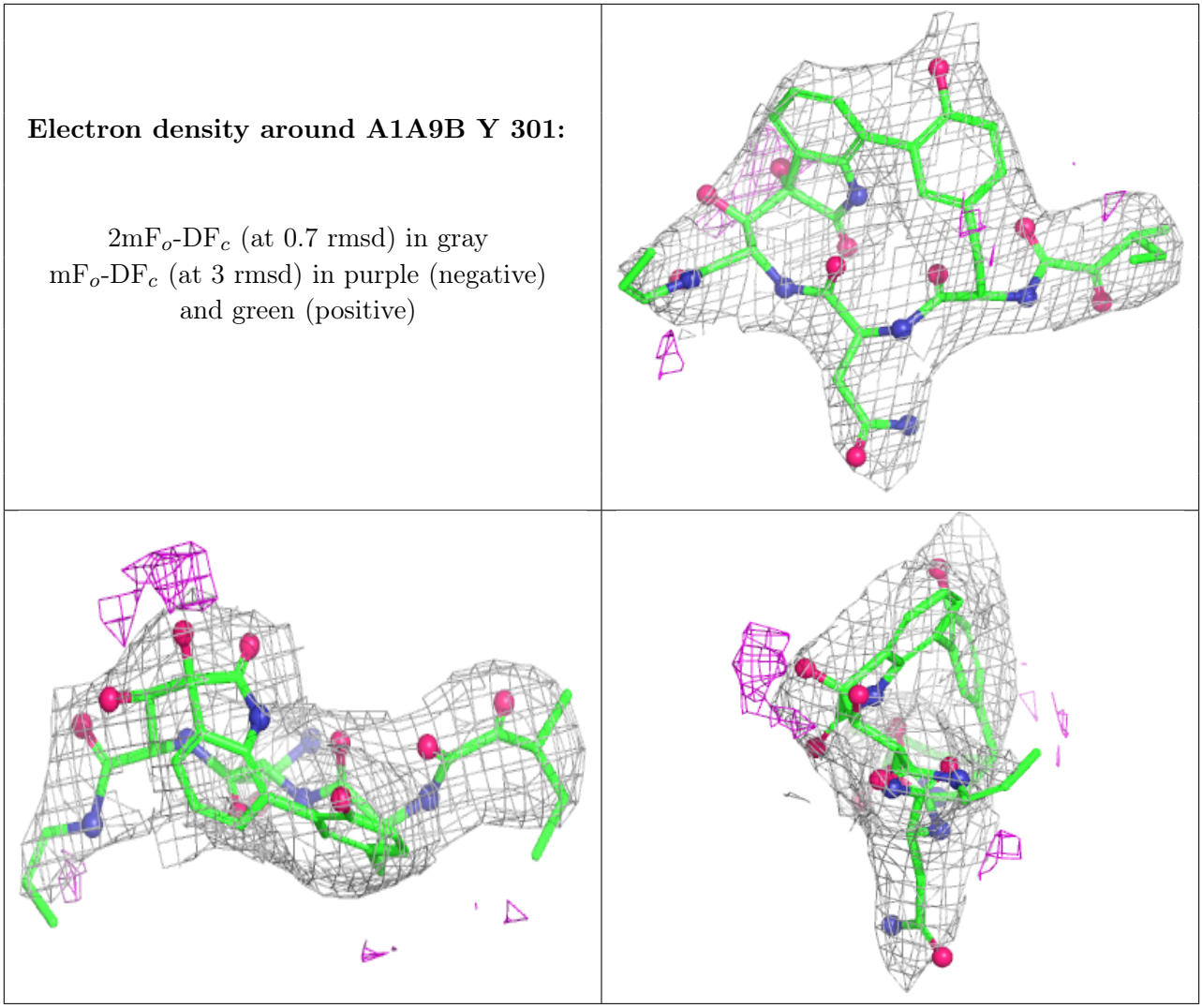






Electron density around A1A9B Y 301:

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



6.5 Other polymers

There are no such residues in this entry.