



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:31 PM UTC

PDB ID : 3UN4 / pdb_00003un4
Title : Yeast 20S proteasome in complex with PR-957 (morpholine)
Authors : Huber, E.; Basler, M.; Schwab, R.; Heinemeyer, W.; Kirk, C.; Groettrup, M.; Groll, M.
Deposited on : 2011-11-15
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

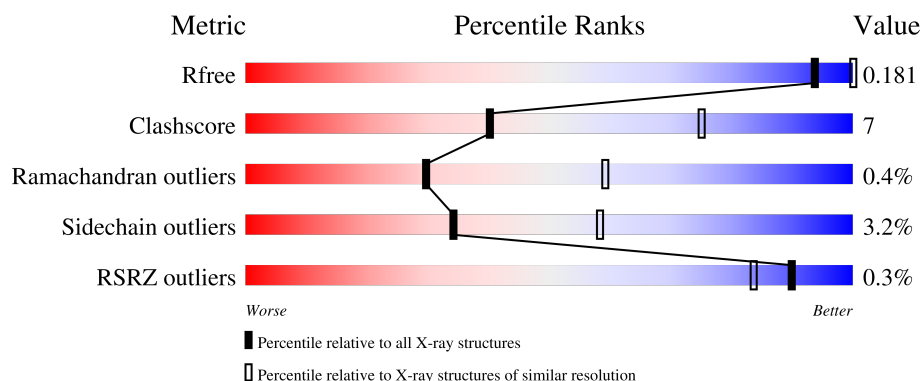
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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

Mol	Chain	Length	Quality of chain
1	A	250	 88% 10% • 2%
1	O	250	 87% 12% • 1%
2	B	258	 76% 18% • 5%
2	P	258	 76% 17% • 5%
3	C	254	 73% 20% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	254	 75%18%5%
4	D	260	 77%15%7%
4	R	260	 78%14%7%
5	E	234	 82%15%
5	S	234	 83%15%
6	F	288	 73%11%15%
6	T	288	 72%11%15%
7	G	252	 80%16%
7	U	252	 79%17%
8	H	232	 81%15%
8	V	232	 82%13%
9	I	205	 83%16%
9	W	205	 83%16%
10	J	198	 80%19%
10	X	198	 79%20%
11	K	212	 83%15%
11	Y	212	 83%15%
12	L	222	 82%17%
12	Z	222	 84%15%
13	M	233	 84%15%
13	a	233	 82%16%
14	N	196	 85%14%
14	b	196	 84%15%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51112 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome component Y7.

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

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			
4	R	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

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

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

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

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			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 component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

Continued on next page...

Continued from previous page...

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

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

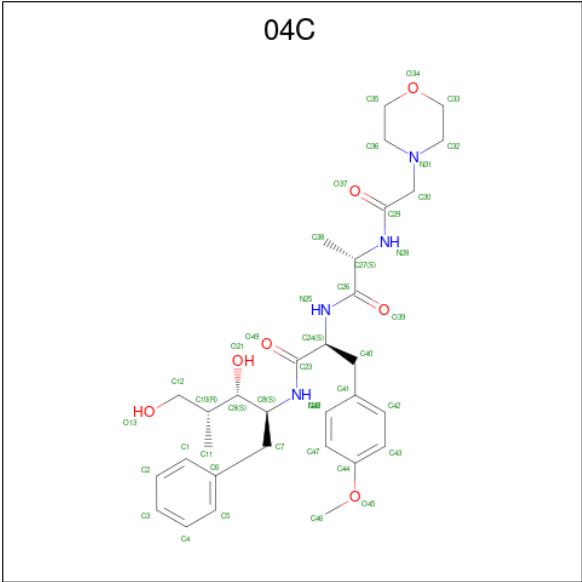
- Molecule 13 is a protein called Proteasome component PRE4.

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

- Molecule 14 is a protein called Proteasome component PRE3.

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

- Molecule 15 is 1,2,4-trideoxy-4-methyl-2-{[N-(morpholin-4-ylacetyl)-L-alanyl-O-methyl-L-tyrosyl]amino}-1-phenyl-D-xylitol (CCD ID: 04C) (formula: C₃₁H₄₄N₄O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			42	31	4	7		
15	K	1	Total	C	N	O	0	0
			42	31	4	7		
15	N	1	Total	C	N	O	0	0
			42	31	4	7		
15	V	1	Total	C	N	O	0	0
			42	31	4	7		
15	Y	1	Total	C	N	O	0	0
			42	31	4	7		
15	b	1	Total	C	N	O	0	0
			42	31	4	7		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	56	Total	O	0	0
			56	56		
16	B	38	Total	O	0	0
			38	38		
16	C	42	Total	O	0	0
			42	42		
16	D	38	Total	O	0	0
			38	38		
16	E	23	Total	O	0	0
			23	23		
16	F	48	Total	O	0	0
			48	48		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	61	Total O 61 61	0	0
16	H	49	Total O 49 49	0	0
16	I	62	Total O 62 62	0	0
16	J	54	Total O 54 54	0	0
16	K	46	Total O 46 46	0	0
16	L	55	Total O 55 55	0	0
16	M	72	Total O 72 72	0	0
16	N	51	Total O 51 51	0	0
16	O	32	Total O 32 32	0	0
16	P	30	Total O 30 30	0	0
16	Q	30	Total O 30 30	0	0
16	R	27	Total O 27 27	0	0
16	S	20	Total O 20 20	0	0
16	T	41	Total O 41 41	0	0
16	U	61	Total O 61 61	0	0
16	V	45	Total O 45 45	0	0
16	W	57	Total O 57 57	0	0
16	X	52	Total O 52 52	0	0
16	Y	49	Total O 49 49	0	0
16	Z	50	Total O 50 50	0	0
16	a	75	Total O 75 75	0	0

Continued on next page...

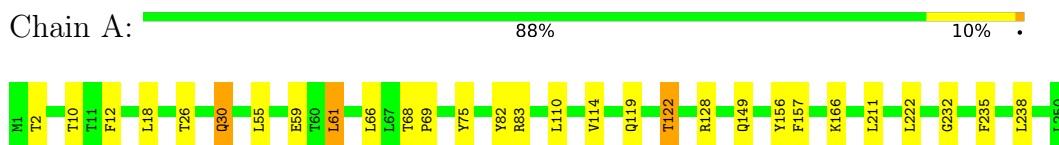
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	b	58	Total	O	0	0
			58	58		

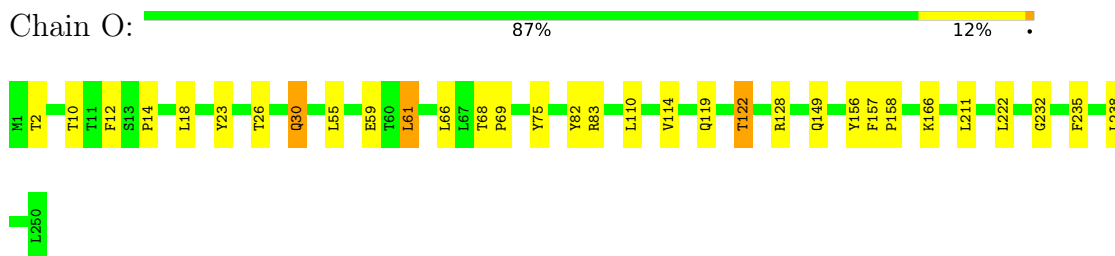
3 Residue-property plots

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

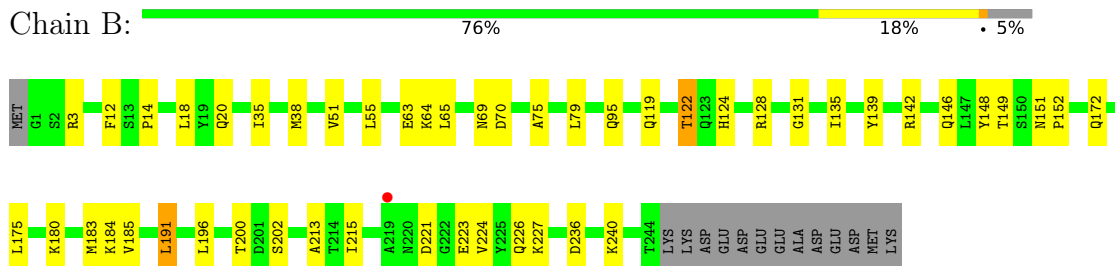
• Molecule 1: Proteasome component Y7



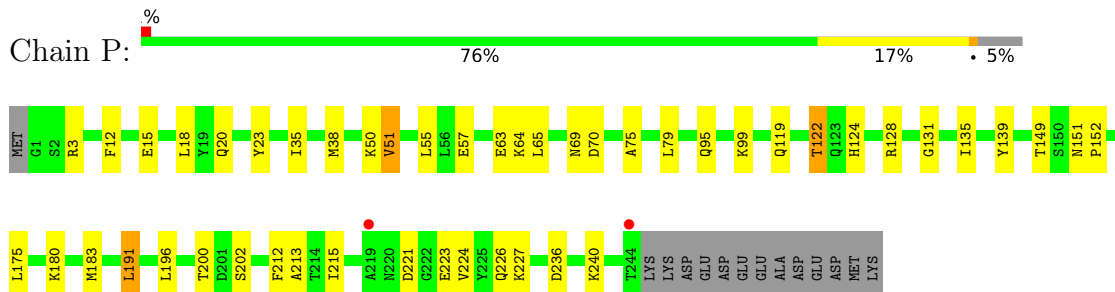
• Molecule 1: Proteasome component Y7



• Molecule 2: Proteasome component Y13

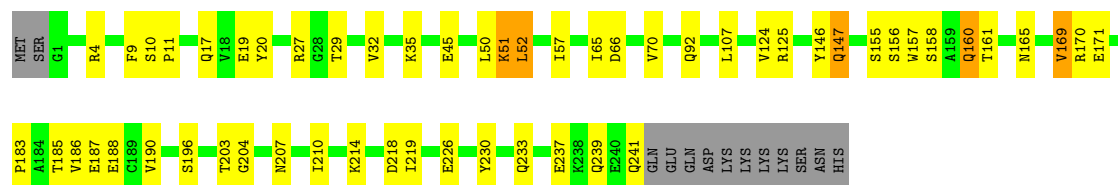


• Molecule 2: Proteasome component Y13



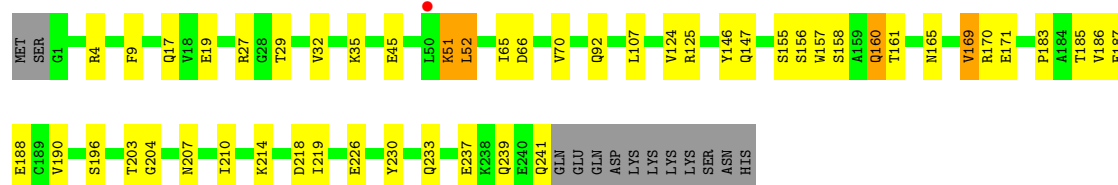
- Molecule 3: Proteasome component PRE6

Chain C:  73% 20% 5%



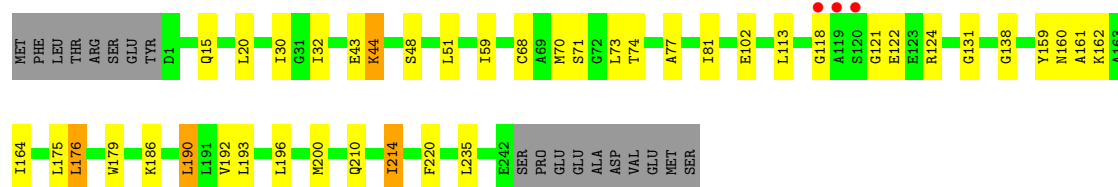
- Molecule 3: Proteasome component PRE6

Chain Q:  75% 18% 5%



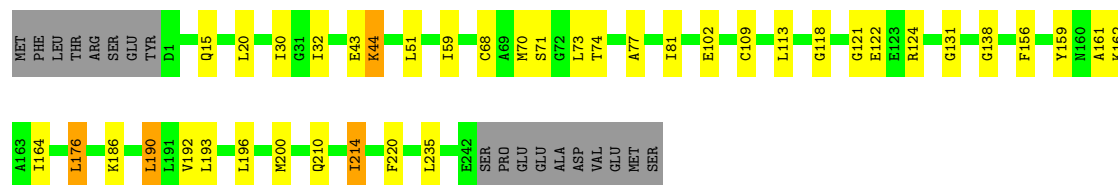
- Molecule 4: Proteasome component PUP2

Chain D:  77% 15% 7%



- Molecule 4: Proteasome component PUP2

Chain R:  78% 14% 7%

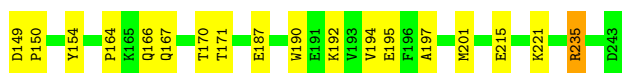


- Molecule 5: Proteasome component PRE5

Chain E:  82% 15% 3%

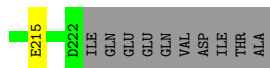






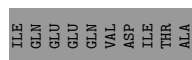
• Molecule 8: Proteasome component PUP1

Chain H: 81% 15%



• Molecule 8: Proteasome component PUP1

Chain V: 82% 13%



• Molecule 9: Proteasome component PUP3

Chain I: 83% 16%



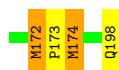
• Molecule 9: Proteasome component PUP3

Chain W: 83% 16%

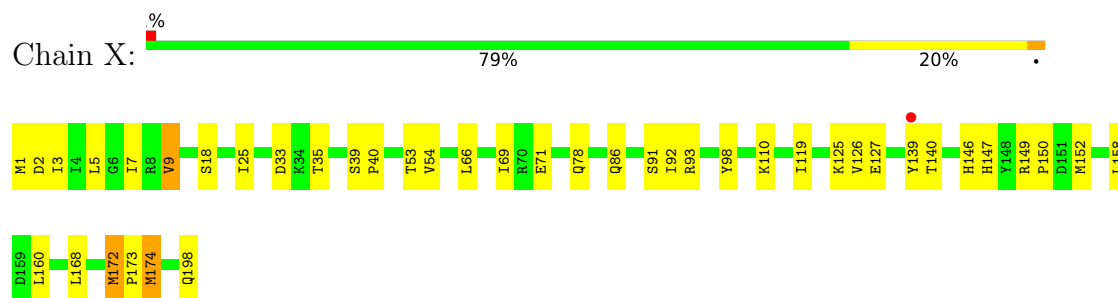


• Molecule 10: Proteasome component C11

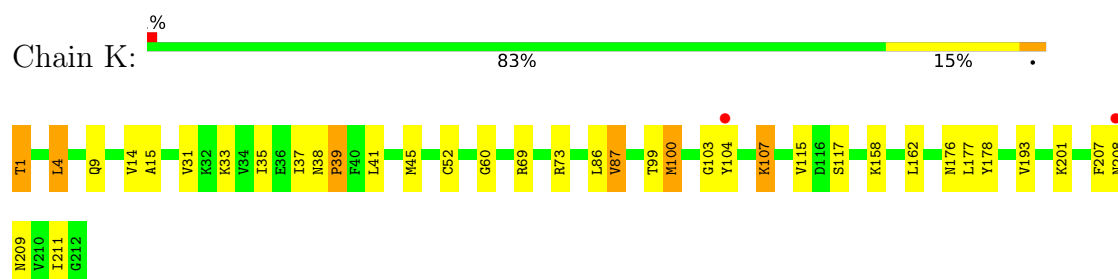
Chain J: 80% 19%



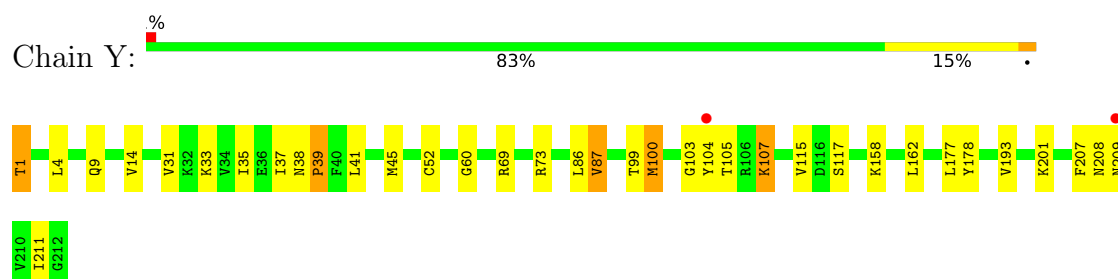
- Molecule 10: Proteasome component C11



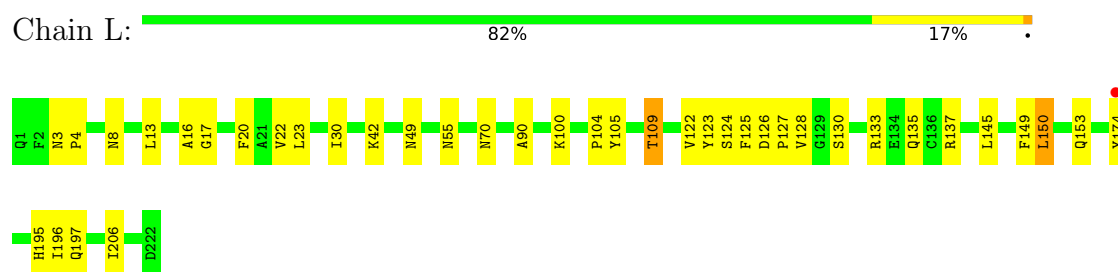
- Molecule 11: Proteasome component PRE2



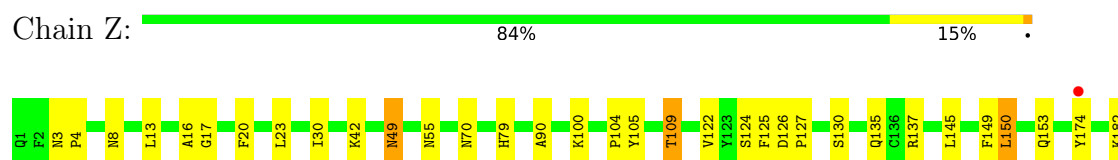
- Molecule 11: Proteasome component PRE2

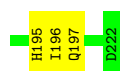


- Molecule 12: Proteasome component C5



- Molecule 12: Proteasome component C5





- Molecule 13: Proteasome component PRE4

Chain M: 84% 15% .



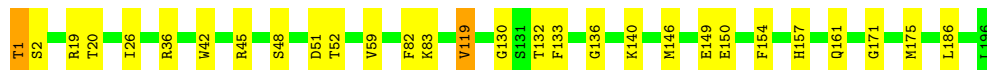
- Molecule 13: Proteasome component PRE4

Chain a: 82% 16% .



- Molecule 14: Proteasome component PRE3

Chain N: 85% 14% .



- Molecule 14: Proteasome component PRE3

Chain b: 84% 15% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.41Å 300.78Å 143.82Å 90.00° 112.75° 90.00°	Depositor
Resolution (Å)	15.00 – 3.40 15.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (15.00-3.40) 97.2 (15.00-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 3.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.179 , 0.219 (Not available) , 0.181	Depositor DCC
R_{free} test set	7082 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.8	Xtriage
Anisotropy	0.786	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	51112	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 04C

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	0.47	0/1952	0.77	0/2642
1	O	0.47	0/1952	0.77	0/2642
2	B	0.45	0/1934	0.77	0/2618
2	P	0.45	0/1934	0.77	0/2618
3	C	0.46	0/1919	0.78	0/2598
3	Q	0.46	0/1919	0.78	0/2598
4	D	0.52	0/1886	0.75	0/2541
4	R	0.52	0/1886	0.75	0/2541
5	E	0.46	0/1823	0.75	0/2463
5	S	0.46	0/1823	0.76	0/2463
6	F	0.58	0/1936	0.82	0/2614
6	T	0.58	0/1936	0.82	0/2614
7	G	0.47	0/1959	0.77	0/2652
7	U	0.47	0/1959	0.77	0/2652
8	H	0.66	1/1715 (0.1%)	0.75	0/2326
8	V	0.66	1/1715 (0.1%)	0.75	0/2326
9	I	0.45	0/1611	0.76	0/2174
9	W	0.45	0/1611	0.76	0/2174
10	J	0.48	0/1613	0.79	2/2173 (0.1%)
10	X	0.47	0/1613	0.79	2/2173 (0.1%)
11	K	0.63	1/1681 (0.1%)	0.76	0/2274
11	Y	0.62	1/1681 (0.1%)	0.76	0/2274
12	L	0.50	0/1795	0.77	0/2420
12	Z	0.50	0/1795	0.77	0/2420
13	M	0.45	0/1855	0.75	0/2514
13	a	0.45	0/1855	0.74	0/2514
14	N	0.62	1/1541 (0.1%)	0.78	0/2087
14	b	0.60	1/1541 (0.1%)	0.79	1/2087 (0.0%)
All	All	0.52	6/50440 (0.0%)	0.77	5/68192 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
14	b	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	1	THR	C-N	12.09	1.48	1.33
14	b	1	THR	C-N	11.17	1.49	1.33
8	V	1	THR	C-N	10.03	1.47	1.33
8	H	1	THR	C-N	9.88	1.46	1.33
11	K	1	THR	C-N	9.62	1.46	1.33
11	Y	1	THR	C-N	8.89	1.45	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1	THR	N-CA-C	5.80	127.24	111.00
10	J	172	MET	CA-C-N	5.35	125.17	119.28
10	J	172	MET	C-N-CA	5.35	125.17	119.28
10	X	172	MET	CA-C-N	5.25	125.06	119.28
10	X	172	MET	C-N-CA	5.25	125.06	119.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	b	1	THR	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	18	0
1	O	1915	0	1929	21	0
2	B	1904	0	1904	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1904	0	1904	31	0
3	C	1890	0	1903	40	0
3	Q	1890	0	1903	34	0
4	D	1861	0	1839	20	0
4	R	1861	0	1839	21	0
5	E	1795	0	1800	32	0
5	S	1795	0	1800	31	0
6	F	1896	0	1889	21	0
6	T	1896	0	1889	22	0
7	G	1921	0	1913	26	0
7	U	1921	0	1913	31	0
8	H	1684	0	1686	21	0
8	V	1684	0	1686	19	0
9	I	1581	0	1574	25	0
9	W	1581	0	1574	24	0
10	J	1585	0	1590	40	0
10	X	1585	0	1590	37	0
11	K	1644	0	1593	26	0
11	Y	1644	0	1593	22	0
12	L	1757	0	1711	28	0
12	Z	1757	0	1711	29	0
13	M	1824	0	1832	25	0
13	a	1824	0	1832	27	0
14	N	1512	0	1479	23	0
14	b	1512	0	1479	31	0
15	H	42	0	42	0	0
15	K	42	0	42	5	0
15	N	42	0	42	4	0
15	V	42	0	42	0	0
15	Y	42	0	42	2	0
15	b	42	0	42	8	0
16	A	56	0	0	0	0
16	B	38	0	0	1	0
16	C	42	0	0	0	0
16	D	38	0	0	0	0
16	E	23	0	0	0	0
16	F	48	0	0	0	0
16	G	61	0	0	0	0
16	H	49	0	0	0	0
16	I	62	0	0	1	0
16	J	54	0	0	3	0
16	K	46	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	L	55	0	0	0	0
16	M	72	0	0	0	0
16	N	51	0	0	0	0
16	O	32	0	0	0	0
16	P	30	0	0	0	0
16	Q	30	0	0	0	0
16	R	27	0	0	2	0
16	S	20	0	0	0	0
16	T	41	0	0	0	0
16	U	61	0	0	0	0
16	V	45	0	0	0	0
16	W	57	0	0	0	0
16	X	52	0	0	3	0
16	Y	49	0	0	0	0
16	Z	50	0	0	0	0
16	a	75	0	0	0	0
16	b	58	0	0	0	0
All	All	51112	0	49536	659	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 (659) 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)
10:J:174:MET:HE3	10:X:174:MET:HE3	1.28	1.11
14:b:1:THR:HG22	14:b:2:SER:N	1.66	1.10
14:b:1:THR:HG22	14:b:2:SER:H	0.97	1.07
14:b:1:THR:CG2	14:b:2:SER:H	1.68	1.07
14:b:45:ARG:NH1	15:b:201:04C:H44	1.84	0.92
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.13	0.91
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.19	0.91
11:K:209:ASN:HB3	16:X:234:HOH:O	1.77	0.85
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.63	0.80
1:O:12:PHE:H	2:P:20:GLN:HE22	1.27	0.80
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.62	0.80
10:J:139:TYR:HD1	16:J:228:HOH:O	1.65	0.79
2:P:200:THR:HG22	2:P:202:SER:H	1.49	0.78
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.64	0.78
2:B:200:THR:HG22	2:B:202:SER:H	1.49	0.78
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.50	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:PHE:H	3:C:17:GLN:HE22	1.32	0.76
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.50	0.76
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.66	0.76
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.68	0.76
13:a:161:ARG:HG3	13:a:161:ARG:HH11	1.51	0.76
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.50	0.76
5:S:12:PHE:H	6:T:19:GLN:HE22	1.31	0.75
15:N:201:04C:H7	15:N:201:04C:H22	1.68	0.75
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.68	0.75
13:M:43:ILE:HG12	13:M:64:GLU:HG3	1.68	0.75
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	1.85	0.75
13:a:43:ILE:HG12	13:a:64:GLU:HG3	1.67	0.75
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.69	0.74
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.35	0.74
10:J:139:TYR:CE2	10:J:172:MET:HG3	2.23	0.74
14:b:20:THR:HG22	15:b:201:04C:H41	1.70	0.74
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.51	0.73
13:M:48:ASN:H	13:M:48:ASN:HD22	1.35	0.72
10:X:139:TYR:CE2	10:X:172:MET:HG3	2.24	0.72
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.71	0.72
4:R:161:ALA:HB3	5:S:55:LEU:HD23	1.71	0.71
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.72	0.71
13:a:48:ASN:H	13:a:48:ASN:HD22	1.36	0.71
5:E:12:PHE:H	6:F:19:GLN:HE22	1.37	0.71
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.39	0.71
3:C:9:PHE:H	4:D:15:GLN:HE22	1.39	0.71
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	1.87	0.71
5:S:205:LEU:HA	5:S:209:ASN:HD22	1.56	0.70
5:E:205:LEU:HA	5:E:209:ASN:HD22	1.56	0.70
2:B:122:THR:HG22	3:C:125:ARG:HH21	1.55	0.70
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.71	0.70
1:A:12:PHE:H	2:B:20:GLN:HE22	1.37	0.70
10:X:39:SER:HB2	10:X:40:PRO:HD2	1.73	0.70
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.56	0.70
10:J:39:SER:HB2	10:J:40:PRO:HD2	1.73	0.70
12:L:195:HIS:HD2	12:L:197:GLN:H	1.40	0.70
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.74	0.70
13:a:179:ASN:HD22	13:a:182:ARG:HH11	1.39	0.69
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.41	0.69
11:K:209:ASN:ND2	9:W:37:ASN:HD21	1.90	0.69
5:E:92:ASN:HD21	12:L:70:ASN:ND2	1.89	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:45:MET:HE2	15:K:301:04C:H44	1.75	0.69
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.40	0.68
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.40	0.68
7:U:92:ALA:HA	7:U:103:MET:HE2	1.75	0.68
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.74	0.68
10:J:150:PRO:HG3	11:Y:208:ASN:HD21	1.59	0.68
7:G:92:ALA:HA	7:G:103:MET:HE2	1.74	0.68
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.74	0.68
11:K:73:ARG:NH2	11:K:104:TYR:O	2.27	0.67
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.40	0.67
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.25	0.67
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.77	0.67
11:K:208:ASN:HD21	10:X:150:PRO:HG3	1.60	0.67
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.28	0.67
2:P:122:THR:HG22	3:Q:125:ARG:HH21	1.60	0.66
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.24	0.66
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.42	0.65
8:V:35:HIS:CB	8:V:56:THR:HG21	2.27	0.65
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.78	0.65
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.77	0.65
9:I:148:MET:HE3	9:I:152:LEU:HD11	1.79	0.65
9:I:37:ASN:HD21	11:Y:209:ASN:ND2	1.94	0.64
6:F:32:THR:HG22	6:F:47:GLU:OE2	1.97	0.64
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.62	0.64
5:E:92:ASN:ND2	12:L:70:ASN:HD21	1.91	0.64
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.63	0.64
9:W:148:MET:HE3	9:W:152:LEU:HD11	1.80	0.64
14:b:1:THR:CG2	14:b:2:SER:N	2.37	0.64
8:H:35:HIS:CB	8:H:56:THR:HG21	2.27	0.64
6:T:32:THR:HG22	6:T:47:GLU:OE2	1.98	0.64
7:G:195:GLU:HG3	7:G:235:ARG:HG3	1.78	0.63
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.62	0.63
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.47	0.63
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.63	0.63
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.79	0.62
14:b:175:MET:HB2	14:b:186:LEU:HB2	1.81	0.62
13:M:48:ASN:HD22	13:M:48:ASN:N	1.97	0.62
10:J:174:MET:HE3	10:X:174:MET:CE	2.19	0.61
5:E:205:LEU:HA	5:E:209:ASN:ND2	2.15	0.61
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.65	0.61
6:F:31:THR:HG21	6:F:47:GLU:O	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.65	0.61
14:N:1:THR:HG22	14:N:2:SER:N	2.15	0.61
6:T:31:THR:HG21	6:T:47:GLU:O	2.00	0.61
2:B:180:LYS:HG3	2:B:183:MET:HG3	1.83	0.61
5:S:205:LEU:HA	5:S:209:ASN:ND2	2.15	0.61
9:I:37:ASN:ND2	9:I:37:ASN:H	1.99	0.60
4:R:73:LEU:HD12	4:R:131:GLY:HA3	1.83	0.60
3:C:161:THR:HG21	3:C:169:VAL:HG13	1.83	0.60
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.83	0.60
5:S:127:TYR:O	5:S:148:PRO:HB3	2.01	0.60
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.82	0.60
2:B:63:GLU:HG3	2:B:64:LYS:HG3	1.82	0.60
13:a:179:ASN:HD22	13:a:182:ARG:NH1	1.99	0.60
13:a:48:ASN:HD22	13:a:48:ASN:N	1.98	0.60
10:J:149:ARG:HB2	10:J:152:MET:HG3	1.84	0.60
11:K:87:VAL:HG11	11:K:117:SER:HA	1.83	0.60
11:K:208:ASN:ND2	10:X:150:PRO:HG3	2.16	0.60
2:P:63:GLU:HG3	2:P:64:LYS:HG3	1.82	0.60
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.83	0.60
5:E:127:TYR:O	5:E:148:PRO:HB3	2.01	0.60
10:J:1:MET:HG2	10:J:2:ASP:H	1.67	0.59
4:D:73:LEU:HD12	4:D:131:GLY:HA3	1.84	0.59
1:A:30:GLN:HE21	1:A:30:GLN:HA	1.67	0.59
10:J:150:PRO:HG3	11:Y:208:ASN:ND2	2.16	0.59
10:X:149:ARG:HB2	10:X:152:MET:HG3	1.84	0.59
7:G:117:GLN:O	7:G:120:THR:HB	2.02	0.59
9:I:36:SER:HB2	10:J:126:VAL:HG21	1.84	0.59
6:T:91:GLU:HG3	6:T:111:ARG:HH11	1.67	0.59
12:Z:126:ASP:HB2	12:Z:130:SER:HB3	1.85	0.59
13:a:227:GLY:HA3	13:a:231:GLN:HB3	1.84	0.59
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.83	0.59
10:X:3:ILE:HD13	10:X:168:LEU:HD13	1.83	0.59
2:B:18:LEU:HD13	2:B:122:THR:HG23	1.83	0.59
6:F:91:GLU:HG3	6:F:111:ARG:HH11	1.66	0.59
13:M:179:ASN:HD22	13:M:182:ARG:NH1	1.99	0.59
2:P:18:LEU:HD13	2:P:122:THR:HG23	1.85	0.58
5:E:197:SER:HA	5:E:200:LEU:HG	1.84	0.58
11:K:38:ASN:HB2	11:K:39:PRO:HD2	1.85	0.58
8:H:62:ASN:HB3	8:H:82:MET:HE1	1.85	0.58
1:O:30:GLN:HA	1:O:30:GLN:HE21	1.68	0.58
3:C:204:GLY:HA3	3:C:207:ASN:HB2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:1:MET:HG2	10:X:2:ASP:H	1.69	0.58
11:Y:87:VAL:HG11	11:Y:117:SER:HA	1.83	0.58
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	1.86	0.58
10:J:3:ILE:HD13	10:J:168:LEU:HD13	1.85	0.58
12:L:126:ASP:HB2	12:L:130:SER:HB3	1.86	0.58
7:U:117:GLN:O	7:U:120:THR:HB	2.04	0.58
2:P:180:LYS:HG3	2:P:183:MET:HG3	1.84	0.57
5:S:197:SER:HA	5:S:200:LEU:HG	1.85	0.57
9:W:37:ASN:ND2	9:W:37:ASN:H	2.01	0.57
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.84	0.57
13:M:227:GLY:HA3	13:M:231:GLN:HB3	1.85	0.57
7:G:103:MET:HE3	7:G:108:LEU:HB2	1.87	0.57
1:O:119:GLN:O	1:O:122:THR:HB	2.05	0.57
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.85	0.57
9:W:36:SER:HB2	10:X:126:VAL:HG21	1.86	0.57
11:K:87:VAL:CG1	11:K:117:SER:HA	2.35	0.57
2:B:122:THR:CG2	3:C:125:ARG:HH21	2.18	0.57
2:B:215:ILE:HG12	2:B:226:GLN:HG2	1.87	0.57
9:I:97:ARG:HD2	16:I:360:HOH:O	2.05	0.57
8:V:62:ASN:HB3	8:V:82:MET:HE1	1.86	0.57
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.87	0.56
9:W:148:MET:HE2	9:W:172:ASN:HB2	1.88	0.56
10:X:147:HIS:HB2	10:X:160:LEU:HD11	1.87	0.56
1:A:119:GLN:O	1:A:122:THR:HB	2.05	0.56
11:Y:87:VAL:CG1	11:Y:117:SER:HA	2.34	0.56
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.88	0.56
3:Q:204:GLY:HA3	3:Q:207:ASN:HB2	1.87	0.56
10:J:25:ILE:O	10:X:139:TYR:OH	2.23	0.56
2:P:215:ILE:HG12	2:P:226:GLN:HG2	1.87	0.56
4:D:176:LEU:HD22	5:E:55:LEU:HD13	1.88	0.56
10:J:139:TYR:OH	10:X:25:ILE:O	2.24	0.55
10:J:174:MET:CE	10:X:174:MET:HE3	2.20	0.55
2:P:75:ALA:HB3	2:P:135:ILE:HB	1.88	0.55
9:I:148:MET:HE2	9:I:172:ASN:HB2	1.88	0.55
9:W:14:MET:HB3	9:W:162:LEU:HD11	1.87	0.55
2:B:3:ARG:HB2	5:E:122:TYR:OH	2.06	0.55
14:N:1:THR:CG2	14:N:2:SER:N	2.70	0.55
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.88	0.55
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.71	0.55
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.89	0.55
11:Y:107:LYS:H	11:Y:107:LYS:HD2	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	1.87	0.55
15:N:201:04C:H24	15:N:201:04C:H8	1.88	0.55
11:Y:45:MET:HE2	15:Y:301:04C:H44	1.89	0.55
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.88	0.55
10:J:46:PHE:HD1	10:J:53:THR:HG1	1.54	0.55
10:J:147:HIS:HB2	10:J:160:LEU:HD11	1.89	0.55
7:U:103:MET:HE3	7:U:108:LEU:HB2	1.89	0.55
9:W:94:LEU:HD11	9:W:106:PRO:HG2	1.88	0.55
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.38	0.54
14:b:20:THR:HG21	15:b:201:04C:H42	1.89	0.54
9:I:14:MET:HB3	9:I:162:LEU:HD11	1.88	0.54
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.72	0.54
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.90	0.54
10:X:7:ILE:HD11	10:X:160:LEU:HD23	1.89	0.54
11:K:107:LYS:H	11:K:107:LYS:HD2	1.73	0.54
3:C:185:THR:HB	3:C:188:GLU:HG2	1.89	0.54
13:a:209:LYS:HB3	13:a:212:LEU:HD11	1.90	0.54
13:M:209:LYS:HB3	13:M:212:LEU:HD11	1.90	0.54
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.88	0.54
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.42	0.54
14:b:20:THR:HG22	15:b:201:04C:C5	2.37	0.54
1:A:55:LEU:HD12	7:G:170:THR:HG23	1.89	0.53
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.89	0.53
2:B:75:ALA:HB3	2:B:135:ILE:HB	1.90	0.53
5:E:12:PHE:HB2	6:F:19:GLN:HE22	1.73	0.53
11:K:45:MET:HG2	11:K:52:CYS:HB3	1.90	0.53
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.38	0.53
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.43	0.53
10:J:7:ILE:HD11	10:J:160:LEU:HD23	1.90	0.53
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.90	0.53
14:b:19:ARG:HG3	14:b:26:ILE:HG23	1.91	0.53
13:a:15:LYS:HB3	13:a:20:VAL:HG12	1.90	0.53
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.44	0.53
5:S:205:LEU:HD23	5:S:205:LEU:H	1.74	0.53
10:J:139:TYR:HE1	16:X:236:HOH:O	1.91	0.53
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.44	0.53
9:I:52:ILE:HB	9:I:59:VAL:HG13	1.92	0.52
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.44	0.52
8:H:165:ASN:HD22	13:a:156:ARG:HH11	1.56	0.52
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.92	0.52
5:E:227:GLU:CD	5:E:227:GLU:H	2.17	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.44	0.52
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.91	0.52
2:B:69:ASN:ND2	2:B:70:ASP:H	2.07	0.52
9:I:35:VAL:HG13	16:J:242:HOH:O	2.08	0.52
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.73	0.52
15:b:201:04C:H22	15:b:201:04C:H8	1.91	0.52
5:E:205:LEU:H	5:E:205:LEU:HD23	1.75	0.52
1:O:68:THR:HB	1:O:69:PRO:HD2	1.92	0.52
5:S:227:GLU:CD	5:S:227:GLU:H	2.16	0.52
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.92	0.52
14:N:19:ARG:HG3	14:N:26:ILE:HG23	1.92	0.51
1:A:68:THR:HB	1:A:69:PRO:HD2	1.91	0.51
7:U:103:MET:HE3	7:U:108:LEU:HD13	1.92	0.51
3:C:35:LYS:HG2	3:C:158:SER:O	2.10	0.51
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.22	0.51
13:M:15:LYS:HB3	13:M:20:VAL:HG12	1.91	0.51
12:Z:90:ALA:HA	12:Z:125:PHE:HZ	1.75	0.51
6:F:33:SER:HB3	6:F:46:VAL:HG23	1.92	0.51
8:H:1:THR:HG23	8:H:33:LYS:HD3	1.93	0.51
6:T:31:THR:HG23	6:T:47:GLU:HB3	1.91	0.51
13:a:27:LEU:HB2	13:a:192:SER:HB2	1.93	0.51
14:N:157:HIS:HD2	14:b:140:LYS:NZ	2.09	0.51
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.10	0.51
3:C:66:ASP:HA	10:J:69:ILE:HD13	1.93	0.51
3:Q:157:TRP:CE2	4:R:51:LEU:HD23	2.46	0.51
5:S:226:GLY:O	5:S:229:VAL:HG22	2.11	0.51
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.46	0.51
12:L:8:ASN:HA	12:L:30:ILE:O	2.10	0.51
12:L:135:GLN:HG3	12:L:174:TYR:OH	2.11	0.51
13:M:161:ARG:HG3	13:M:161:ARG:NH1	2.24	0.51
14:N:45:ARG:HD2	14:N:52:THR:HB	1.93	0.51
3:Q:27:ARG:HH11	3:Q:27:ARG:HB2	1.76	0.51
14:b:20:THR:CG2	15:b:201:04C:H42	2.41	0.51
2:B:35:ILE:HD12	2:B:196:LEU:HG	1.92	0.51
10:X:119:ILE:HG12	10:X:125:LYS:HG3	1.92	0.51
14:b:146:MET:HE1	14:b:154:PHE:HB2	1.94	0.51
6:F:31:THR:HG23	6:F:47:GLU:HB3	1.93	0.50
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.93	0.50
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.93	0.50
3:C:29:THR:HB	3:C:45:GLU:HG3	1.93	0.50
2:P:69:ASN:ND2	2:P:70:ASP:H	2.08	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:126:ASP:CB	12:Z:130:SER:HB3	2.41	0.50
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.93	0.50
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.46	0.50
11:Y:99:THR:HG22	11:Y:115:VAL:O	2.11	0.50
14:N:140:LYS:NZ	14:b:157:HIS:HD2	2.09	0.50
6:T:158:GLY:O	7:U:54:LEU:HB3	2.11	0.50
2:B:119:GLN:O	2:B:122:THR:HB	2.11	0.50
12:Z:135:GLN:HG3	12:Z:174:TYR:OH	2.11	0.50
12:L:126:ASP:CB	12:L:130:SER:HB3	2.42	0.50
14:N:132:THR:O	14:b:133:PHE:HA	2.12	0.50
1:A:110:LEU:O	1:A:114:VAL:HG23	2.11	0.50
5:E:200:LEU:HD11	5:E:205:LEU:HD22	1.94	0.50
7:G:78:ILE:N	7:G:79:PRO:HD2	2.26	0.50
13:M:27:LEU:HB2	13:M:192:SER:HB2	1.93	0.50
4:R:43:GLU:HG3	4:R:200:MET:HE3	1.93	0.50
5:S:230:ALA:HA	5:S:233:ILE:HD12	1.94	0.50
7:U:78:ILE:N	7:U:79:PRO:HD2	2.26	0.50
3:C:214:LYS:HB2	3:C:218:ASP:HB3	1.94	0.50
4:D:43:GLU:HG3	4:D:200:MET:HE3	1.94	0.50
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.47	0.50
10:X:152:MET:HE1	10:X:160:LEU:HD22	1.93	0.50
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.77	0.50
3:C:27:ARG:HB2	3:C:27:ARG:HH11	1.77	0.49
13:M:16:TYR:CE2	13:M:170:VAL:HG22	2.47	0.49
2:P:119:GLN:O	2:P:122:THR:HB	2.12	0.49
2:P:175:LEU:HD23	2:P:191:LEU:HD22	1.93	0.49
3:Q:27:ARG:HB2	3:Q:27:ARG:NH1	2.27	0.49
10:X:7:ILE:CD1	10:X:160:LEU:HD23	2.42	0.49
5:E:226:GLY:O	5:E:229:VAL:HG22	2.11	0.49
7:G:187:GLU:HG2	7:G:192:LYS:CB	2.42	0.49
12:L:90:ALA:HA	12:L:125:PHE:HZ	1.76	0.49
7:U:63:ILE:HD12	7:U:215:GLU:HG2	1.94	0.49
3:C:65:ILE:HG21	3:C:107:LEU:HD21	1.95	0.49
6:F:8:ASN:HB3	6:F:123:ASN:HA	1.94	0.49
5:S:68:HIS:HE1	5:S:102:LEU:O	1.95	0.49
13:a:16:TYR:CE2	13:a:170:VAL:HG22	2.47	0.49
5:E:193:VAL:HG13	5:E:205:LEU:HD11	1.94	0.49
7:G:63:ILE:HD12	7:G:215:GLU:HG2	1.95	0.49
13:M:193:ARG:HG3	13:M:214:VAL:HB	1.93	0.49
3:Q:65:ILE:HG21	3:Q:107:LEU:HD21	1.95	0.49
3:Q:214:LYS:HB2	3:Q:218:ASP:HB3	1.94	0.49

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:119:THR:HA	1.95	0.49
6:T:33:SER:HB3	6:T:46:VAL:HG23	1.93	0.49
2:B:223:GLU:HG2	2:B:224:VAL:H	1.77	0.49
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.93	0.49
10:J:119:ILE:HG12	10:J:125:LYS:HG3	1.94	0.49
1:A:211:LEU:HD22	1:A:238:LEU:HD12	1.95	0.49
3:C:27:ARG:HB2	3:C:27:ARG:NH1	2.28	0.49
3:C:239:GLN:C	3:C:241:GLN:H	2.21	0.49
7:G:103:MET:HE3	7:G:108:LEU:HD13	1.93	0.49
14:N:133:PHE:HA	14:b:132:THR:O	2.12	0.49
2:P:99:LYS:HG2	10:X:86:GLN:HE22	1.78	0.49
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.94	0.49
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.94	0.49
8:H:84:LYS:HG3	8:H:85:GLN:N	2.28	0.49
1:O:110:LEU:O	1:O:114:VAL:HG23	2.13	0.49
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.78	0.49
12:L:109:THR:HG23	12:L:125:PHE:HB2	1.94	0.49
10:J:139:TYR:OH	10:X:25:ILE:HG12	2.13	0.48
10:J:152:MET:HE1	10:J:160:LEU:HD22	1.95	0.48
3:C:155:SER:HB2	4:D:51:LEU:HD21	1.95	0.48
10:J:7:ILE:CD1	10:J:160:LEU:HD23	2.43	0.48
14:N:146:MET:HE1	14:N:154:PHE:HB2	1.94	0.48
5:E:68:HIS:HE1	5:E:102:LEU:O	1.95	0.48
7:G:30:ASN:HD22	7:G:164:PRO:HG2	1.78	0.48
5:S:193:VAL:HG13	5:S:205:LEU:HD11	1.95	0.48
1:O:211:LEU:HD22	1:O:238:LEU:HD12	1.95	0.48
2:P:122:THR:CG2	3:Q:125:ARG:HH21	2.26	0.48
5:S:134:ILE:HD12	5:S:215:VAL:HG12	1.94	0.48
2:B:175:LEU:HD23	2:B:191:LEU:HD22	1.94	0.48
5:E:80:ALA:HB2	5:E:129:VAL:HG21	1.96	0.48
5:E:230:ALA:HA	5:E:233:ILE:HD12	1.95	0.48
2:P:35:ILE:HD12	2:P:196:LEU:HG	1.95	0.48
3:Q:29:THR:HB	3:Q:45:GLU:HG3	1.94	0.48
3:Q:239:GLN:C	3:Q:241:GLN:H	2.21	0.48
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.96	0.48
10:X:139:TYR:HE2	10:X:172:MET:HG3	1.75	0.48
12:L:145:LEU:O	9:W:147:GLY:HA3	2.14	0.48
5:S:80:ALA:HB2	5:S:129:VAL:HG21	1.95	0.48
5:S:200:LEU:HD11	5:S:205:LEU:HD22	1.95	0.48
3:C:185:THR:HG22	3:C:187:GLU:H	1.78	0.48
5:S:49:LYS:HB3	5:S:58:TYR:HB3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:TYR:OH	3:C:57:ILE:HB	2.14	0.47
12:L:124:SER:CB	12:L:137:ARG:HG2	2.43	0.47
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.49	0.47
8:V:3:ILE:HG22	8:V:16:ALA:HB2	1.96	0.47
9:W:62:LEU:CD1	9:W:104:VAL:HG21	2.43	0.47
7:G:3:TYR:C	7:G:5:ARG:H	2.22	0.47
13:a:161:ARG:HG3	13:a:161:ARG:NH1	2.25	0.47
14:b:45:ARG:HD2	14:b:52:THR:HB	1.96	0.47
13:a:193:ARG:HG3	13:a:214:VAL:HB	1.94	0.47
2:B:142:ARG:HB2	16:B:332:HOH:O	2.14	0.47
2:B:172:GLN:HG2	3:C:50:LEU:HD12	1.96	0.47
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.95	0.47
13:a:27:LEU:HD11	13:a:34:LEU:HB3	1.96	0.47
9:I:62:LEU:CD1	9:I:104:VAL:HG21	2.45	0.47
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.60	0.47
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.97	0.47
7:U:187:GLU:HG2	7:U:192:LYS:CB	2.43	0.47
8:V:84:LYS:HG3	8:V:85:GLN:N	2.29	0.47
3:C:92:GLN:HG3	10:J:66:LEU:HB2	1.97	0.47
15:K:301:04C:H7	15:K:301:04C:H24	1.97	0.47
5:E:9:THR:HG21	5:E:119:THR:HA	1.95	0.47
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.95	0.47
5:E:70:GLY:HA3	5:E:221:PHE:CE2	2.49	0.47
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.14	0.47
4:R:44:LYS:HE3	4:R:210:GLN:HB2	1.96	0.47
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.50	0.47
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.96	0.47
12:Z:124:SER:CB	12:Z:137:ARG:HG2	2.44	0.47
9:I:53:THR:O	9:I:104:VAL:HA	2.15	0.47
11:K:99:THR:HG22	11:K:115:VAL:O	2.15	0.47
12:L:42:LYS:HD2	12:L:55:ASN:ND2	2.30	0.47
7:U:70:ILE:HG21	7:U:108:LEU:HD23	1.97	0.47
9:I:10:ILE:HD11	9:I:174:ALA:HB2	1.97	0.46
4:R:113:LEU:HB2	16:R:315:HOH:O	2.15	0.46
6:T:110:ASP:O	6:T:114:GLN:HG2	2.15	0.46
12:L:124:SER:HB3	12:L:137:ARG:HG2	1.97	0.46
13:M:161:ARG:HH11	13:M:161:ARG:CG	2.26	0.46
9:W:10:ILE:HD11	9:W:174:ALA:HB2	1.97	0.46
5:E:49:LYS:HB3	5:E:58:TYR:HB3	1.96	0.46
2:P:79:LEU:HD23	2:P:131:GLY:HA3	1.97	0.46
2:P:223:GLU:HG2	2:P:224:VAL:H	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:77:ALA:O	4:R:81:ILE:HG12	2.15	0.46
9:W:185:VAL:HG21	9:W:196:LYS:HE3	1.97	0.46
12:Z:17:GLY:HA3	12:Z:20:PHE:CE2	2.51	0.46
12:Z:109:THR:HG23	12:Z:125:PHE:HB2	1.97	0.46
14:N:20:THR:HG22	15:N:201:04C:C5	2.46	0.46
12:L:126:ASP:OD2	12:L:127:PRO:HD2	2.15	0.46
1:O:26:THR:O	1:O:30:GLN:HG2	2.15	0.46
6:T:8:ASN:HB3	6:T:123:ASN:HA	1.96	0.46
12:Z:124:SER:HB3	12:Z:137:ARG:HG2	1.98	0.46
5:E:134:ILE:HD12	5:E:215:VAL:HG12	1.96	0.46
9:I:147:GLY:HA3	12:Z:145:LEU:O	2.15	0.46
7:U:55:LEU:O	7:U:57:PRO:HD3	2.16	0.46
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.96	0.46
7:U:30:ASN:HD22	7:U:164:PRO:HG2	1.79	0.46
2:B:79:LEU:HD23	2:B:131:GLY:HA3	1.98	0.46
4:D:44:LYS:HE3	4:D:210:GLN:HB2	1.97	0.46
13:M:27:LEU:HD11	13:M:34:LEU:HB3	1.98	0.46
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.98	0.46
5:E:231:LYS:H	5:E:231:LYS:HD2	1.81	0.45
10:J:53:THR:HG23	10:J:54:VAL:N	2.32	0.45
12:Z:126:ASP:OD2	12:Z:127:PRO:HD2	2.17	0.45
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.22	0.45
12:Z:49:ASN:HD22	12:Z:49:ASN:HA	1.63	0.45
8:H:22:GLN:HG3	8:H:27:ALA:HB2	1.97	0.45
14:b:48:SER:HB3	14:b:51:ASP:HB2	1.98	0.45
12:L:17:GLY:HA3	12:L:20:PHE:CE2	2.52	0.45
7:U:3:TYR:C	7:U:5:ARG:H	2.24	0.45
11:Y:201:LYS:HG3	11:Y:207:PHE:HB2	1.99	0.45
14:b:45:ARG:CZ	15:b:201:04C:H44	2.45	0.45
6:F:110:ASP:O	6:F:114:GLN:HG2	2.17	0.45
7:G:70:ILE:HG21	7:G:108:LEU:HD23	1.99	0.45
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.52	0.45
11:Y:100:MET:HE2	11:Y:100:MET:HB2	1.82	0.45
1:A:149:GLN:O	1:A:156:TYR:HA	2.17	0.45
8:H:3:ILE:HG22	8:H:16:ALA:HB2	1.99	0.45
11:K:162:LEU:HD12	11:K:193:VAL:HG13	1.98	0.45
14:b:59:VAL:HG11	14:b:82:PHE:CE2	2.52	0.45
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.46	0.45
1:O:149:GLN:O	1:O:156:TYR:HA	2.16	0.45
14:N:146:MET:HE2	14:N:150:GLU:HB3	1.99	0.45
4:R:71:SER:HB3	4:R:164:ILE:HD12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:231:LYS:H	5:S:231:LYS:HD2	1.82	0.45
1:A:26:THR:O	1:A:30:GLN:HG2	2.17	0.45
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.99	0.45
4:D:186:LYS:O	4:D:190:LEU:HD22	2.16	0.45
6:F:66:VAL:HG11	6:F:108:PHE:CE1	2.52	0.45
10:J:146:HIS:HD2	10:J:147:HIS:CE1	2.35	0.45
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.17	0.45
3:Q:190:VAL:HG13	3:Q:210:ILE:HG21	1.99	0.45
4:R:186:LYS:O	4:R:190:LEU:HD22	2.17	0.45
10:X:5:LEU:HD21	10:X:140:THR:HG21	1.99	0.45
10:X:91:SER:HG	10:X:98:TYR:H	1.62	0.45
5:E:12:PHE:HB2	6:F:19:GLN:NE2	2.32	0.44
7:G:55:LEU:O	7:G:57:PRO:HD3	2.17	0.44
10:J:172:MET:HA	10:J:173:PRO:HD3	1.79	0.44
4:R:159:TYR:CG	4:R:162:LYS:HB2	2.51	0.44
5:S:155:LEU:HD23	6:T:55:LEU:HA	1.98	0.44
9:W:53:THR:O	9:W:104:VAL:HA	2.17	0.44
14:b:146:MET:HE2	14:b:150:GLU:HB3	1.99	0.44
3:C:51:LYS:O	3:C:52:LEU:HB2	2.16	0.44
10:J:1:MET:HG2	10:J:2:ASP:N	2.32	0.44
11:K:31:VAL:HG11	15:K:301:04C:C4	2.47	0.44
5:S:70:GLY:HA3	5:S:221:PHE:CZ	2.52	0.44
3:C:190:VAL:HG13	3:C:210:ILE:HG21	1.99	0.44
7:G:52:ASP:HB3	7:G:55:LEU:HG	1.99	0.44
10:J:158:LEU:HD13	10:J:198:GLN:HE22	1.82	0.44
9:W:73:TYR:CE1	9:W:77:GLU:HG3	2.52	0.44
11:Y:31:VAL:HG11	15:Y:301:04C:C4	2.47	0.44
11:Y:162:LEU:HD12	11:Y:193:VAL:HG13	1.99	0.44
9:I:8:GLY:HA2	9:I:140:THR:HG21	1.99	0.44
10:J:25:ILE:HG12	10:X:139:TYR:OH	2.18	0.44
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.52	0.44
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.52	0.44
8:H:78:SER:O	8:H:82:MET:HG3	2.17	0.44
9:I:37:ASN:ND2	9:I:37:ASN:N	2.64	0.44
6:T:205:GLU:HG3	6:T:206:LYS:HG3	2.00	0.44
10:X:33:ASP:OD2	10:X:35:THR:HG22	2.18	0.44
14:b:45:ARG:NH1	14:b:53:GLN:HG3	2.32	0.44
4:D:71:SER:HB3	4:D:164:ILE:HD12	1.99	0.44
11:K:201:LYS:HG3	11:K:207:PHE:HB2	2.00	0.44
4:R:59:ILE:HG22	4:R:220:PHE:HZ	1.83	0.44
7:U:45:ILE:HD13	7:U:197:ALA:CB	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.00	0.44
10:X:158:LEU:HD13	10:X:198:GLN:HE22	1.82	0.44
11:Y:158:LYS:HB2	11:Y:177:LEU:HD11	1.99	0.44
6:F:158:GLY:O	7:G:54:LEU:HB3	2.18	0.44
7:G:66:ILE:HG21	7:G:108:LEU:HD21	1.99	0.44
2:P:3:ARG:HB2	5:S:122:TYR:OH	2.17	0.44
6:T:39:ASN:N	6:T:39:ASN:HD22	2.16	0.44
8:V:78:SER:O	8:V:82:MET:HG3	2.17	0.44
10:X:53:THR:HG23	10:X:54:VAL:N	2.33	0.44
10:X:172:MET:HA	10:X:173:PRO:HD3	1.79	0.44
3:Q:70:VAL:HG13	3:Q:219:ILE:HD13	1.99	0.44
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.00	0.44
14:N:2:SER:OG	14:N:130:GLY:HA3	2.17	0.44
5:S:227:GLU:CD	5:S:227:GLU:N	2.76	0.44
12:Z:42:LYS:HD2	12:Z:55:ASN:ND2	2.33	0.44
1:A:10:THR:HG22	1:A:18:LEU:HD22	2.00	0.43
3:C:70:VAL:HG13	3:C:219:ILE:HD13	2.00	0.43
11:K:158:LYS:HB2	11:K:177:LEU:HD11	2.01	0.43
13:a:25:ASP:HA	13:a:195:PHE:HA	2.01	0.43
1:A:66:LEU:HD12	1:A:235:PHE:CD2	2.52	0.43
4:D:59:ILE:HG22	4:D:220:PHE:HZ	1.82	0.43
6:F:39:ASN:N	6:F:39:ASN:HD22	2.16	0.43
8:H:167:LEU:HD22	12:Z:196:ILE:O	2.18	0.43
12:L:100:LYS:HD3	12:L:105:TYR:CE1	2.53	0.43
14:N:59:VAL:HG11	14:N:82:PHE:CE2	2.53	0.43
6:T:66:VAL:HG11	6:T:108:PHE:CE1	2.53	0.43
4:D:159:TYR:CG	4:D:162:LYS:HB2	2.53	0.43
3:Q:92:GLN:HG3	10:X:66:LEU:HB2	1.99	0.43
7:U:66:ILE:HG21	7:U:108:LEU:HD21	2.00	0.43
8:V:80:LEU:HD12	8:V:113:ILE:HD11	2.01	0.43
2:B:213:ALA:HA	2:B:227:LYS:O	2.19	0.43
2:B:223:GLU:HG2	2:B:224:VAL:N	2.34	0.43
10:X:3:ILE:HB	10:X:18:SER:HB3	2.00	0.43
9:I:73:TYR:CE1	9:I:77:GLU:HG3	2.53	0.43
3:Q:155:SER:HB2	4:R:51:LEU:HD21	2.00	0.43
13:M:25:ASP:HA	13:M:195:PHE:HA	2.00	0.43
3:C:32:VAL:HG23	3:C:161:THR:HB	2.00	0.43
5:E:227:GLU:CD	5:E:227:GLU:N	2.77	0.43
8:H:77:VAL:HB	13:a:230:THR:HG22	2.01	0.43
14:N:136:GLY:HA2	14:b:161:GLN:NE2	2.32	0.43
8:V:215:GLU:HG3	9:W:197:ARG:HG2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:201:04C:H19	15:b:201:04C:O13	2.18	0.43
5:E:70:GLY:HA3	5:E:221:PHE:CZ	2.53	0.43
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.54	0.43
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.47	0.43
13:M:174:GLU:O	13:M:178:VAL:HG23	2.19	0.43
7:U:70:ILE:HD11	7:U:103:MET:O	2.18	0.43
14:b:2:SER:OG	14:b:130:GLY:HA3	2.18	0.43
7:G:45:ILE:HD13	7:G:197:ALA:CB	2.49	0.42
14:N:26:ILE:HB	13:a:187:ARG:HA	2.01	0.42
1:O:55:LEU:HD12	7:U:170:THR:HG23	2.01	0.42
13:M:179:ASN:ND2	13:M:182:ARG:HH11	2.12	0.42
14:N:161:GLN:NE2	14:b:136:GLY:HA2	2.33	0.42
2:P:213:ALA:HA	2:P:227:LYS:O	2.19	0.42
3:C:226:GLU:O	3:C:230:TYR:HD1	2.03	0.42
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.55	0.42
8:H:215:GLU:HG3	9:I:197:ARG:HG2	2.02	0.42
9:I:185:VAL:HG21	9:I:196:LYS:HE3	2.00	0.42
2:P:236:ASP:O	2:P:240:LYS:HG2	2.19	0.42
4:D:77:ALA:O	4:D:81:ILE:HG12	2.19	0.42
4:R:159:TYR:CE2	4:R:162:LYS:HD3	2.54	0.42
7:U:149:ASP:HB2	7:U:150:PRO:HD2	2.01	0.42
9:W:62:LEU:HD12	9:W:104:VAL:HG21	2.00	0.42
10:X:146:HIS:HD2	10:X:147:HIS:CE1	2.37	0.42
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.45	0.42
13:a:127:LEU:HG	13:a:142:LEU:HD12	2.01	0.42
15:K:301:04C:H11	12:L:128:VAL:HG22	2.02	0.42
10:J:9:VAL:HB	10:J:152:MET:O	2.20	0.42
1:O:66:LEU:HD12	1:O:235:PHE:CD2	2.54	0.42
6:F:7:SER:HB3	6:F:10:VAL:HG23	2.02	0.42
10:J:139:TYR:HE2	10:J:172:MET:HG3	1.76	0.42
7:U:52:ASP:HB3	7:U:55:LEU:HG	2.00	0.42
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.49	0.42
12:Z:100:LYS:O	12:Z:104:PRO:HA	2.20	0.42
12:L:100:LYS:O	12:L:104:PRO:HA	2.20	0.42
10:X:78:GLN:HB2	16:X:213:HOH:O	2.20	0.42
12:Z:195:HIS:CD2	12:Z:197:GLN:H	2.29	0.42
11:K:1:THR:HG23	11:K:33:LYS:HD3	2.02	0.42
2:P:223:GLU:HG2	2:P:224:VAL:N	2.35	0.42
3:Q:165:ASN:O	3:Q:169:VAL:HG12	2.20	0.42
4:R:30:ILE:HD12	4:R:196:LEU:HG	2.02	0.42
10:J:33:ASP:OD2	10:J:35:THR:HG22	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:209:ASN:O	9:W:38:LYS:NZ	2.53	0.42
6:T:78:ILE:HB	6:T:79:PRO:HD3	2.02	0.42
10:X:92:ILE:HG23	10:X:93:ARG:HG3	2.00	0.42
11:Y:1:THR:HG23	11:Y:33:LYS:HD3	2.01	0.42
6:F:205:GLU:HG3	6:F:206:LYS:HG3	2.01	0.41
12:L:149:PHE:CE1	12:L:153:GLN:HG3	2.54	0.41
12:L:196:ILE:O	8:V:167:LEU:HD22	2.19	0.41
6:T:201:GLU:O	6:T:204:LYS:HD2	2.20	0.41
8:V:1:THR:HA	8:V:33:LYS:HZ3	1.85	0.41
8:V:4:VAL:HG22	8:V:159:ILE:HD11	2.02	0.41
9:W:8:GLY:HA2	9:W:140:THR:HG21	2.02	0.41
1:A:30:GLN:HE21	1:A:30:GLN:CA	2.33	0.41
6:F:154:TRP:CZ3	7:G:60:VAL:HA	2.55	0.41
12:L:22:VAL:HG12	12:L:206:ILE:HG13	2.02	0.41
15:N:201:04C:H22	15:N:201:04C:C35	2.46	0.41
3:Q:66:ASP:HA	10:X:69:ILE:HD13	2.02	0.41
4:R:109:CYS:SG	4:R:156:PHE:HB3	2.60	0.41
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.01	0.41
4:D:70:MET:HG3	4:D:74:THR:HG22	2.02	0.41
9:I:36:SER:CB	10:J:126:VAL:HG21	2.50	0.41
10:J:3:ILE:HB	10:J:18:SER:HB3	2.02	0.41
7:U:35:ALA:HB2	7:U:44:VAL:HG12	2.03	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.50	0.41
9:I:11:VAL:HG22	9:I:24:CYS:HB3	2.01	0.41
10:J:139:TYR:CD1	16:J:228:HOH:O	2.53	0.41
12:L:123:TYR:CE1	12:L:133:ARG:HB2	2.56	0.41
3:Q:226:GLU:O	3:Q:230:TYR:HD1	2.03	0.41
3:Q:233:GLN:O	3:Q:237:GLU:HG2	2.20	0.41
3:C:165:ASN:O	3:C:169:VAL:HG12	2.20	0.41
10:J:36:ARG:HA	10:J:36:ARG:HD3	1.91	0.41
11:K:176:ASN:HD22	11:K:176:ASN:HA	1.74	0.41
1:O:10:THR:HG22	1:O:18:LEU:HD22	2.03	0.41
9:W:11:VAL:HG22	9:W:24:CYS:HB3	2.02	0.41
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	2.02	0.41
2:B:236:ASP:O	2:B:240:LYS:HG2	2.19	0.41
4:D:113:LEU:HD12	5:E:78:PRO:HB2	2.01	0.41
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.56	0.41
8:H:172:ASN:HD22	8:H:192:THR:HA	1.84	0.41
9:I:62:LEU:HD12	9:I:104:VAL:HG21	2.02	0.41
11:K:14:VAL:HB	11:K:178:TYR:HB2	2.01	0.41
11:K:37:ILE:HG23	11:K:60:GLY:HA2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:83:ARG:HH21	7:U:114:ASN:HD22	1.68	0.41
5:S:12:PHE:HB2	6:T:19:GLN:HE22	1.85	0.41
7:U:190:TRP:O	7:U:194:VAL:HG23	2.20	0.41
8:V:172:ASN:HD22	8:V:192:THR:HA	1.86	0.41
10:X:1:MET:HG2	10:X:2:ASP:N	2.34	0.41
13:a:161:ARG:HH11	13:a:161:ARG:CG	2.26	0.41
6:F:41:GLY:HA3	6:F:215:CYS:O	2.20	0.41
7:G:190:TRP:O	7:G:194:VAL:HG23	2.21	0.41
8:H:4:VAL:HG22	8:H:159:ILE:HD11	2.02	0.41
10:J:53:THR:HG23	10:J:54:VAL:HG23	2.02	0.41
1:O:158:PRO:HB2	2:P:57:GLU:HB3	2.02	0.41
6:T:41:GLY:HA3	6:T:215:CYS:O	2.20	0.41
14:b:65:LEU:HG	14:b:69:GLN:HE21	1.86	0.41
2:B:180:LYS:CG	2:B:183:MET:HG3	2.49	0.41
3:C:233:GLN:O	3:C:237:GLU:HG2	2.21	0.41
6:F:107:ALA:O	6:F:111:ARG:HG2	2.21	0.41
4:R:70:MET:HG3	4:R:74:THR:HG22	2.02	0.41
3:C:147:GLN:HE21	3:C:147:GLN:HB3	1.61	0.41
11:K:86:LEU:C	11:K:86:LEU:HD13	2.46	0.41
13:M:48:ASN:N	13:M:48:ASN:ND2	2.68	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.01	0.41
1:O:59:GLU:C	1:O:61:LEU:H	2.29	0.41
1:O:83:ARG:HE	7:U:114:ASN:HD21	1.69	0.41
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.21	0.41
4:R:176:LEU:HD22	5:S:55:LEU:HD13	2.02	0.41
12:Z:100:LYS:HD3	12:Z:105:TYR:CE1	2.56	0.41
14:b:20:THR:OG1	14:b:28:ASN:HB3	2.21	0.41
3:C:10:SER:HB2	3:C:11:PRO:HD2	2.03	0.41
4:D:161:ALA:HB1	4:D:175:LEU:HD22	2.02	0.41
2:P:15:GLU:O	3:Q:27:ARG:NH1	2.54	0.41
6:T:9:SER:O	7:U:126:ARG:HD3	2.21	0.41
11:Y:14:VAL:HB	11:Y:178:TYR:HB2	2.03	0.41
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.56	0.40
2:B:184:LYS:HD3	2:B:185:VAL:N	2.36	0.40
3:C:146:TYR:CE1	3:C:156:SER:HB3	2.56	0.40
4:D:30:ILE:HD12	4:D:196:LEU:HG	2.02	0.40
7:G:35:ALA:HB2	7:G:44:VAL:HG12	2.04	0.40
8:H:200:GLN:HG2	12:Z:182:LYS:HA	2.03	0.40
11:K:100:MET:HE2	11:K:100:MET:HB2	1.83	0.40
13:M:7:THR:HA	13:M:55:GLY:O	2.21	0.40
10:X:53:THR:HG23	10:X:54:VAL:HG23	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:7:THR:HA	13:a:55:GLY:O	2.21	0.40
1:A:59:GLU:C	1:A:61:LEU:H	2.28	0.40
8:H:80:LEU:HD12	8:H:113:ILE:HD11	2.02	0.40
11:K:31:VAL:HG11	15:K:301:04C:C3	2.51	0.40
3:Q:32:VAL:HG23	3:Q:161:THR:HB	2.02	0.40
9:W:73:TYR:CZ	9:W:77:GLU:HG3	2.56	0.40
3:C:157:TRP:CZ3	4:D:48:SER:HB3	2.56	0.40
7:G:70:ILE:HD11	7:G:103:MET:O	2.20	0.40
11:K:41:LEU:HD23	11:K:103:GLY:HA3	2.02	0.40
14:N:83:LYS:HG3	14:N:119:VAL:HG22	2.03	0.40
2:P:50:LYS:HG2	2:P:51:VAL:HG23	2.03	0.40
12:Z:149:PHE:CE1	12:Z:153:GLN:HG3	2.56	0.40
13:a:174:GLU:O	13:a:178:VAL:HG23	2.21	0.40
10:J:5:LEU:HD21	10:J:140:THR:HG21	2.02	0.40
3:Q:146:TYR:CE1	3:Q:156:SER:HB3	2.57	0.40
10:X:9:VAL:HB	10:X:152:MET:O	2.22	0.40
11:Y:41:LEU:HD23	11:Y:103:GLY:HA3	2.03	0.40
11:Y:105:THR:HB	11:Y:107:LYS:HD2	2.03	0.40
13:a:179:ASN:ND2	13:a:182:ARG:HH11	2.12	0.40
1:A:83:ARG:HH21	7:G:114:ASN:HD22	1.70	0.40
3:C:186:VAL:O	3:C:190:VAL:HG23	2.21	0.40
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.52	0.40
5:E:155:LEU:HD23	6:F:55:LEU:HA	2.03	0.40
10:J:92:ILE:HG23	10:J:93:ARG:HG3	2.02	0.40
11:K:4:LEU:CD1	11:K:15:ALA:HB3	2.52	0.40
16:R:318:HOH:O	12:Z:79:HIS:HE1	2.04	0.40
9:W:120:ILE:HD12	9:W:136:ILE:HG12	2.02	0.40
13:a:129:TYR:HE1	13:a:144:THR:HG22	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	239 (96%)	7 (3%)	2 (1%)	16	44
1	O	248/250 (99%)	239 (96%)	7 (3%)	2 (1%)	16	44
2	B	242/258 (94%)	230 (95%)	10 (4%)	2 (1%)	16	44
2	P	242/258 (94%)	231 (96%)	9 (4%)	2 (1%)	16	44
3	C	239/254 (94%)	227 (95%)	9 (4%)	3 (1%)	9	33
3	Q	239/254 (94%)	227 (95%)	9 (4%)	3 (1%)	9	33
4	D	240/260 (92%)	230 (96%)	7 (3%)	3 (1%)	9	33
4	R	240/260 (92%)	230 (96%)	7 (3%)	3 (1%)	9	33
5	E	231/234 (99%)	218 (94%)	12 (5%)	1 (0%)	30	59
5	S	231/234 (99%)	218 (94%)	12 (5%)	1 (0%)	30	59
6	F	242/288 (84%)	232 (96%)	10 (4%)	0	100	100
6	T	242/288 (84%)	232 (96%)	10 (4%)	0	100	100
7	G	241/252 (96%)	232 (96%)	9 (4%)	0	100	100
7	U	241/252 (96%)	231 (96%)	10 (4%)	0	100	100
8	H	220/232 (95%)	212 (96%)	8 (4%)	0	100	100
8	V	220/232 (95%)	210 (96%)	10 (4%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	196/198 (99%)	187 (95%)	8 (4%)	1 (0%)	24	54
10	X	196/198 (99%)	187 (95%)	8 (4%)	1 (0%)	24	54
11	K	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	24	54
11	Y	210/212 (99%)	201 (96%)	8 (4%)	1 (0%)	24	54
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%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	186 (96%)	7 (4%)	1 (0%)	24	54
All	All	6312/6588 (96%)	6042 (96%)	243 (4%)	27 (0%)	30	59

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	52	LEU
3	Q	52	LEU
1	A	166	LYS
3	C	203	THR
4	D	122	GLU
5	E	201	ARG
1	O	166	LYS
3	Q	203	THR
4	R	122	GLU
5	S	201	ARG
14	b	2	SER
1	A	2	THR
2	B	221	ASP
4	D	121	GLY
11	K	39	PRO
1	O	2	THR
2	P	221	ASP
4	R	121	GLY
11	Y	39	PRO
2	B	51	VAL
3	C	183	PRO
2	P	51	VAL
3	Q	183	PRO
10	J	9	VAL
10	X	9	VAL
4	D	118	GLY
4	R	118	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	205 (98%)	4 (2%)	50	66
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	66
2	B	203/216 (94%)	197 (97%)	6 (3%)	36	59
2	P	203/216 (94%)	196 (97%)	7 (3%)	32	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	213/226 (94%)	206 (97%)	7 (3%)	33	57
3	Q	213/226 (94%)	206 (97%)	7 (3%)	33	57
4	D	198/215 (92%)	188 (95%)	10 (5%)	21	48
4	R	198/215 (92%)	188 (95%)	10 (5%)	21	48
5	E	192/193 (100%)	185 (96%)	7 (4%)	31	56
5	S	192/193 (100%)	185 (96%)	7 (4%)	31	56
6	F	201/239 (84%)	191 (95%)	10 (5%)	22	49
6	T	201/239 (84%)	191 (95%)	10 (5%)	22	49
7	G	207/210 (99%)	200 (97%)	7 (3%)	32	57
7	U	207/210 (99%)	200 (97%)	7 (3%)	32	57
8	H	181/190 (95%)	177 (98%)	4 (2%)	45	63
8	V	181/190 (95%)	178 (98%)	3 (2%)	53	67
9	I	172/173 (99%)	170 (99%)	2 (1%)	63	72
9	W	172/173 (99%)	170 (99%)	2 (1%)	63	72
10	J	175/175 (100%)	171 (98%)	4 (2%)	44	63
10	X	175/175 (100%)	171 (98%)	4 (2%)	44	63
11	K	169/169 (100%)	161 (95%)	8 (5%)	23	50
11	Y	169/169 (100%)	161 (95%)	8 (5%)	23	50
12	L	185/185 (100%)	181 (98%)	4 (2%)	45	63
12	Z	185/185 (100%)	181 (98%)	4 (2%)	45	63
13	M	199/199 (100%)	190 (96%)	9 (4%)	24	51
13	a	199/199 (100%)	190 (96%)	9 (4%)	24	51
14	N	162/162 (100%)	160 (99%)	2 (1%)	63	72
14	b	162/162 (100%)	160 (99%)	2 (1%)	63	72
All	All	5332/5522 (97%)	5164 (97%)	168 (3%)	34	58

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
2	B	38	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	55	LEU
2	B	65	LEU
2	B	122	THR
2	B	149	THR
2	B	191	LEU
3	C	4	ARG
3	C	19	GLU
3	C	51	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	171	GLU
4	D	20	LEU
4	D	44	LYS
4	D	68	CYS
4	D	102	GLU
4	D	124	ARG
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
5	E	9	THR
5	E	29	LYS
5	E	188	LEU
5	E	198	GLN
5	E	205	LEU
5	E	227	GLU
5	E	231	LYS
6	F	31	THR
6	F	39	ASN
6	F	117	GLN
6	F	123	ASN
6	F	140	ASN
6	F	172	LEU
6	F	181	GLU
6	F	186	ARG
6	F	201	GLU
6	F	221	ASN
7	G	83	ASN
7	G	115	LEU
7	G	166	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	201	MET
7	G	221	LYS
7	G	235	ARG
7	G	236	LEU
8	H	34	LEU
8	H	43	CYS
8	H	55	VAL
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	71	GLU
10	J	110	LYS
10	J	127	GLU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	69	ARG
11	K	87	VAL
11	K	100	MET
11	K	107	LYS
11	K	211	ILE
12	L	23	LEU
12	L	49	ASN
12	L	109	THR
12	L	150	LEU
13	M	48	ASN
13	M	69	ASP
13	M	70	LEU
13	M	104	ARG
13	M	146	PHE
13	M	161	ARG
13	M	170	VAL
13	M	171	GLN
13	M	226	LYS
14	N	119	VAL
14	N	149	GLU
1	O	30	GLN
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
2	P	38	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	55	LEU
2	P	65	LEU
2	P	122	THR
2	P	149	THR
2	P	191	LEU
2	P	212	PHE
3	Q	4	ARG
3	Q	19	GLU
3	Q	51	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	171	GLU
4	R	20	LEU
4	R	44	LYS
4	R	68	CYS
4	R	102	GLU
4	R	124	ARG
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
5	S	9	THR
5	S	29	LYS
5	S	188	LEU
5	S	198	GLN
5	S	205	LEU
5	S	227	GLU
5	S	231	LYS
6	T	31	THR
6	T	39	ASN
6	T	117	GLN
6	T	123	ASN
6	T	140	ASN
6	T	172	LEU
6	T	181	GLU
6	T	186	ARG
6	T	201	GLU
6	T	221	ASN
7	U	83	ASN
7	U	115	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	154	TYR
7	U	166	GLN
7	U	201	MET
7	U	221	LYS
7	U	235	ARG
8	V	34	LEU
8	V	43	CYS
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	71	GLU
10	X	110	LYS
10	X	127	GLU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	69	ARG
11	Y	87	VAL
11	Y	100	MET
11	Y	107	LYS
11	Y	211	ILE
12	Z	23	LEU
12	Z	49	ASN
12	Z	109	THR
12	Z	150	LEU
13	a	48	ASN
13	a	69	ASP
13	a	70	LEU
13	a	104	ARG
13	a	146	PHE
13	a	161	ARG
13	a	170	VAL
13	a	171	GLN
13	a	226	LYS
14	b	119	VAL
14	b	149	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (208) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	143	ASN
1	A	149	GLN
2	B	20	GLN
2	B	69	ASN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	146	GLN
2	B	155	ASN
2	B	176	GLN
2	B	220	ASN
3	C	17	GLN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	165	ASN
3	C	228	ASN
3	C	241	GLN
4	D	15	GLN
4	D	91	HIS
4	D	146	GLN
4	D	160	ASN
4	D	198	GLN
4	D	210	GLN
4	D	225	ASN
5	E	4	ASN
5	E	59	GLN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	184	ASN
5	E	198	GLN
5	E	209	ASN
6	F	19	GLN
6	F	39	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
7	G	186	ASN
7	G	231	ASN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
8	H	219	ASN
9	I	37	ASN
9	I	44	HIS
9	I	88	GLN
9	I	156	ASN
9	I	203	GLN
10	J	37	GLN
10	J	55	GLN
10	J	63	ASN
10	J	78	GLN
10	J	86	GLN
10	J	146	HIS
10	J	198	GLN
11	K	9	GLN
11	K	24	ASN
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN
11	K	209	ASN
12	L	1	GLN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	76	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	80	ASN
12	L	165	ASN
12	L	195	HIS
12	L	197	GLN
13	M	2	GLN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	149	HIS
13	M	171	GLN
13	M	179	ASN
13	M	213	GLN
14	N	69	GLN
14	N	141	ASN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	30	GLN
1	O	143	ASN
1	O	149	GLN
2	P	20	GLN
2	P	69	ASN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
2	P	220	ASN
3	Q	17	GLN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	165	ASN
3	Q	228	ASN
3	Q	241	GLN
4	R	15	GLN
4	R	91	HIS
4	R	146	GLN
4	R	160	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	R	210	GLN
4	R	225	ASN
5	S	4	ASN
5	S	59	GLN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
5	S	198	GLN
5	S	209	ASN
6	T	19	GLN
6	T	39	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
7	U	231	ASN
8	V	30	ASN
8	V	66	HIS
8	V	116	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
8	V	219	ASN
9	W	37	ASN
9	W	44	HIS
9	W	88	GLN
9	W	156	ASN
9	W	203	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	X	37	GLN
10	X	55	GLN
10	X	63	ASN
10	X	78	GLN
10	X	86	GLN
10	X	146	HIS
10	X	147	HIS
10	X	166	GLN
10	X	198	GLN
11	Y	9	GLN
11	Y	24	ASN
11	Y	85	ASN
11	Y	133	GLN
11	Y	176	ASN
11	Y	208	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	76	HIS
12	Z	80	ASN
12	Z	165	ASN
12	Z	195	HIS
12	Z	197	GLN
13	a	2	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	149	HIS
13	a	171	GLN
13	a	179	ASN
13	a	213	GLN
14	b	69	GLN
14	b	141	ASN
14	b	145	ASN
14	b	157	HIS
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
15	04C	K	301	11	44,44,44	1.32	2 (4%)	54,58,58	1.12	3 (5%)
15	04C	b	201	14	44,44,44	1.56	6 (13%)	54,58,58	1.42	7 (12%)
15	04C	H	301	8	44,44,44	1.42	4 (9%)	54,58,58	0.94	4 (7%)
15	04C	N	201	14	44,44,44	1.50	6 (13%)	54,58,58	1.17	4 (7%)
15	04C	Y	301	11	44,44,44	1.43	3 (6%)	54,58,58	1.03	3 (5%)
15	04C	V	301	8	44,44,44	1.47	3 (6%)	54,58,58	0.87	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	04C	K	301	11	-	12/44/52/52	0/3/3/3
15	04C	b	201	14	-	12/44/52/52	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	04C	H	301	8	-	13/44/52/52	0/3/3/3
15	04C	N	201	14	-	13/44/52/52	0/3/3/3
15	04C	Y	301	11	-	13/44/52/52	0/3/3/3
15	04C	V	301	8	-	14/44/52/52	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	301	04C	C12-C10	4.67	1.57	1.52
15	b	201	04C	C12-C10	4.38	1.57	1.52
15	b	201	04C	C10-C9	4.16	1.60	1.53
15	K	301	04C	C12-C10	4.09	1.57	1.52
15	N	201	04C	C10-C9	3.97	1.60	1.53
15	V	301	04C	C12-C10	3.85	1.57	1.52
15	H	301	04C	C12-C10	3.79	1.56	1.52
15	N	201	04C	C12-C10	3.71	1.56	1.52
15	Y	301	04C	C10-C9	3.56	1.59	1.53
15	K	301	04C	C10-C9	3.50	1.59	1.53
15	V	301	04C	C10-C9	3.37	1.59	1.53
15	H	301	04C	C10-C9	3.26	1.59	1.53
15	b	201	04C	C7-C8	2.76	1.59	1.53
15	b	201	04C	C9-C8	2.65	1.58	1.53
15	b	201	04C	O45-C44	2.42	1.42	1.37
15	V	301	04C	C9-C8	2.32	1.57	1.53
15	H	301	04C	C9-C8	2.29	1.57	1.53
15	N	201	04C	C2-C1	2.26	1.42	1.38
15	N	201	04C	C4-C5	2.21	1.42	1.38
15	N	201	04C	C9-C8	2.12	1.57	1.53
15	H	301	04C	C4-C5	2.10	1.42	1.38
15	Y	301	04C	O45-C44	2.04	1.41	1.37
15	b	201	04C	C47-C44	2.02	1.42	1.38
15	N	201	04C	C7-C6	2.02	1.56	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	201	04C	C11-C10-C12	-5.52	102.74	109.76
15	N	201	04C	C11-C10-C12	-4.99	103.41	109.76
15	Y	301	04C	C6-C7-C8	4.41	120.88	113.40
15	K	301	04C	C11-C10-C12	-4.04	104.62	109.76
15	K	301	04C	C6-C7-C8	3.99	120.17	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	201	04C	C6-C7-C8	3.73	119.72	113.40
15	b	201	04C	C35-C36-N31	-3.67	104.55	110.12
15	b	201	04C	C30-N31-C32	3.54	116.64	111.14
15	b	201	04C	C30-N31-C36	3.41	116.45	111.14
15	H	301	04C	C32-N31-C36	2.94	115.17	108.84
15	K	301	04C	C30-N31-C36	2.83	115.54	111.14
15	V	301	04C	C6-C7-C8	2.72	118.01	113.40
15	V	301	04C	C11-C10-C12	-2.70	106.32	109.76
15	H	301	04C	C6-C7-C8	2.55	117.73	113.40
15	b	201	04C	C33-O34-C35	2.54	118.09	109.88
15	H	301	04C	C11-C10-C12	-2.51	106.57	109.76
15	b	201	04C	C29-C30-N31	-2.44	107.75	113.41
15	Y	301	04C	C30-N31-C32	2.24	114.63	111.14
15	V	301	04C	C32-N31-C36	2.21	113.59	108.84
15	b	201	04C	C33-C32-N31	-2.20	106.78	110.12
15	N	201	04C	C32-N31-C36	2.06	113.28	108.84
15	N	201	04C	C33-O34-C35	2.06	116.53	109.88
15	H	301	04C	C35-C36-N31	2.01	113.17	110.12
15	Y	301	04C	C7-C8-N22	-2.00	107.24	110.08

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	H	301	04C	C6-C7-C8-N22
15	H	301	04C	C6-C7-C8-C9
15	K	301	04C	C9-C10-C12-O13
15	N	201	04C	C9-C10-C12-O13
15	V	301	04C	C6-C7-C8-C9
15	Y	301	04C	C11-C10-C9-C8
15	Y	301	04C	C12-C10-C9-C8
15	b	201	04C	C9-C10-C12-O13
15	V	301	04C	C43-C44-O45-C46
15	H	301	04C	C47-C44-O45-C46
15	H	301	04C	C43-C44-O45-C46
15	K	301	04C	C43-C44-O45-C46
15	N	201	04C	C47-C44-O45-C46
15	N	201	04C	C43-C44-O45-C46
15	V	301	04C	C47-C44-O45-C46
15	K	301	04C	C47-C44-O45-C46
15	Y	301	04C	C47-C44-O45-C46
15	Y	301	04C	C43-C44-O45-C46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b	201	04C	C47-C44-O45-C46
15	b	201	04C	C43-C44-O45-C46
15	b	201	04C	C23-C24-C40-C41
15	b	201	04C	N25-C24-C40-C41
15	H	301	04C	N25-C24-C40-C41
15	K	301	04C	C5-C6-C7-C8
15	V	301	04C	C5-C6-C7-C8
15	H	301	04C	C23-C24-C40-C41
15	V	301	04C	C1-C6-C7-C8
15	K	301	04C	N25-C24-C40-C41
15	K	301	04C	C1-C6-C7-C8
15	K	301	04C	C23-C24-C40-C41
15	N	201	04C	N25-C24-C40-C41
15	b	201	04C	N28-C29-C30-N31
15	V	301	04C	C11-C10-C9-C8
15	K	301	04C	C11-C10-C12-O13
15	b	201	04C	C11-C10-C12-O13
15	H	301	04C	N28-C29-C30-N31
15	K	301	04C	C6-C7-C8-N22
15	V	301	04C	C6-C7-C8-N22
15	Y	301	04C	C6-C7-C8-N22
15	H	301	04C	C5-C6-C7-C8
15	H	301	04C	C1-C6-C7-C8
15	Y	301	04C	C5-C6-C7-C8
15	Y	301	04C	C1-C6-C7-C8
15	V	301	04C	C11-C10-C9-O21
15	V	301	04C	N28-C29-C30-N31
15	H	301	04C	O37-C29-C30-N31
15	V	301	04C	O37-C29-C30-N31
15	N	201	04C	C1-C6-C7-C8
15	N	201	04C	C5-C6-C7-C8
15	K	301	04C	N28-C29-C30-N31
15	b	201	04C	O37-C29-C30-N31
15	N	201	04C	C30-C29-N28-C27
15	b	201	04C	C5-C6-C7-C8
15	N	201	04C	C23-C24-C40-C41
15	b	201	04C	C1-C6-C7-C8
15	b	201	04C	C11-C10-C9-C8
15	Y	301	04C	C11-C10-C9-O21
15	N	201	04C	C6-C7-C8-N22
15	K	301	04C	O37-C29-C30-N31
15	V	301	04C	C29-C30-N31-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	V	301	04C	C29-C30-N31-C32
15	V	301	04C	N25-C24-C40-C41
15	N	201	04C	O37-C29-N28-C27
15	H	301	04C	C29-C30-N31-C32
15	N	201	04C	C29-C30-N31-C32
15	Y	301	04C	C12-C10-C9-O21
15	H	301	04C	C29-C30-N31-C36
15	b	201	04C	C29-C30-N31-C36
15	K	301	04C	C6-C7-C8-C9
15	V	301	04C	C23-C24-C40-C41
15	Y	301	04C	O49-C23-C24-N25
15	Y	301	04C	C6-C7-C8-C9
15	H	301	04C	C11-C10-C9-O21
15	N	201	04C	C29-C30-N31-C36
15	Y	301	04C	N25-C24-C40-C41
15	N	201	04C	N25-C26-C27-N28
15	Y	301	04C	N22-C23-C24-N25

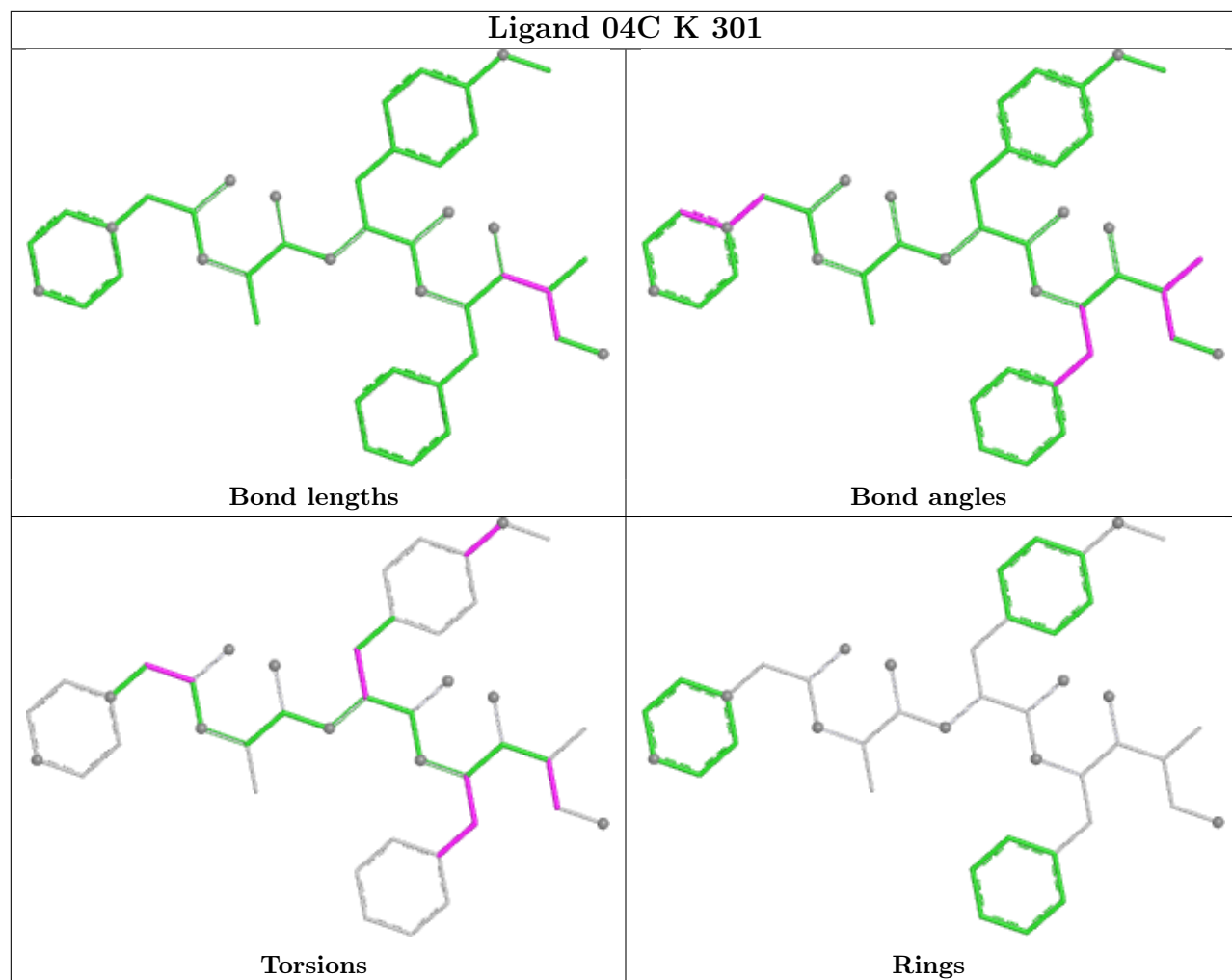
There are no ring outliers.

4 monomers are involved in 19 short contacts:

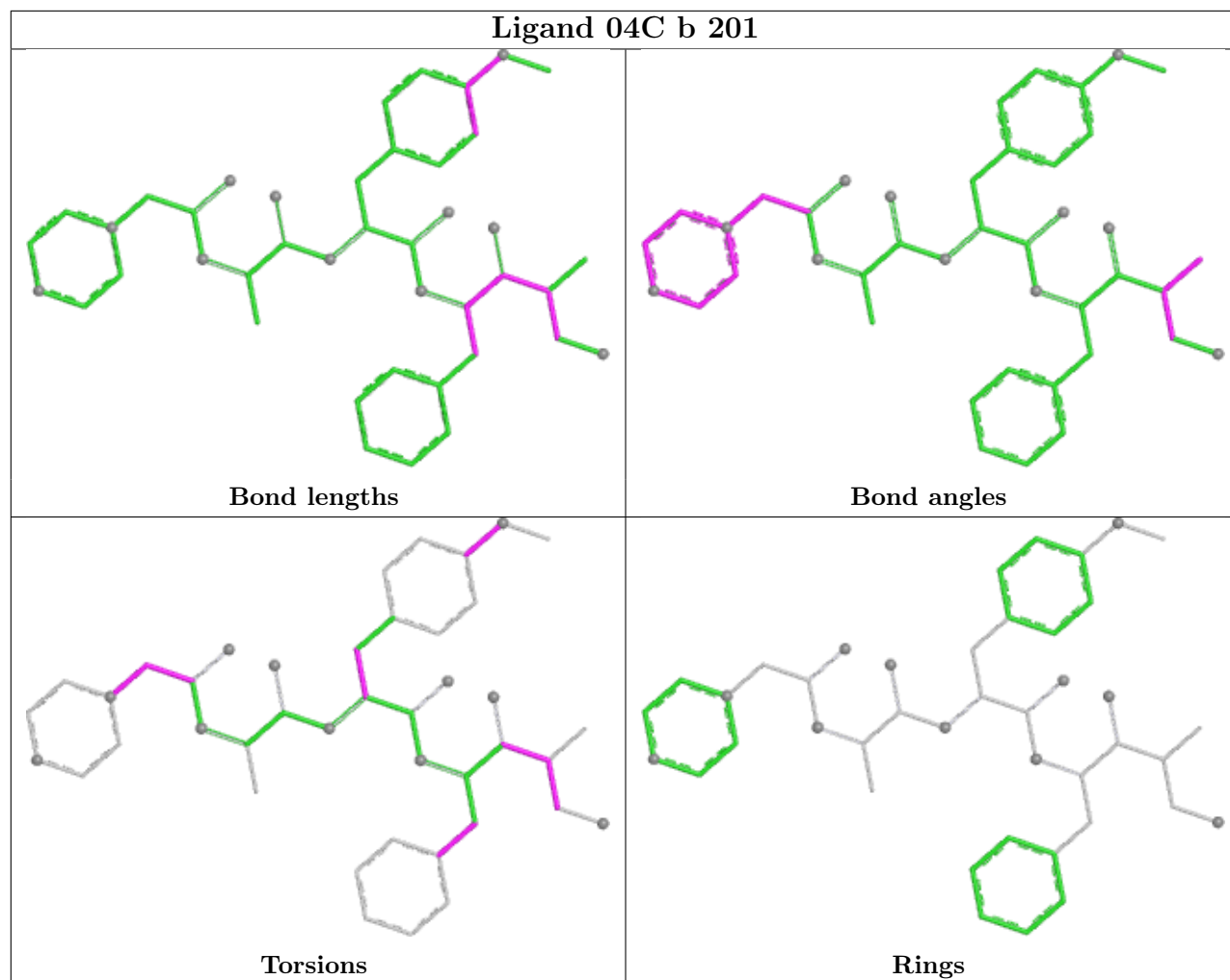
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	K	301	04C	5	0
15	b	201	04C	8	0
15	N	201	04C	4	0
15	Y	301	04C	2	0

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

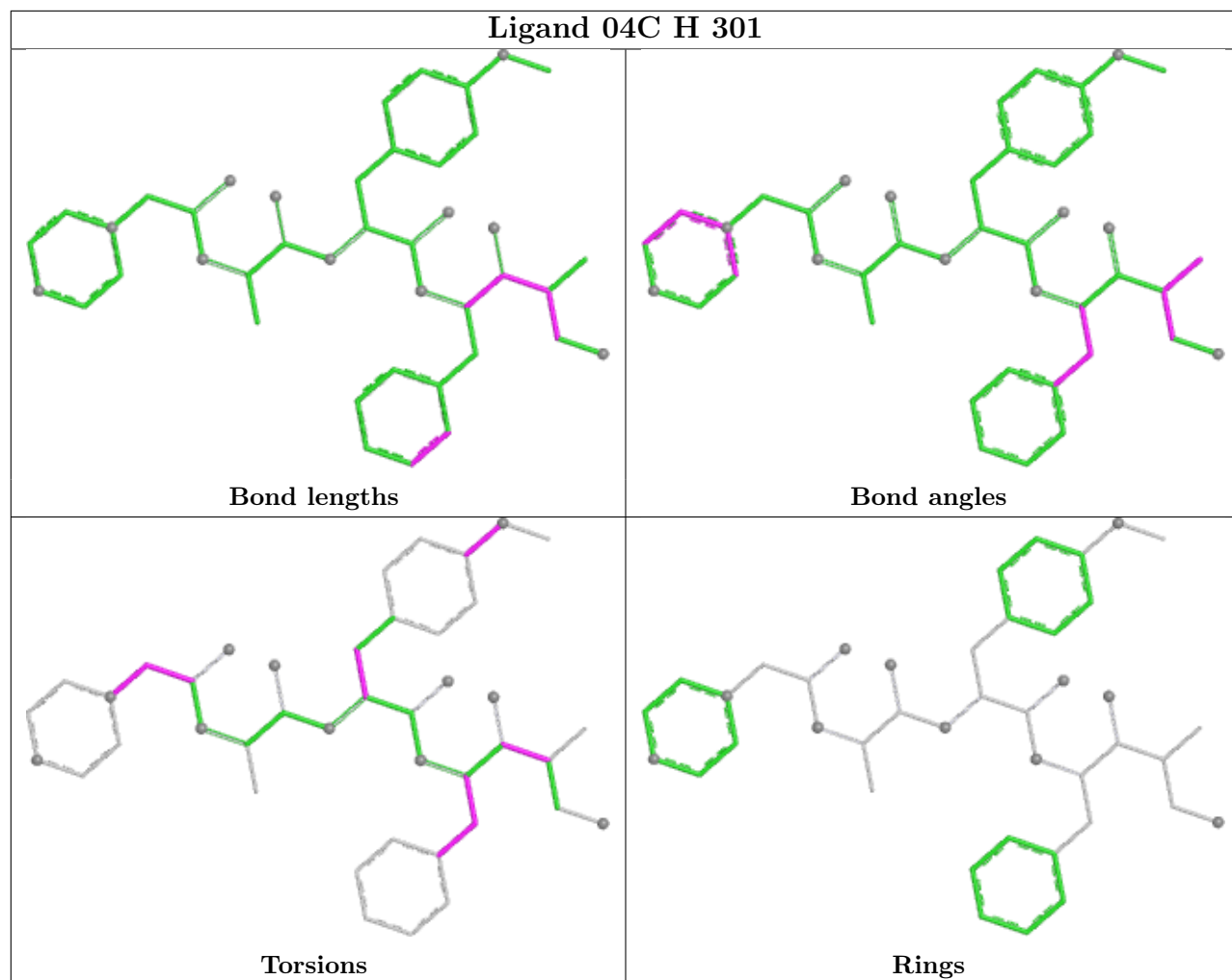
Ligand 04C K 301

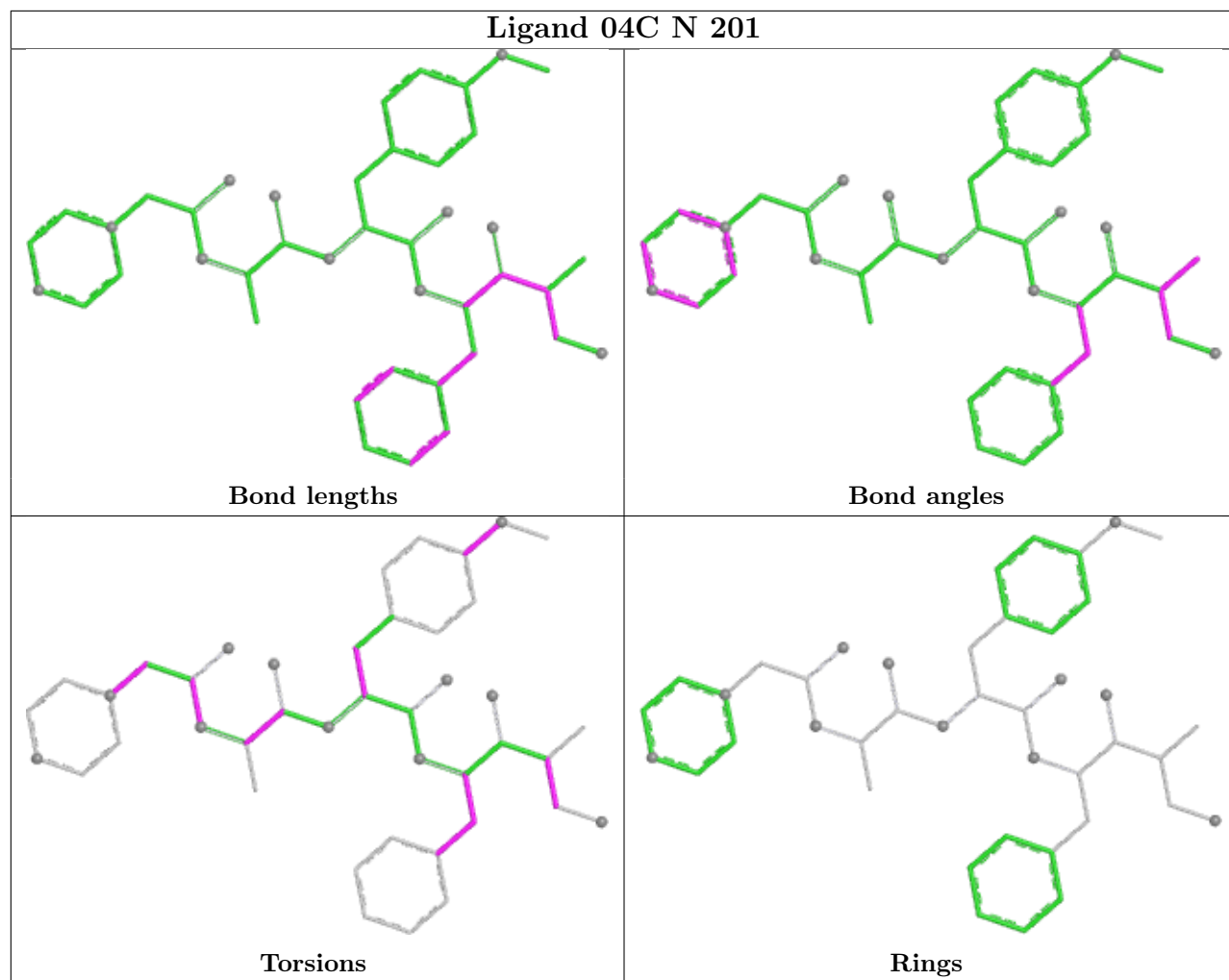


Ligand 04C b 201

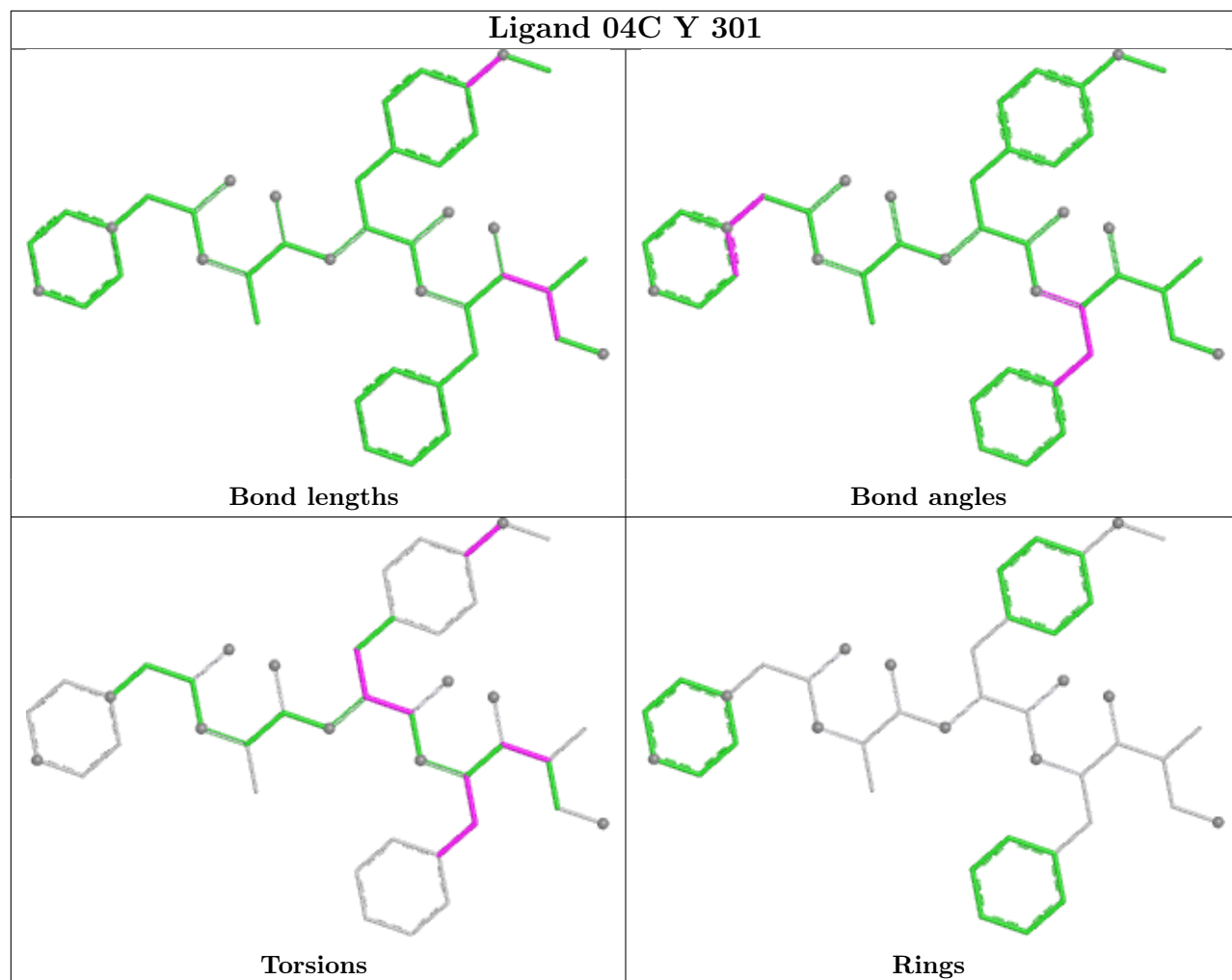


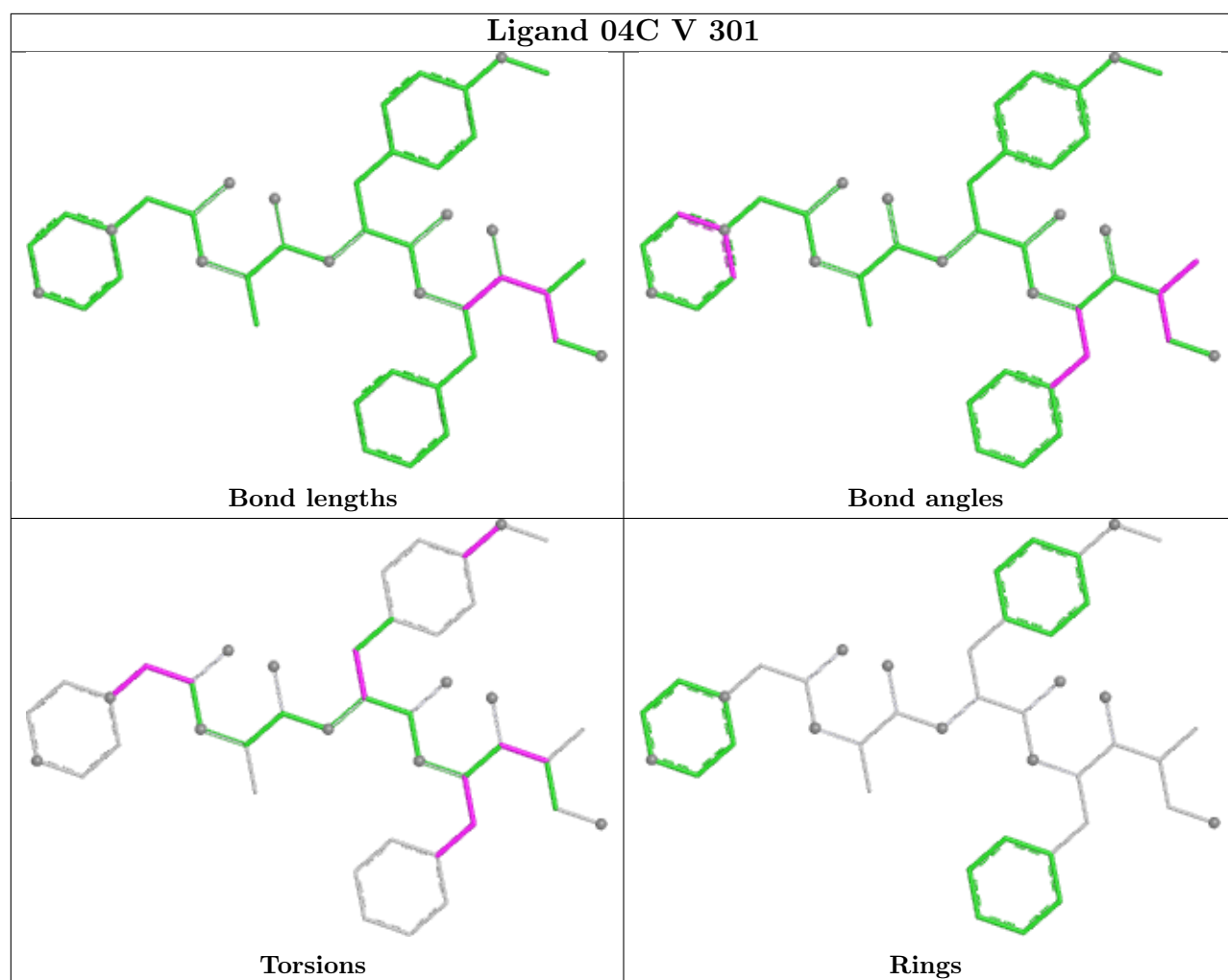
Ligand 04C H 301





Ligand 04C Y 301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.80	0 100 100	46, 72, 111, 148	0
1	O	250/250 (100%)	-0.76	0 100 100	59, 80, 119, 157	0
2	B	244/258 (94%)	-0.65	1 (0%) 88 81	54, 80, 132, 166	0
2	P	244/258 (94%)	-0.59	2 (0%) 82 71	55, 80, 123, 174	0
3	C	241/254 (94%)	-0.63	0 100 100	50, 79, 133, 170	0
3	Q	241/254 (94%)	-0.58	1 (0%) 88 81	62, 94, 160, 208	0
4	D	242/260 (93%)	-0.67	3 (1%) 76 63	58, 82, 128, 160	0
4	R	242/260 (93%)	-0.57	0 100 100	66, 92, 141, 182	0
5	E	233/234 (99%)	-0.62	0 100 100	60, 88, 131, 155	0
5	S	233/234 (99%)	-0.48	0 100 100	67, 98, 146, 184	0
6	F	244/288 (84%)	-0.70	0 100 100	61, 83, 132, 154	0
6	T	244/288 (84%)	-0.60	0 100 100	63, 91, 142, 177	0
7	G	243/252 (96%)	-0.72	0 100 100	53, 76, 118, 184	0
7	U	243/252 (96%)	-0.70	0 100 100	59, 78, 113, 163	0
8	H	222/232 (95%)	-0.86	0 100 100	18, 70, 104, 147	0
8	V	222/232 (95%)	-0.79	1 (0%) 87 78	10, 72, 105, 148	0
9	I	204/205 (99%)	-0.85	0 100 100	43, 65, 96, 117	0
9	W	204/205 (99%)	-0.86	0 100 100	46, 64, 98, 117	0
10	J	198/198 (100%)	-0.79	0 100 100	44, 64, 94, 164	0
10	X	198/198 (100%)	-0.81	1 (0%) 87 78	50, 67, 95, 168	0
11	K	212/212 (100%)	-0.74	2 (0%) 81 68	18, 65, 100, 116	0
11	Y	212/212 (100%)	-0.71	2 (0%) 81 68	14, 69, 102, 126	0
12	L	222/222 (100%)	-0.71	1 (0%) 87 78	48, 69, 104, 134	0
12	Z	222/222 (100%)	-0.75	1 (0%) 87 78	50, 69, 106, 132	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%)	-0.79	1 (0%) 88 81	49, 72, 107, 149	0
13	a	233/233 (100%)	-0.81	0 100 100	47, 68, 100, 142	0
14	N	196/196 (100%)	-0.87	0 100 100	11, 66, 97, 117	0
14	b	196/196 (100%)	-0.84	0 100 100	6, 66, 96, 115	0
All	All	6368/6588 (96%)	-0.72	16 (0%) 90 84	6, 75, 126, 208	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	244	THR	3.6
3	Q	50	LEU	3.5
11	Y	209	ASN	3.5
12	Z	174	TYR	3.3
12	L	174	TYR	3.3
4	D	118	GLY	3.2
13	M	227	GLY	3.1
11	K	104	TYR	2.9
11	Y	104	TYR	2.7
8	V	1	THR	2.6
4	D	119	ALA	2.6
11	K	208	ASN	2.4
4	D	120	SER	2.4
10	X	139	TYR	2.2
2	P	219	ALA	2.2
2	B	219	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

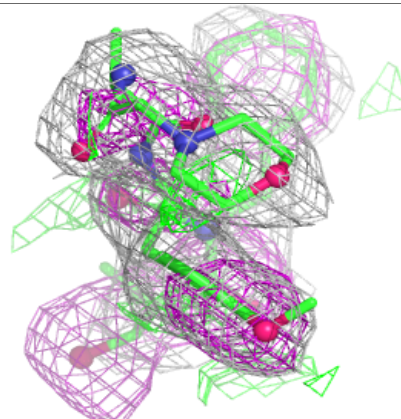
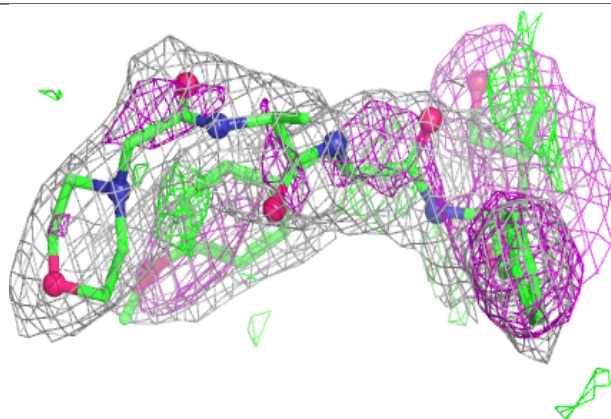
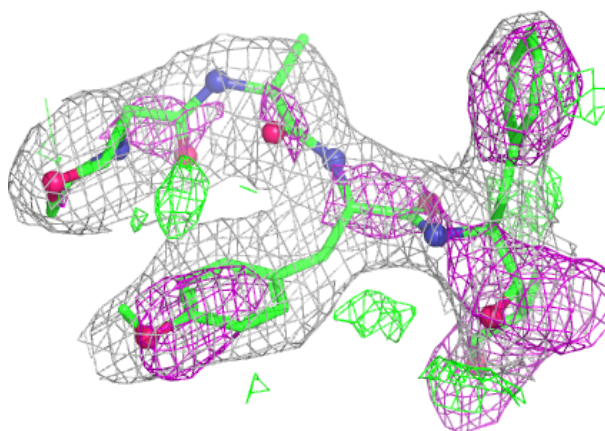
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	04C	H	301	42/42	0.91	0.11	13,26,45,51	0
15	04C	b	201	42/42	0.91	0.12	4,11,27,40	0
15	04C	V	301	42/42	0.92	0.12	9,13,54,141	0
15	04C	N	201	42/42	0.92	0.11	6,10,19,25	0
15	04C	Y	301	42/42	0.93	0.10	11,31,53,59	0
15	04C	K	301	42/42	0.94	0.10	17,31,47,55	0

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

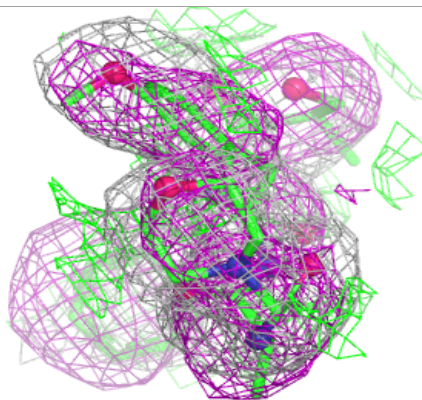
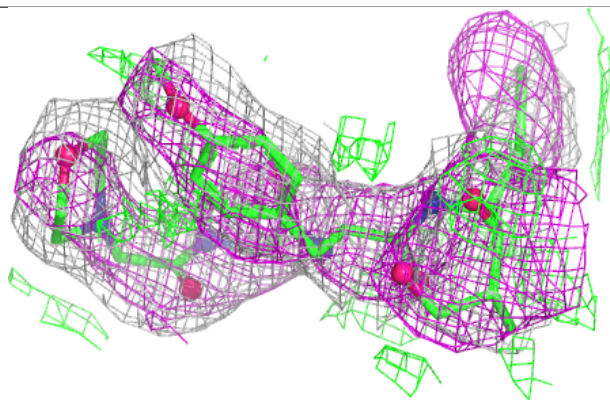
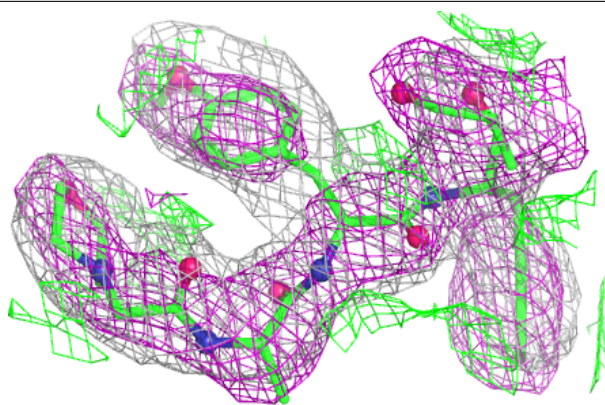
Electron density around 04C H 301:

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



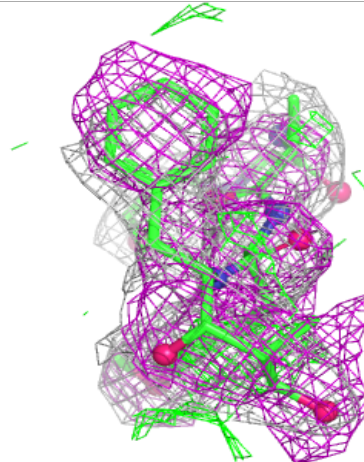
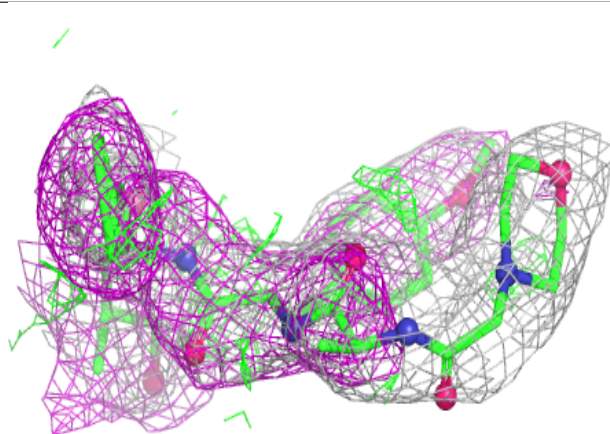
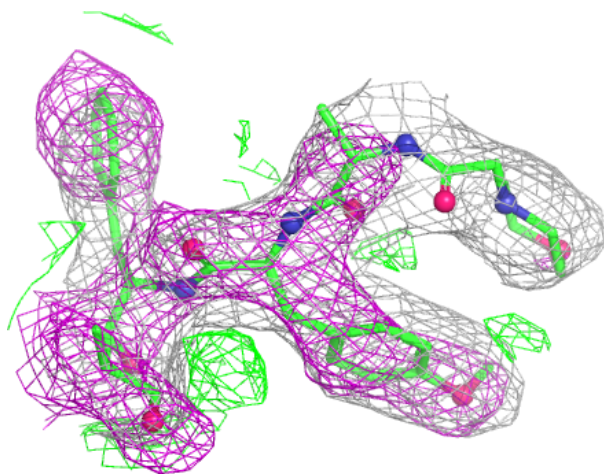
Electron density around 04C b 201:

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



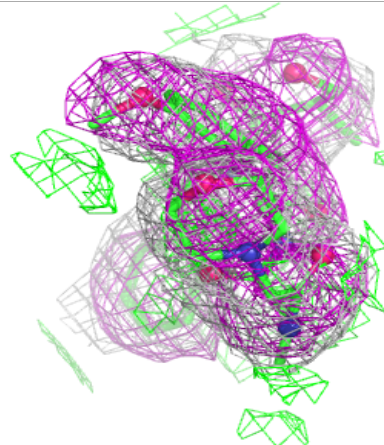
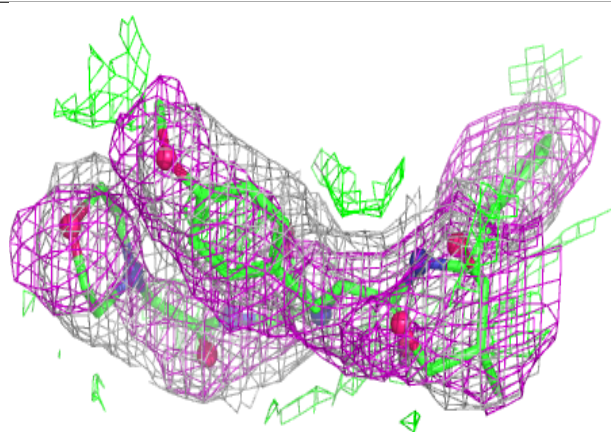
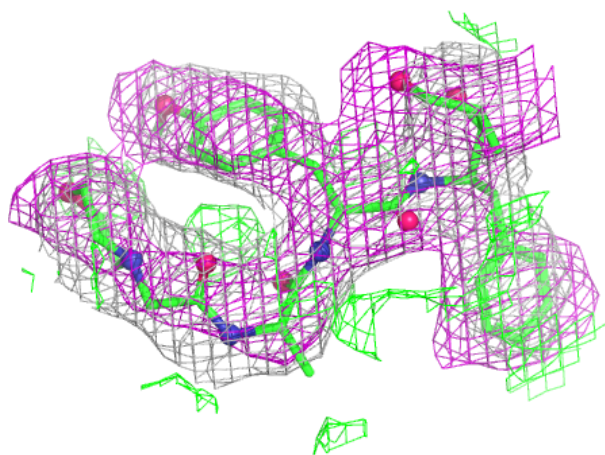
Electron density around 04C V 301:

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



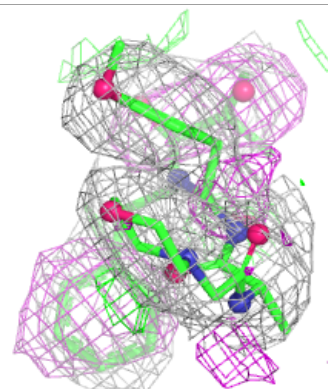
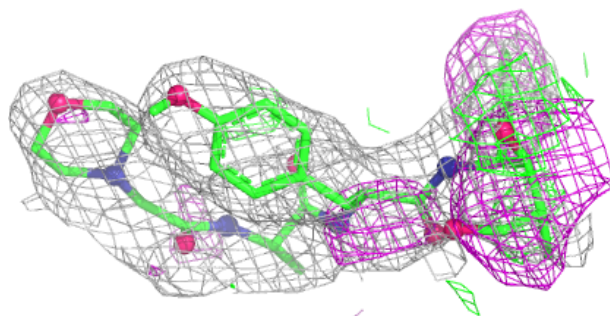
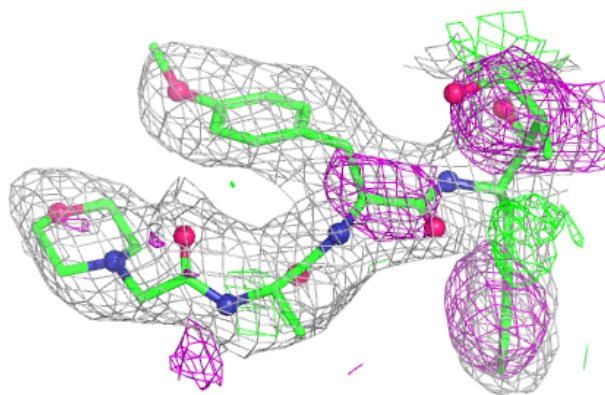
Electron density around 04C N 201:

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

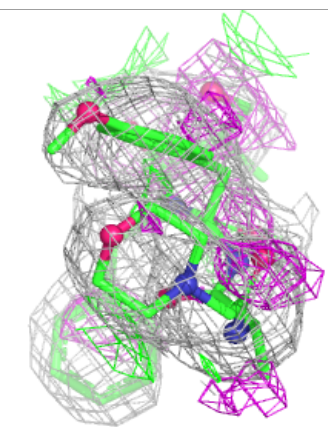
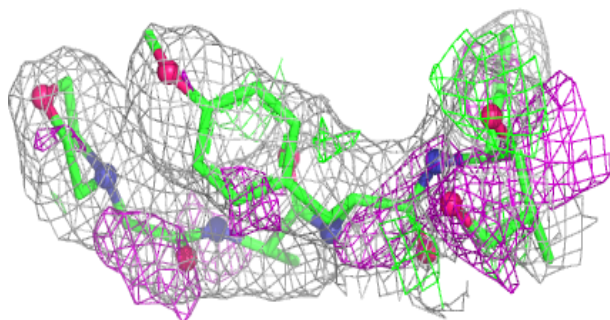
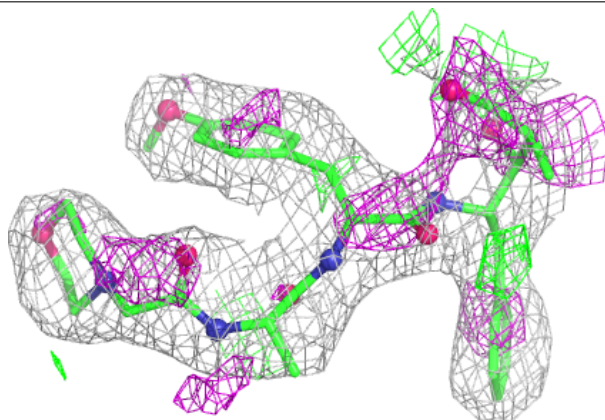


Electron density around 04C Y 301:

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

**Electron density around 04C 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.