



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:33 pm BST

PDB ID : 4INR
Title : Yeast 20S proteasome in complex with the vinyl sulfone LU102
Authors : Geurink, P.P.; van der Linden, W.A.; Mirabella, A.C.; Gallastegui, N.; de Bruin, G.; Blom, A.E.M.; Voges, M.J.; Mock, E.D.; Florea, B.I.; van der Marel, G.A.; Driessen, C.; van der Stelt, M.; Groll, M.; Overkleeft, H.S.; Kisselev, A.F.
Deposited on : 2013-01-06
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

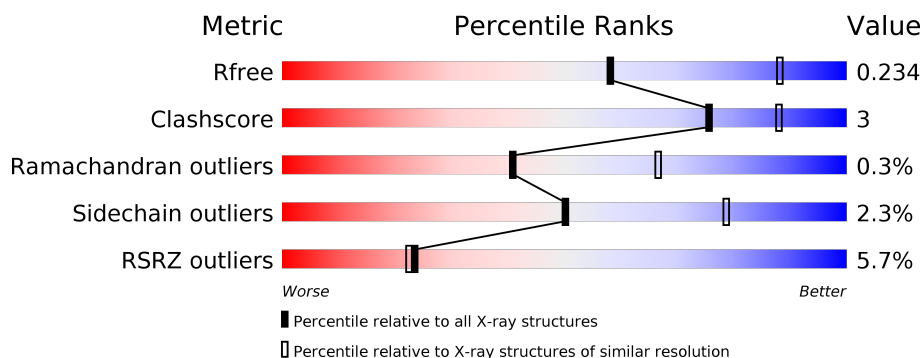
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	O	250	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
2	B	258	<div> <div>9%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>5%</div> </div> </div>
2	P	258	<div> <div>10%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>5%</div> </div> </div>
3	C	254	<div> <div>11%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </div> </div>
3	Q	254	<div> <div>16%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	233	
13	a	233	
14	N	196	
14	b	196	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51061 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			

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

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

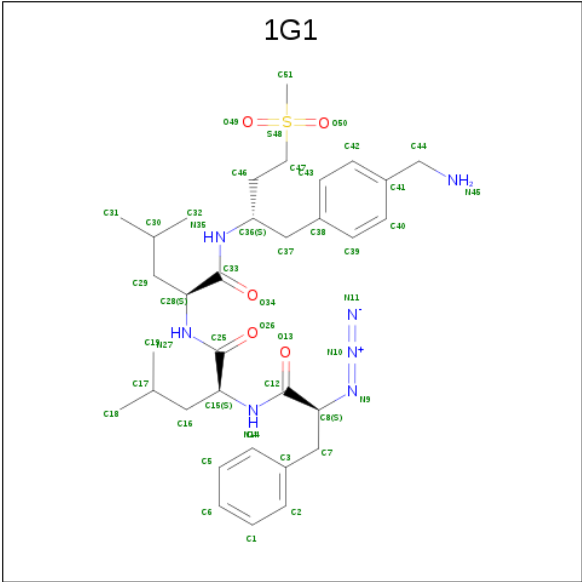
- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	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 N3Phe-Leu-Leu-Phe(4-NH₂CH₂)-methyl vinyl sulfone, bound form (three-letter code: 1G1) (formula: C₃₃H₄₉N₇O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	H	1	Total	C	N	O	S	0	0
			46	33	7	5	1		
15	K	1	Total	C	N	O	S	0	0
			46	33	7	5	1		
15	V	1	Total	C	N	O	S	0	0
			46	33	7	5	1		
15	Y	1	Total	C	N	O	S	0	0
			46	33	7	5	1		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	58	Total	O	0	0
			58	58		
16	B	37	Total	O	0	0
			37	37		
16	C	43	Total	O	0	0
			43	43		
16	D	37	Total	O	0	0
			37	37		
16	E	21	Total	O	0	0
			21	21		
16	F	47	Total	O	0	0
			47	47		
16	G	60	Total	O	0	0
			60	60		
16	H	54	Total	O	0	0
			54	54		

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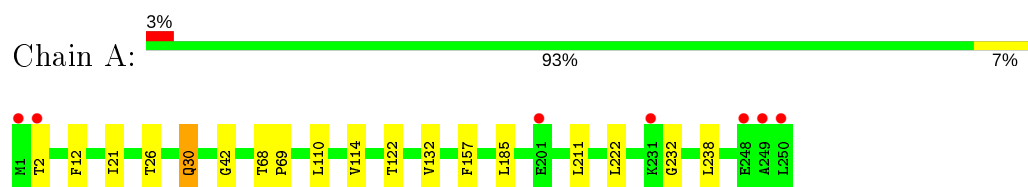
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	I	68	Total O 68 68	0	0
16	J	53	Total O 53 53	0	0
16	K	48	Total O 48 48	0	0
16	L	57	Total O 57 57	0	0
16	M	75	Total O 75 75	0	0
16	N	55	Total O 55 55	0	0
16	O	35	Total O 35 35	0	0
16	P	28	Total O 28 28	0	0
16	Q	29	Total O 29 29	0	0
16	R	27	Total O 27 27	0	0
16	S	17	Total O 17 17	0	0
16	T	42	Total O 42 42	0	0
16	U	60	Total O 60 60	0	0
16	V	50	Total O 50 50	0	0
16	W	57	Total O 57 57	0	0
16	X	46	Total O 46 46	0	0
16	Y	52	Total O 52 52	0	0
16	Z	49	Total O 49 49	0	0
16	a	77	Total O 77 77	0	0
16	b	57	Total O 57 57	0	0

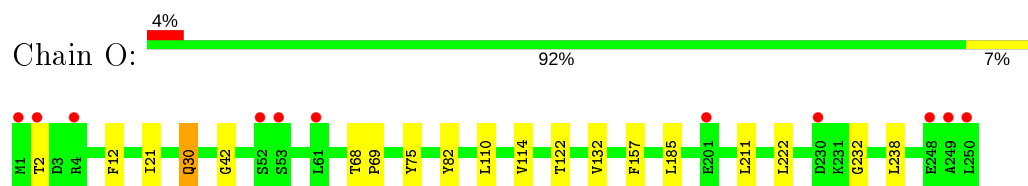
3 Residue-property plots [i](#)

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

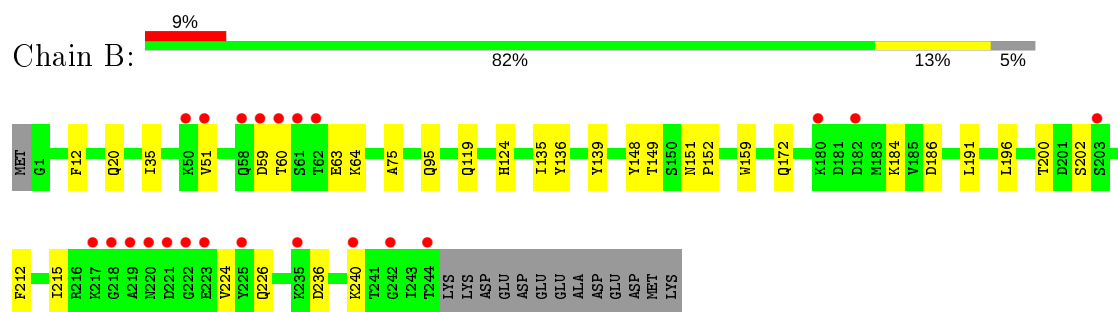
- Molecule 1: Proteasome component Y7



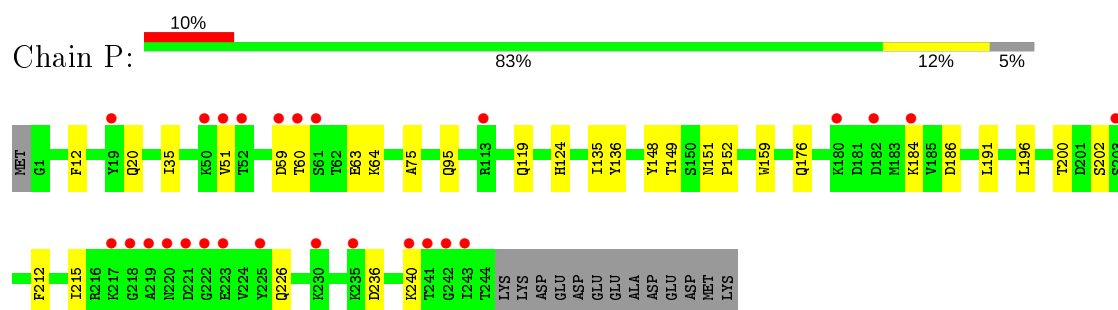
- Molecule 1: Proteasome component Y7



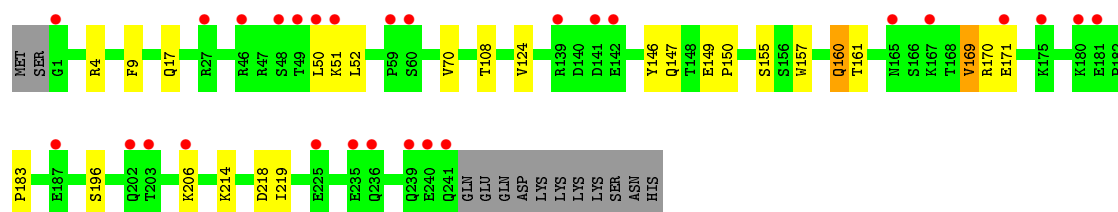
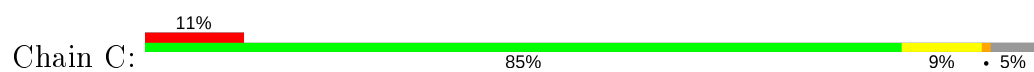
- Molecule 2: Proteasome component Y13



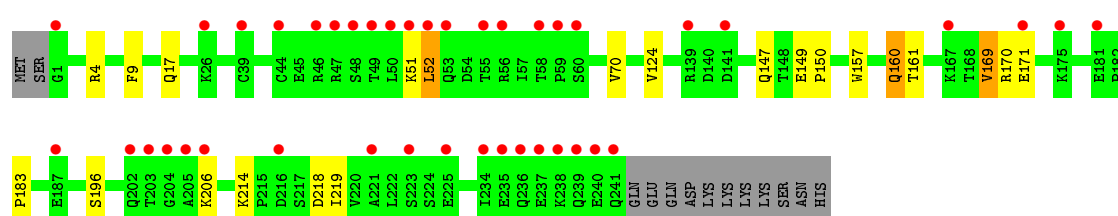
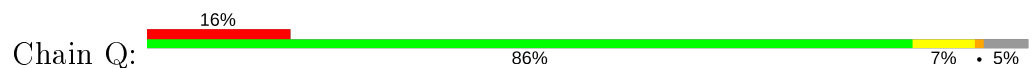
- Molecule 2: Proteasome component Y13



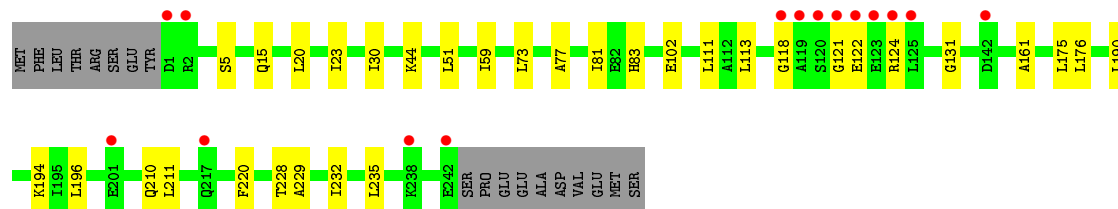
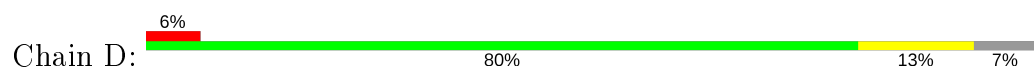
- Molecule 3: Proteasome component PRE6



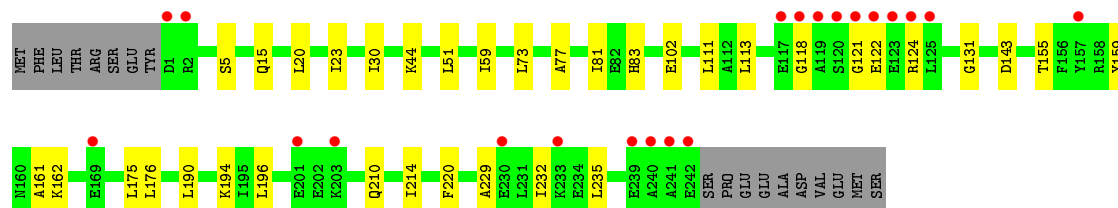
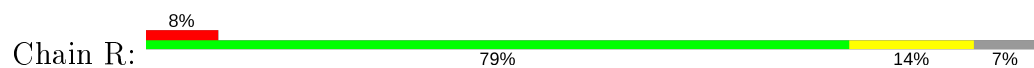
• Molecule 3: Proteasome component PRE6



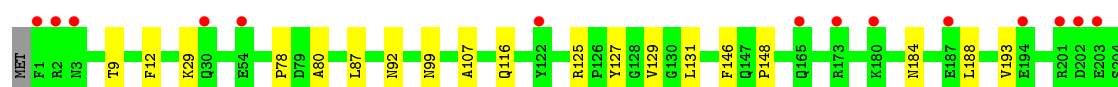
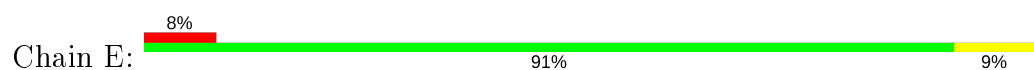
• Molecule 4: Proteasome component PUP2

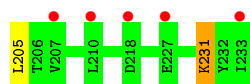


• Molecule 4: Proteasome component PUP2

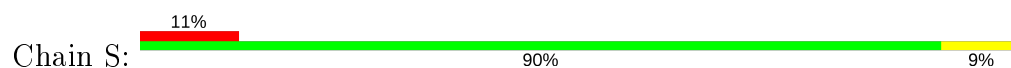


• Molecule 5: Proteasome component PRE5

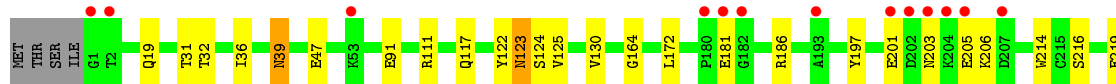
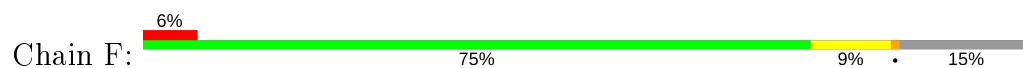




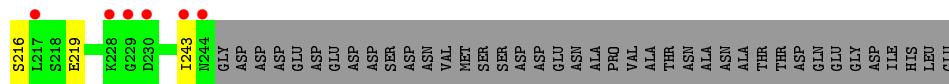
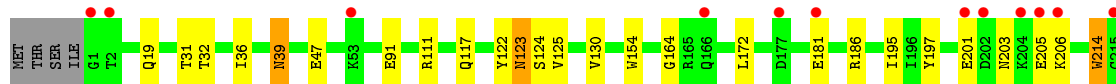
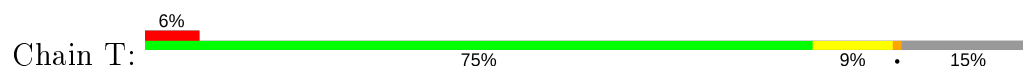
• Molecule 5: Proteasome component PRE5



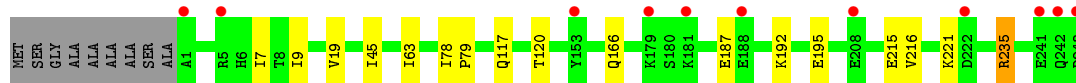
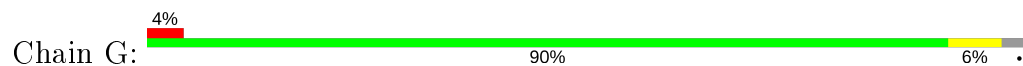
• Molecule 6: Proteasome component C1



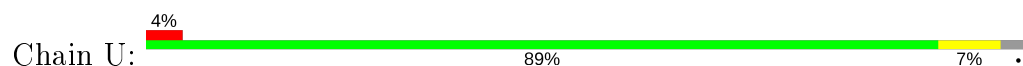
• Molecule 6: Proteasome component C1



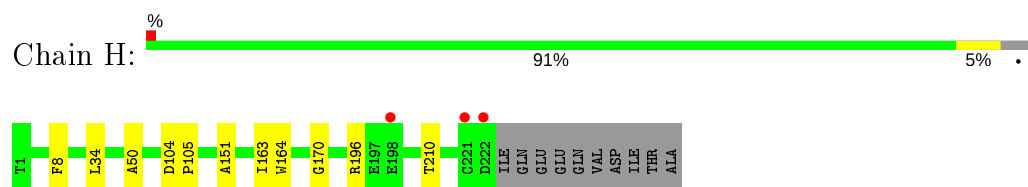
• Molecule 7: Proteasome component C7-alpha



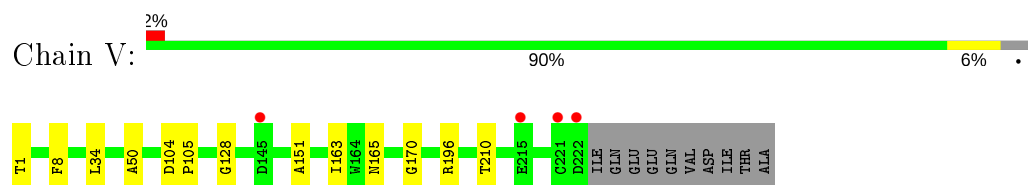
• Molecule 7: Proteasome component C7-alpha



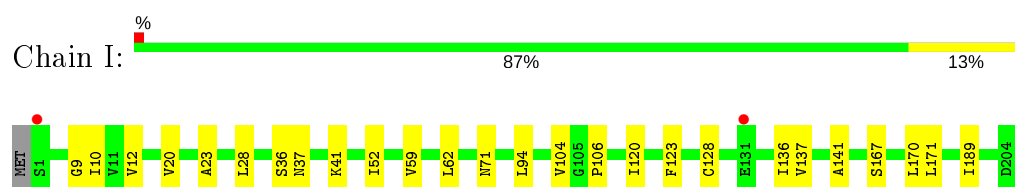
- Molecule 8: Proteasome component PUP1



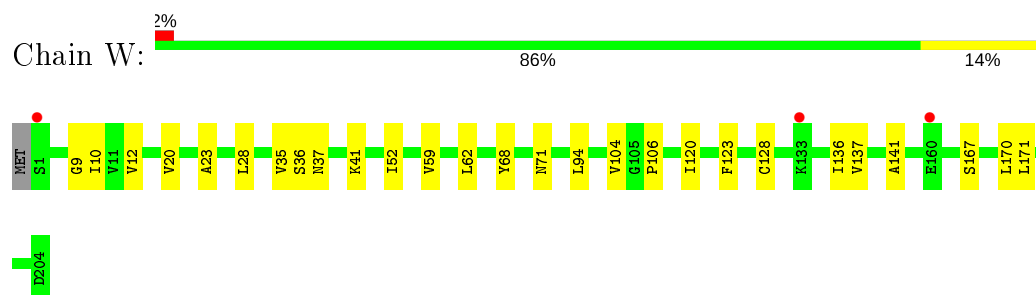
- Molecule 8: Proteasome component PUP1



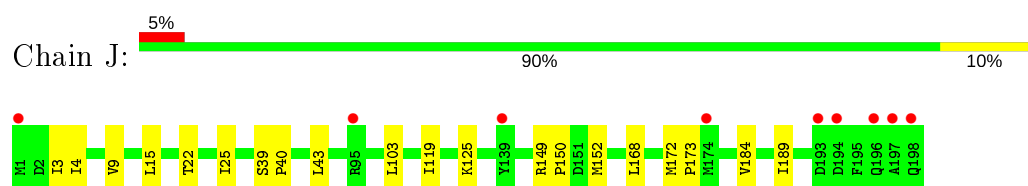
- Molecule 9: Proteasome component PUP3



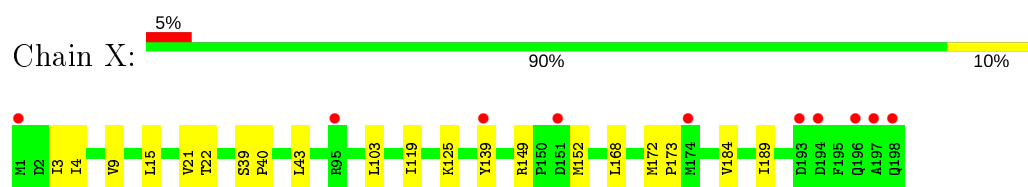
- Molecule 9: Proteasome component PUP3



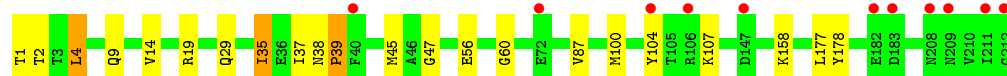
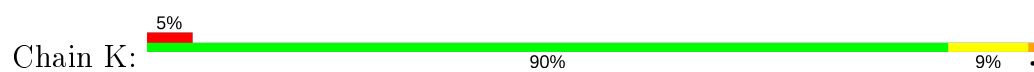
- Molecule 10: Proteasome component C11



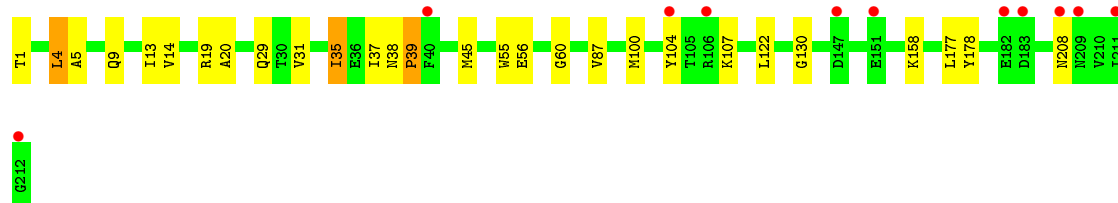
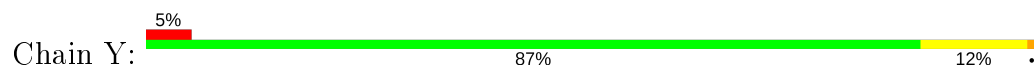
- Molecule 10: Proteasome component C11



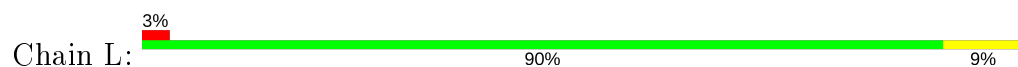
- Molecule 11: Proteasome component PRE2



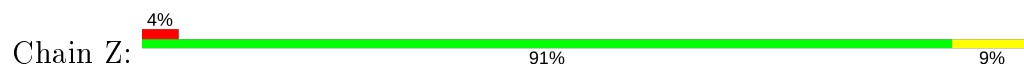
- Molecule 11: Proteasome component PRE2



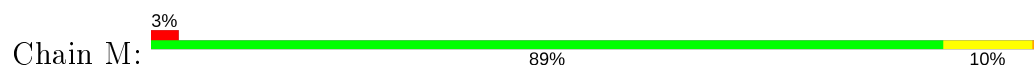
- Molecule 12: Proteasome component C5



- Molecule 12: Proteasome component C5



- Molecule 13: Proteasome component PRE4

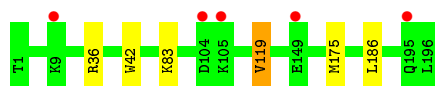


- Molecule 13: Proteasome component PRE4

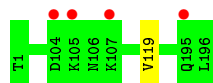


- Molecule 14: Proteasome component PRE3





- Molecule 14: Proteasome component PRE3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.32Å 301.05Å 144.32Å 90.00° 113.13° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (15.00-2.70) 98.9 (15.00-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.231 0.228 , 0.234	Depositor DCC
R_{free} test set	14301 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.2	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	51061	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: 1G1

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	0.36	0/1952	0.46	0/2642
1	O	0.36	0/1952	0.46	0/2642
2	B	0.33	0/1934	0.46	0/2618
2	P	0.33	0/1934	0.46	0/2618
3	C	0.33	0/1919	0.47	0/2598
3	Q	0.33	0/1919	0.47	0/2598
4	D	0.36	0/1886	0.47	0/2541
4	R	0.36	0/1886	0.47	0/2541
5	E	0.31	0/1823	0.45	0/2463
5	S	0.31	0/1823	0.45	0/2463
6	F	0.41	0/1936	0.45	0/2614
6	T	0.41	1/1936 (0.1%)	0.45	0/2614
7	G	0.34	0/1959	0.46	0/2652
7	U	0.34	0/1959	0.46	0/2652
8	H	0.44	1/1715 (0.1%)	0.46	0/2326
8	V	0.44	0/1715	0.47	0/2326
9	I	0.34	0/1611	0.46	0/2174
9	W	0.34	0/1611	0.47	0/2174
10	J	0.31	0/1613	0.45	0/2173
10	X	0.31	0/1613	0.45	0/2173
11	K	0.50	0/1681	0.49	1/2274 (0.0%)
11	Y	0.50	1/1681 (0.1%)	0.49	1/2274 (0.0%)
12	L	0.36	1/1795 (0.1%)	0.45	0/2420
12	Z	0.36	0/1795	0.45	0/2420
13	M	0.36	0/1855	0.48	0/2514
13	a	0.36	0/1855	0.48	0/2514
14	N	0.39	0/1541	0.44	0/2087
14	b	0.39	0/1541	0.44	0/2087
All	All	0.37	4/50440 (0.0%)	0.46	2/68192 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	214	TRP	CD2-CE2	5.06	1.47	1.41
12	L	74	TRP	CD2-CE2	5.01	1.47	1.41
8	H	164	TRP	CD2-CE2	5.01	1.47	1.41
11	Y	55	TRP	CD2-CE2	5.01	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	4	LEU	CA-CB-CG	5.33	127.56	115.30
11	K	4	LEU	CA-CB-CG	5.24	127.36	115.30

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	1915	0	1929	9	0
1	O	1915	0	1929	9	0
2	B	1904	0	1904	16	0
2	P	1904	0	1904	16	0
3	C	1890	0	1903	15	0
3	Q	1890	0	1903	12	0
4	D	1861	0	1839	16	0
4	R	1861	0	1839	18	0
5	E	1795	0	1800	11	0
5	S	1795	0	1800	12	0
6	F	1896	0	1889	14	0
6	T	1896	0	1889	16	0
7	G	1921	0	1913	7	0
7	U	1921	0	1913	8	0
8	H	1684	0	1687	6	0
8	V	1684	0	1687	12	0
9	I	1581	0	1574	14	0
9	W	1581	0	1574	16	0
10	J	1585	0	1590	13	0
10	X	1585	0	1590	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	1644	0	1594	10	0
11	Y	1644	0	1594	15	0
12	L	1757	0	1711	11	0
12	Z	1757	0	1711	11	0
13	M	1824	0	1832	16	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	3	0
14	b	1512	0	1481	0	0
15	H	46	0	48	1	0
15	K	46	0	48	1	0
15	V	46	0	48	4	0
15	Y	46	0	48	6	0
16	A	58	0	0	0	0
16	B	37	0	0	0	0
16	C	43	0	0	0	0
16	D	37	0	0	0	0
16	E	21	0	0	0	0
16	F	47	0	0	0	0
16	G	60	0	0	0	0
16	H	54	0	0	0	0
16	I	68	0	0	0	0
16	J	53	0	0	0	0
16	K	48	0	0	0	0
16	L	57	0	0	0	0
16	M	75	0	0	0	0
16	N	55	0	0	0	0
16	O	35	0	0	0	0
16	P	28	0	0	0	0
16	Q	29	0	0	0	0
16	R	27	0	0	0	0
16	S	17	0	0	0	0
16	T	42	0	0	0	0
16	U	60	0	0	0	0
16	V	50	0	0	0	0
16	W	57	0	0	0	0
16	X	46	0	0	1	0
16	Y	52	0	0	3	0
16	Z	49	0	0	0	0
16	a	77	0	0	0	0
16	b	57	0	0	0	0
All	All	51061	0	49484	285	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 3.

All (285) 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)
15:Y:301:1G1:H19	16:Y:442:HOH:O	1.74	0.87
12:L:109:THR:HG23	12:L:125:PHE:HB2	1.66	0.77
10:X:4:ILE:HG22	10:X:103:LEU:HD12	1.66	0.76
5:E:12:PHE:H	6:F:19:GLN:HE22	1.38	0.71
5:S:12:PHE:H	6:T:19:GLN:HE22	1.39	0.71
10:J:4:ILE:HG22	10:J:103:LEU:HD12	1.70	0.71
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.37	0.70
3:C:9:PHE:H	4:D:15:GLN:HE22	1.38	0.70
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.56	0.70
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.56	0.69
13:M:161:ARG:HH11	13:M:161:ARG:HG3	1.56	0.69
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.75	0.68
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.75	0.68
4:D:44:LYS:HE3	4:D:210:GLN:HB2	1.76	0.66
4:R:44:LYS:HE3	4:R:210:GLN:HB2	1.77	0.66
14:N:83:LYS:HG3	14:N:119:VAL:HG22	1.79	0.65
13:M:48:ASN:H	13:M:48:ASN:HD22	1.47	0.63
4:R:161:ALA:HB3	5:S:55:LEU:HD23	1.79	0.63
12:Z:109:THR:HG23	12:Z:125:PHE:HB2	1.80	0.62
8:V:50:ALA:HB2	9:W:128:CYS:HB2	1.82	0.61
1:A:12:PHE:H	2:B:20:GLN:HE22	1.48	0.61
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.82	0.61
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.82	0.61
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.84	0.60
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.84	0.59
2:B:12:PHE:H	3:C:17:GLN:HE22	1.51	0.59
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.85	0.59
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.83	0.58
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.85	0.58
6:F:91:GLU:HG3	6:F:111:ARG:HH11	1.69	0.58
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.84	0.58
15:Y:301:1G1:H8	16:Y:442:HOH:O	2.04	0.58
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.85	0.58
1:O:12:PHE:H	2:P:20:GLN:HE22	1.50	0.58
11:K:35:ILE:HB	11:K:45:MET:HE3	1.86	0.58
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.85	0.58
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.51	0.58
4:D:73:LEU:HD12	4:D:131:GLY:HA3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.86	0.57
8:H:50:ALA:HB2	9:I:128:CYS:HB2	1.86	0.57
11:Y:107:LYS:H	11:Y:107:LYS:HD2	1.70	0.57
11:K:107:LYS:H	11:K:107:LYS:HD2	1.70	0.57
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.85	0.57
4:R:73:LEU:HD12	4:R:131:GLY:HA3	1.87	0.56
6:T:91:GLU:HG3	6:T:111:ARG:HH11	1.68	0.56
11:Y:20:ALA:HA	16:Y:442:HOH:O	2.06	0.56
1:O:21:ILE:HD11	1:O:122:THR:HG21	1.88	0.56
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.87	0.56
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.86	0.56
6:F:39:ASN:HD22	6:F:39:ASN:N	2.04	0.56
10:J:39:SER:HB2	10:J:40:PRO:HD2	1.89	0.55
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.54	0.55
11:K:47:GLY:H	15:K:301:1G1:H5	1.71	0.55
6:T:39:ASN:HD22	6:T:39:ASN:N	2.05	0.55
2:P:200:THR:HG22	2:P:202:SER:H	1.72	0.55
1:A:21:ILE:HD11	1:A:122:THR:HG21	1.87	0.55
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.55	0.54
6:T:31:THR:HG23	6:T:47:GLU:HB3	1.88	0.54
12:L:195:HIS:HD2	12:L:197:GLN:H	1.56	0.54
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.89	0.54
10:J:119:ILE:HG12	10:J:125:LYS:HG3	1.89	0.54
10:J:149:ARG:HB2	10:J:152:MET:HG3	1.90	0.53
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	1.89	0.53
10:X:119:ILE:HG12	10:X:125:LYS:HG3	1.89	0.53
6:T:31:THR:HG21	6:T:47:GLU:O	2.09	0.53
8:V:1:THR:N	15:V:301:1G1:H5	2.23	0.52
9:I:106:PRO:HD2	9:I:123:PHE:HB2	1.91	0.52
2:P:35:ILE:HD12	2:P:196:LEU:HG	1.90	0.52
6:F:39:ASN:HD22	6:F:39:ASN:H	1.57	0.52
2:P:136:TYR:HB2	2:P:148:TYR:HB2	1.90	0.52
1:O:211:LEU:HD22	1:O:238:LEU:HD12	1.90	0.52
2:P:215:ILE:HG12	2:P:226:GLN:HG2	1.92	0.52
11:Y:1:THR:O	11:Y:130:GLY:HA3	2.08	0.52
1:A:211:LEU:HD22	1:A:238:LEU:HD12	1.91	0.52
10:J:168:LEU:O	10:J:172:MET:HB2	2.09	0.52
11:K:35:ILE:HG21	11:K:56:GLU:HB3	1.92	0.52
2:B:136:TYR:HB2	2:B:148:TYR:HB2	1.92	0.51
6:T:36:ILE:HG12	6:T:172:LEU:HD11	1.92	0.51
10:X:39:SER:HB2	10:X:40:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:35:ILE:HG21	11:Y:56:GLU:HB3	1.92	0.51
9:W:106:PRO:HD2	9:W:123:PHE:HB2	1.93	0.51
13:M:129:TYR:HE1	13:M:144:THR:HG22	1.76	0.51
10:X:149:ARG:HB2	10:X:152:MET:HG3	1.93	0.51
2:B:63:GLU:HG3	2:B:64:LYS:HG3	1.92	0.51
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.93	0.51
1:A:68:THR:HB	1:A:69:PRO:HD2	1.93	0.51
3:C:161:THR:HG21	3:C:169:VAL:HG13	1.93	0.51
11:Y:31:VAL:HG11	15:Y:301:1G1:H18	1.93	0.50
4:D:5:SER:HB2	5:E:125:ARG:HD3	1.93	0.50
11:K:38:ASN:HB2	11:K:39:PRO:HD2	1.92	0.50
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.93	0.50
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.93	0.50
2:B:215:ILE:HG12	2:B:226:GLN:HG2	1.93	0.50
2:B:35:ILE:HD12	2:B:196:LEU:HG	1.91	0.50
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.94	0.50
6:F:31:THR:HG21	6:F:47:GLU:O	2.11	0.50
13:M:27:LEU:HB2	13:M:192:SER:HB2	1.94	0.50
7:G:63:ILE:HD12	7:G:215:GLU:HG2	1.94	0.49
3:Q:214:LYS:HB2	3:Q:218:ASP:HB3	1.94	0.49
7:G:78:ILE:N	7:G:79:PRO:HD2	2.26	0.49
4:D:59:ILE:HG22	4:D:220:PHE:HZ	1.78	0.49
8:V:210:THR:HG21	9:W:167:SER:HB3	1.95	0.49
7:U:78:ILE:N	7:U:79:PRO:HD2	2.26	0.49
3:C:214:LYS:HB2	3:C:218:ASP:HB3	1.94	0.49
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.94	0.49
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.61	0.49
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.95	0.49
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.95	0.49
6:T:39:ASN:H	6:T:39:ASN:HD22	1.61	0.49
7:U:63:ILE:HD12	7:U:215:GLU:HG2	1.95	0.48
2:P:63:GLU:HG3	2:P:64:LYS:HG3	1.94	0.48
2:B:200:THR:HG22	2:B:202:SER:H	1.78	0.48
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.96	0.48
2:B:149:THR:HG22	2:B:159:TRP:HE1	1.78	0.48
9:W:12:VAL:HG23	9:W:137:VAL:HG12	1.95	0.48
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.95	0.48
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.95	0.48
6:T:205:GLU:HG3	6:T:206:LYS:HG3	1.96	0.48
6:F:205:GLU:HG3	6:F:206:LYS:HG3	1.96	0.48
11:Y:19:ARG:HH21	11:Y:29:GLN:HE22	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:150:PRO:HG3	11:Y:208:ASN:HD21	1.79	0.48
13:M:161:ARG:NH1	13:M:161:ARG:HG3	2.27	0.48
10:J:15:LEU:HD12	10:J:43:LEU:HD23	1.94	0.47
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.95	0.47
6:F:36:ILE:HG12	6:F:172:LEU:HD11	1.95	0.47
11:K:14:VAL:HB	11:K:178:TYR:HB2	1.95	0.47
1:O:110:LEU:O	1:O:114:VAL:HG23	2.15	0.47
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.63	0.47
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.96	0.47
5:S:80:ALA:HB2	5:S:129:VAL:HG21	1.96	0.47
10:J:22:THR:HG21	10:X:173:PRO:HB3	1.96	0.47
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.97	0.47
2:B:75:ALA:HB3	2:B:135:ILE:HB	1.95	0.47
9:I:23:ALA:HB1	9:I:170:LEU:HD22	1.95	0.47
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.96	0.47
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.61	0.47
8:V:1:THR:N	15:V:301:1G1:C47	2.78	0.47
1:A:110:LEU:O	1:A:114:VAL:HG23	2.15	0.47
2:P:149:THR:HG22	2:P:159:TRP:HE1	1.78	0.47
10:X:15:LEU:HD12	10:X:43:LEU:HD23	1.97	0.47
5:E:231:LYS:H	5:E:231:LYS:HD2	1.78	0.47
12:L:111:ILE:HG12	12:L:125:PHE:HE1	1.80	0.47
13:M:27:LEU:HD11	13:M:34:LEU:HB3	1.97	0.47
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.96	0.47
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.96	0.47
8:V:1:THR:O	8:V:128:GLY:HA3	2.15	0.47
11:Y:14:VAL:HB	11:Y:178:TYR:HB2	1.97	0.47
5:S:127:TYR:O	5:S:148:PRO:HB3	2.15	0.46
5:S:231:LYS:HD2	5:S:231:LYS:H	1.80	0.46
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.96	0.46
9:I:12:VAL:HG23	9:I:137:VAL:HG12	1.97	0.46
2:P:75:ALA:HB3	2:P:135:ILE:HB	1.97	0.46
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.97	0.46
10:X:168:LEU:O	10:X:172:MET:HB2	2.14	0.46
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.62	0.46
9:W:94:LEU:HD11	9:W:106:PRO:HG2	1.97	0.46
10:J:3:ILE:HD13	10:J:168:LEU:HD13	1.97	0.46
3:Q:157:TRP:CE2	4:R:51:LEU:HD23	2.50	0.46
15:H:301:1G1:H20	15:H:301:1G1:H5	1.66	0.46
5:E:80:ALA:HB2	5:E:129:VAL:HG21	1.96	0.46
4:R:229:ALA:HA	4:R:232:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:184:VAL:HG22	10:X:189:ILE:HG12	1.97	0.46
12:Z:126:ASP:HB2	12:Z:130:SER:HB3	1.97	0.46
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.98	0.46
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.97	0.46
1:O:68:THR:HB	1:O:69:PRO:HD2	1.97	0.46
6:T:123:ASN:HD22	6:T:124:SER:N	2.14	0.46
4:D:229:ALA:HA	4:D:232:ILE:HD12	1.97	0.46
5:E:127:TYR:O	5:E:148:PRO:HB3	2.16	0.46
10:J:184:VAL:HG22	10:J:189:ILE:HG12	1.98	0.46
8:V:1:THR:H3	15:V:301:1G1:C47	2.29	0.46
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.50	0.45
13:M:96:LEU:O	13:M:100:MET:HG2	2.16	0.45
4:R:59:ILE:HG22	4:R:220:PHE:HZ	1.80	0.45
10:X:3:ILE:HD13	10:X:168:LEU:HD13	1.98	0.45
4:R:5:SER:HB2	5:S:125:ARG:HD3	1.98	0.45
11:K:158:LYS:HB2	11:K:177:LEU:HD11	1.99	0.45
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.99	0.45
4:D:161:ALA:HB1	4:D:175:LEU:HD22	1.98	0.45
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.99	0.45
6:F:122:TYR:HB2	6:F:125:VAL:HG22	1.97	0.45
8:H:210:THR:HG21	9:I:167:SER:HB3	1.98	0.45
4:R:77:ALA:O	4:R:81:ILE:HG12	2.16	0.45
6:T:122:TYR:HB2	6:T:125:VAL:HG22	1.98	0.45
9:W:28:LEU:HB3	9:W:36:SER:HB3	1.98	0.45
9:W:62:LEU:HD11	9:W:104:VAL:HG21	1.98	0.45
15:Y:301:1G1:C33	15:Y:301:1G1:H4	2.47	0.45
4:R:155:THR:HG22	5:S:77:ALA:HB3	1.99	0.44
4:D:113:LEU:HD12	5:E:78:PRO:HB2	1.99	0.44
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.99	0.44
9:W:120:ILE:HD12	9:W:136:ILE:HG12	1.99	0.44
12:L:24:ALA:HB1	12:L:202:LEU:HD11	1.98	0.44
1:O:42:GLY:HA3	1:O:185:LEU:HD13	1.99	0.44
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.99	0.44
10:J:173:PRO:HB3	10:X:22:THR:HG21	1.98	0.44
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.47	0.44
11:Y:158:LYS:HB2	11:Y:177:LEU:HD11	1.99	0.44
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.46	0.44
5:E:193:VAL:HG13	5:E:205:LEU:HD11	1.99	0.44
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.48	0.44
9:W:23:ALA:HB1	9:W:170:LEU:HD22	1.98	0.44
6:F:31:THR:HG23	6:F:47:GLU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:17:GLY:HA2	12:Z:174:TYR:HE1	1.82	0.44
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.53	0.44
7:G:7:ILE:HG13	7:G:9:ILE:HG12	2.00	0.44
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.46	0.44
9:I:120:ILE:HD12	9:I:136:ILE:HG12	1.99	0.44
5:S:193:VAL:HG13	5:S:205:LEU:HD11	1.99	0.44
11:Y:1:THR:N	15:Y:301:1G1:H5	2.33	0.44
12:Z:24:ALA:HB1	12:Z:202:LEU:HD11	2.00	0.44
1:A:42:GLY:HA3	1:A:185:LEU:HD13	2.00	0.43
6:F:197:TYR:HB3	6:F:243:ILE:HD12	2.00	0.43
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.99	0.43
9:I:28:LEU:HB3	9:I:36:SER:HB3	2.00	0.43
4:D:194:LYS:HB2	4:D:235:LEU:HD21	2.00	0.43
4:R:113:LEU:HD12	5:S:78:PRO:HB2	1.99	0.43
6:T:197:TYR:HB3	6:T:243:ILE:HD12	2.00	0.43
2:B:236:ASP:O	2:B:240:LYS:HG2	2.17	0.43
12:L:126:ASP:HB2	12:L:130:SER:HB3	1.99	0.43
12:Z:111:ILE:HG12	12:Z:125:PHE:HE1	1.83	0.43
6:F:123:ASN:HD22	6:F:124:SER:N	2.17	0.43
7:G:195:GLU:HG3	7:G:235:ARG:HG3	2.00	0.43
7:U:70:ILE:HD11	7:U:103:MET:O	2.18	0.43
9:I:52:ILE:HB	9:I:59:VAL:HG13	2.01	0.43
2:P:236:ASP:O	2:P:240:LYS:HG2	2.19	0.43
4:R:194:LYS:HB2	4:R:235:LEU:HD21	2.00	0.43
3:C:70:VAL:HG13	3:C:219:ILE:HD13	2.00	0.43
3:C:108:THR:HG21	3:C:146:TYR:HB3	2.01	0.43
4:D:77:ALA:O	4:D:81:ILE:HG12	2.18	0.43
7:U:7:ILE:HG13	7:U:9:ILE:HG12	2.01	0.43
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.49	0.43
1:A:30:GLN:HE21	1:A:30:GLN:HA	1.84	0.43
2:P:176:GLN:HG3	3:Q:52:LEU:HD13	2.01	0.43
5:S:131:LEU:HB2	5:S:146:PHE:HB3	2.01	0.42
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.54	0.42
4:D:20:LEU:HA	4:D:23:ILE:HD12	2.02	0.42
3:Q:70:VAL:HG13	3:Q:219:ILE:HD13	2.00	0.42
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.29	0.42
11:K:19:ARG:HH21	11:K:29:GLN:HE22	1.66	0.42
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.68	0.42
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.02	0.42
6:T:32:THR:HB	6:T:164:GLY:H	1.84	0.42
5:E:131:LEU:HB2	5:E:146:PHE:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:62:LEU:HD11	9:I:104:VAL:HG21	2.02	0.42
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.54	0.42
12:L:138:ALA:HB3	12:L:147:MET:HG2	2.02	0.41
9:W:35:VAL:HG13	16:X:222:HOH:O	2.19	0.41
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.02	0.41
4:D:83:HIS:CG	4:D:111:LEU:HD11	2.55	0.41
12:L:17:GLY:HA2	12:L:174:TYR:HE1	1.86	0.41
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.55	0.41
12:Z:161:GLU:HA	12:Z:162:PRO:HD3	1.93	0.41
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.02	0.41
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.21	0.41
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.02	0.41
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.55	0.41
12:Z:93:ILE:HA	12:Z:96:LEU:HD12	2.02	0.41
6:F:32:THR:HB	6:F:164:GLY:H	1.85	0.41
10:J:25:ILE:HG12	10:X:139:TYR:OH	2.21	0.41
11:K:1:THR:CG2	11:K:2:THR:N	2.83	0.41
1:O:30:GLN:HE21	1:O:30:GLN:HA	1.85	0.41
11:Y:35:ILE:HB	11:Y:45:MET:HE3	2.03	0.41
2:B:172:GLN:HG2	3:C:50:LEU:HD12	2.03	0.41
13:M:129:TYR:CE1	13:M:144:THR:HG22	2.56	0.41
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.02	0.41
10:J:172:MET:HA	10:J:173:PRO:HD3	1.85	0.41
13:M:48:ASN:HD22	13:M:48:ASN:N	2.11	0.41
4:R:83:HIS:CG	4:R:111:LEU:HD11	2.55	0.41
7:G:45:ILE:HG13	7:G:216:VAL:HG22	2.03	0.41
13:M:15:LYS:HB3	13:M:20:VAL:HG12	2.02	0.41
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.57	0.41
15:Y:301:1G1:H3	15:Y:301:1G1:H20	1.86	0.41
1:A:26:THR:O	1:A:30:GLN:HG2	2.21	0.40
4:R:159:TYR:CE2	4:R:162:LYS:HD3	2.56	0.40
8:V:1:THR:H1	15:V:301:1G1:H5	1.84	0.40
13:M:43:ILE:HG12	13:M:64:GLU:HG3	2.03	0.40
4:R:161:ALA:HB1	4:R:175:LEU:HD22	2.04	0.40
6:T:172:LEU:HD22	6:T:195:ILE:HD13	2.03	0.40
3:C:155:SER:HB2	4:D:51:LEU:HD21	2.03	0.40
5:E:99:ASN:HB2	13:M:94:GLU:HG2	2.02	0.40
7:G:19:VAL:HG21	7:G:120:THR:HG23	2.03	0.40
2:P:95:GLN:HE21	9:W:68:TYR:HA	1.87	0.40
4:D:211:LEU:HD12	4:D:228:THR:HG23	2.03	0.40
12:L:93:ILE:HA	12:L:96:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:20:LEU:HA	4:R:23:ILE:HD12	2.03	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%)	241 (97%)	6 (2%)	1 (0%)	34	60
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	34	60
2	B	242/258 (94%)	236 (98%)	5 (2%)	1 (0%)	34	60
2	P	242/258 (94%)	236 (98%)	5 (2%)	1 (0%)	34	60
3	C	239/254 (94%)	231 (97%)	6 (2%)	2 (1%)	19	43
3	Q	239/254 (94%)	232 (97%)	5 (2%)	2 (1%)	19	43
4	D	240/260 (92%)	235 (98%)	2 (1%)	3 (1%)	12	30
4	R	240/260 (92%)	235 (98%)	2 (1%)	3 (1%)	12	30
5	E	231/234 (99%)	224 (97%)	7 (3%)	0	100	100
5	S	231/234 (99%)	224 (97%)	7 (3%)	0	100	100
6	F	242/288 (84%)	233 (96%)	9 (4%)	0	100	100
6	T	242/288 (84%)	233 (96%)	9 (4%)	0	100	100
7	G	241/252 (96%)	234 (97%)	7 (3%)	0	100	100
7	U	241/252 (96%)	234 (97%)	7 (3%)	0	100	100
8	H	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
8	V	220/232 (95%)	212 (96%)	8 (4%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	196/198 (99%)	189 (96%)	6 (3%)	1 (0%)	29	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	X	196/198 (99%)	189 (96%)	6 (3%)	1 (0%)	29	54
11	K	210/212 (99%)	203 (97%)	6 (3%)	1 (0%)	29	54
11	Y	210/212 (99%)	200 (95%)	9 (4%)	1 (0%)	29	54
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/233 (99%)	221 (96%)	9 (4%)	1 (0%)	34	60
13	a	231/233 (99%)	222 (96%)	8 (4%)	1 (0%)	34	60
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6312/6588 (96%)	6111 (97%)	181 (3%)	20 (0%)	41	66

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
3	C	52	LEU
4	D	121	GLY
1	O	2	THR
3	Q	52	LEU
2	B	51	VAL
3	C	183	PRO
4	D	122	GLU
11	K	39	PRO
2	P	51	VAL
3	Q	183	PRO
11	Y	39	PRO
4	D	118	GLY
4	R	122	GLU
13	a	229	GLY
13	M	229	GLY
4	R	121	GLY
10	X	9	VAL
10	J	9	VAL
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%)	206 (99%)	3 (1%)	67	86
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	86
2	B	203/216 (94%)	196 (97%)	7 (3%)	37	66
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	66
3	C	213/226 (94%)	206 (97%)	7 (3%)	38	67
3	Q	213/226 (94%)	206 (97%)	7 (3%)	38	67
4	D	198/215 (92%)	194 (98%)	4 (2%)	55	81
4	R	198/215 (92%)	192 (97%)	6 (3%)	41	70
5	E	192/193 (100%)	186 (97%)	6 (3%)	40	69
5	S	192/193 (100%)	186 (97%)	6 (3%)	40	69
6	F	201/239 (84%)	192 (96%)	9 (4%)	27	55
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	55
7	G	207/210 (99%)	203 (98%)	4 (2%)	57	82
7	U	207/210 (99%)	203 (98%)	4 (2%)	57	82
8	H	181/190 (95%)	179 (99%)	2 (1%)	73	90
8	V	181/190 (95%)	179 (99%)	2 (1%)	73	90
9	I	172/173 (99%)	170 (99%)	2 (1%)	71	88
9	W	172/173 (99%)	170 (99%)	2 (1%)	71	88
10	J	175/175 (100%)	175 (100%)	0	100	100
10	X	175/175 (100%)	175 (100%)	0	100	100
11	K	169/169 (100%)	163 (96%)	6 (4%)	35	64
11	Y	169/169 (100%)	163 (96%)	6 (4%)	35	64
12	L	185/185 (100%)	183 (99%)	2 (1%)	73	90
12	Z	185/185 (100%)	183 (99%)	2 (1%)	73	90
13	M	199/199 (100%)	192 (96%)	7 (4%)	36	65
13	a	199/199 (100%)	192 (96%)	7 (4%)	36	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	161 (99%)	1 (1%)	86	95
14	b	162/162 (100%)	161 (99%)	1 (1%)	86	95
All	All	5332/5522 (97%)	5210 (98%)	122 (2%)	50	78

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	132	VAL
1	A	157	PHE
2	B	59	ASP
2	B	60	THR
2	B	119	GLN
2	B	184	LYS
2	B	186	ASP
2	B	191	LEU
2	B	212	PHE
3	C	4	ARG
3	C	51	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	171	GLU
3	C	206	LYS
4	D	102	GLU
4	D	124	ARG
4	D	176	LEU
4	D	190	LEU
5	E	9	THR
5	E	29	LYS
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	231	LYS
6	F	39	ASN
6	F	117	GLN
6	F	123	ASN
6	F	130	VAL
6	F	181	GLU
6	F	186	ARG
6	F	201	GLU

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Mol	Chain	Res	Type
6	F	203	ASN
6	F	214	TRP
7	G	117	GLN
7	G	166	GLN
7	G	221	LYS
7	G	235	ARG
8	H	34	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	87	VAL
11	K	100	MET
11	K	104	TYR
12	L	49	ASN
12	L	109	THR
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	146	PHE
13	M	159	VAL
13	M	161	ARG
13	M	226	LYS
14	N	119	VAL
1	O	30	GLN
1	O	132	VAL
1	O	157	PHE
2	P	59	ASP
2	P	60	THR
2	P	119	GLN
2	P	184	LYS
2	P	186	ASP
2	P	191	LEU
2	P	212	PHE
3	Q	4	ARG
3	Q	51	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	171	GLU

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Mol	Chain	Res	Type
3	Q	206	LYS
4	R	102	GLU
4	R	124	ARG
4	R	143	ASP
4	R	176	LEU
4	R	190	LEU
4	R	214	ILE
5	S	9	THR
5	S	29	LYS
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	231	LYS
6	T	39	ASN
6	T	117	GLN
6	T	123	ASN
6	T	130	VAL
6	T	181	GLU
6	T	186	ARG
6	T	201	GLU
6	T	203	ASN
6	T	214	TRP
7	U	117	GLN
7	U	166	GLN
7	U	221	LYS
7	U	235	ARG
8	V	34	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	87	VAL
11	Y	100	MET
11	Y	104	TYR
12	Z	49	ASN
12	Z	128	VAL
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	146	PHE

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Mol	Chain	Res	Type
13	a	159	VAL
13	a	161	ARG
13	a	226	LYS
14	b	119	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
2	B	20	GLN
2	B	69	ASN
2	B	95	GLN
2	B	119	GLN
2	B	123	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	241	GLN
4	D	15	GLN
4	D	210	GLN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
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
7	G	30	ASN
7	G	83	ASN

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Mol	Chain	Res	Type
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	175	ASN
7	G	186	ASN
8	H	22	GLN
8	H	30	ASN
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
10	J	55	GLN
10	J	118	GLN
10	J	147	HIS
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	165	ASN
12	L	195	HIS
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	171	GLN
13	M	179	ASN
13	M	213	GLN
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
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

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Mol	Chain	Res	Type
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	241	GLN
4	R	15	GLN
4	R	210	GLN
4	R	225	ASN
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
7	U	6	HIS
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	186	ASN
8	V	30	ASN
8	V	141	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
10	X	55	GLN
10	X	118	GLN
10	X	147	HIS
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN

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Mol	Chain	Res	Type
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	158	ASN
12	Z	165	ASN
12	Z	195	HIS
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	171	GLN
13	a	179	ASN
13	a	213	GLN
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	1G1	K	301	11	46,47,47	1.15	4 (8%)	59,63,63	1.50	5 (8%)
15	1G1	Y	301	11	46,47,47	1.17	3 (6%)	59,63,63	1.63	5 (8%)
15	1G1	H	301	8	46,47,47	1.20	4 (8%)	59,63,63	1.58	7 (11%)
15	1G1	V	301	8	46,47,47	1.27	4 (8%)	59,63,63	1.57	5 (8%)

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	1G1	K	301	11	-	15/51/51/51	0/2/2/2
15	1G1	Y	301	11	-	14/51/51/51	0/2/2/2
15	1G1	H	301	8	-	16/51/51/51	0/2/2/2
15	1G1	V	301	8	-	10/51/51/51	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	301	1G1	C46-C47	4.42	1.57	1.52
15	H	301	1G1	C46-C47	4.00	1.56	1.52
15	Y	301	1G1	C46-C47	3.57	1.56	1.52
15	K	301	1G1	C46-C47	3.51	1.56	1.52
15	V	301	1G1	C47-S48	3.05	1.82	1.78
15	Y	301	1G1	C46-C36	2.73	1.58	1.53
15	Y	301	1G1	C47-S48	2.57	1.81	1.78
15	H	301	1G1	C47-S48	2.52	1.81	1.78
15	V	301	1G1	C46-C36	2.39	1.58	1.53
15	K	301	1G1	C46-C36	2.28	1.57	1.53
15	K	301	1G1	C47-S48	2.27	1.81	1.78
15	H	301	1G1	C46-C36	2.24	1.57	1.53
15	K	301	1G1	C8-N9	-2.15	1.45	1.48
15	H	301	1G1	C8-N9	-2.11	1.45	1.48
15	V	301	1G1	C8-N9	-2.01	1.45	1.48

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	301	1G1	C8-N9-N10	9.34	125.06	115.24
15	V	301	1G1	C8-N9-N10	8.22	123.88	115.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	301	1G1	C8-N9-N10	8.19	123.85	115.24
15	H	301	1G1	C8-N9-N10	7.71	123.35	115.24
15	V	301	1G1	O49-S48-C47	4.72	111.65	108.34
15	H	301	1G1	C38-C37-C36	3.99	122.84	113.78
15	Y	301	1G1	O49-S48-C47	3.98	111.13	108.34
15	K	301	1G1	C38-C37-C36	3.35	121.39	113.78
15	K	301	1G1	C12-C8-N9	-3.19	101.26	108.85
15	H	301	1G1	C12-C8-N9	-3.08	101.52	108.85
15	H	301	1G1	C46-C36-C37	-3.00	106.25	111.14
15	Y	301	1G1	C7-C8-C12	2.70	115.28	109.55
15	V	301	1G1	C12-C8-N9	-2.64	102.58	108.85
15	Y	301	1G1	C12-C8-N9	-2.63	102.60	108.85
15	H	301	1G1	C37-C38-C43	-2.52	115.90	120.91
15	K	301	1G1	C46-C36-C37	-2.52	107.04	111.14
15	K	301	1G1	C37-C38-C43	-2.40	116.15	120.91
15	H	301	1G1	C7-C8-C12	2.38	114.60	109.55
15	V	301	1G1	O50-S48-C51	-2.19	106.70	108.91
15	H	301	1G1	C46-C36-N35	-2.14	107.53	110.54
15	Y	301	1G1	C37-C36-N35	2.11	114.45	110.39
15	V	301	1G1	C7-C8-C12	2.03	113.86	109.55

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	K	301	1G1	N11-N10-N9-C8
15	K	301	1G1	C46-C47-S48-O50
15	K	301	1G1	C46-C47-S48-O49
15	K	301	1G1	C46-C47-S48-C51
15	Y	301	1G1	N14-C12-C8-N9
15	Y	301	1G1	C46-C47-S48-O50
15	Y	301	1G1	C46-C47-S48-O49
15	Y	301	1G1	N35-C36-C46-C47
15	H	301	1G1	C46-C47-S48-O49
15	V	301	1G1	N11-N10-N9-C8
15	V	301	1G1	C46-C47-S48-O50
15	V	301	1G1	C46-C47-S48-O49
15	V	301	1G1	C46-C36-C37-C38
15	K	301	1G1	N14-C15-C16-C17
15	Y	301	1G1	C36-C46-C47-S48
15	V	301	1G1	C36-C46-C47-S48
15	Y	301	1G1	N14-C15-C16-C17

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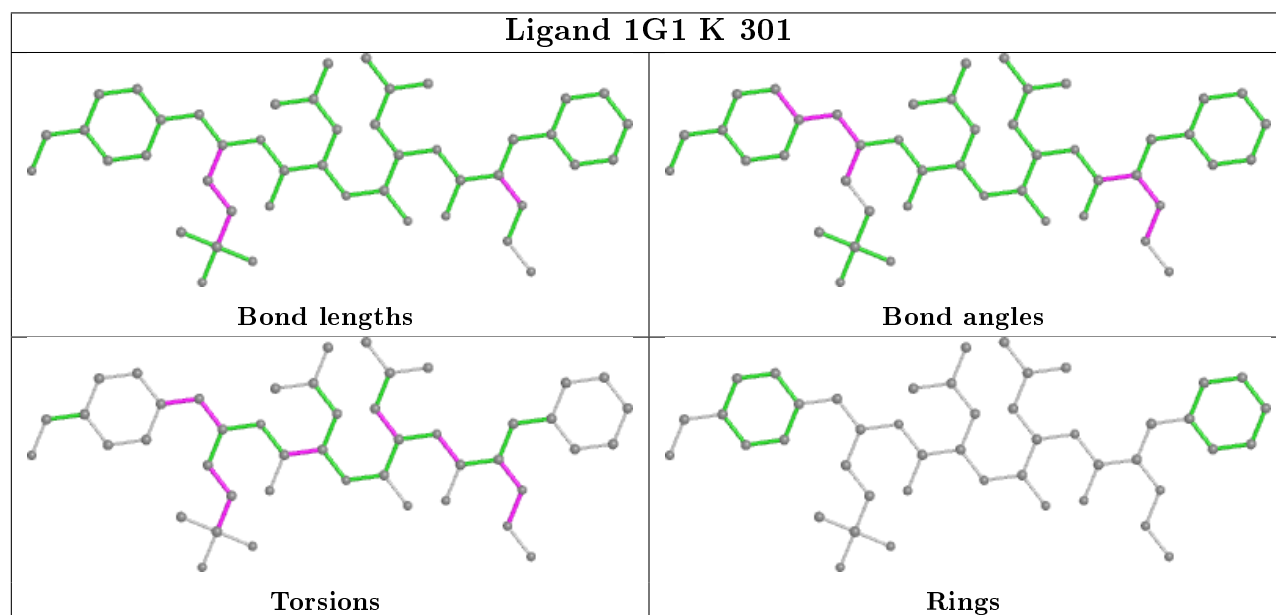
Mol	Chain	Res	Type	Atoms
15	K	301	1G1	C25-C15-C16-C17
15	Y	301	1G1	C25-C15-C16-C17
15	H	301	1G1	N14-C15-C16-C17
15	K	301	1G1	C36-C37-C38-C39
15	H	301	1G1	C25-C15-C16-C17
15	V	301	1G1	C36-C37-C38-C39
15	K	301	1G1	C36-C37-C38-C43
15	K	301	1G1	C46-C36-C37-C38
15	Y	301	1G1	C46-C36-C37-C38
15	K	301	1G1	C36-C46-C47-S48
15	H	301	1G1	C36-C46-C47-S48
15	V	301	1G1	C36-C37-C38-C43
15	H	301	1G1	C15-C16-C17-C19
15	V	301	1G1	N35-C36-C37-C38
15	H	301	1G1	N35-C36-C46-C47
15	H	301	1G1	C36-C37-C38-C39
15	H	301	1G1	C37-C36-C46-C47
15	H	301	1G1	C15-C16-C17-C18
15	H	301	1G1	C36-C37-C38-C43
15	K	301	1G1	N35-C36-C37-C38
15	Y	301	1G1	C36-C37-C38-C39
15	Y	301	1G1	C36-C37-C38-C43
15	Y	301	1G1	C37-C36-C46-C47
15	K	301	1G1	C12-C8-N9-N10
15	H	301	1G1	C46-C36-C37-C38
15	H	301	1G1	C46-C47-S48-O50
15	V	301	1G1	N35-C36-C46-C47
15	K	301	1G1	O13-C12-N14-C15
15	Y	301	1G1	N35-C36-C37-C38
15	K	301	1G1	N27-C28-C33-O34
15	H	301	1G1	C28-C29-C30-C31
15	H	301	1G1	N35-C36-C37-C38
15	K	301	1G1	N27-C28-C33-N35
15	Y	301	1G1	C42-C41-C44-N45
15	H	301	1G1	C28-C29-C30-C32
15	Y	301	1G1	C46-C47-S48-C51
15	H	301	1G1	C46-C47-S48-C51
15	V	301	1G1	C46-C47-S48-C51

There are no ring outliers.

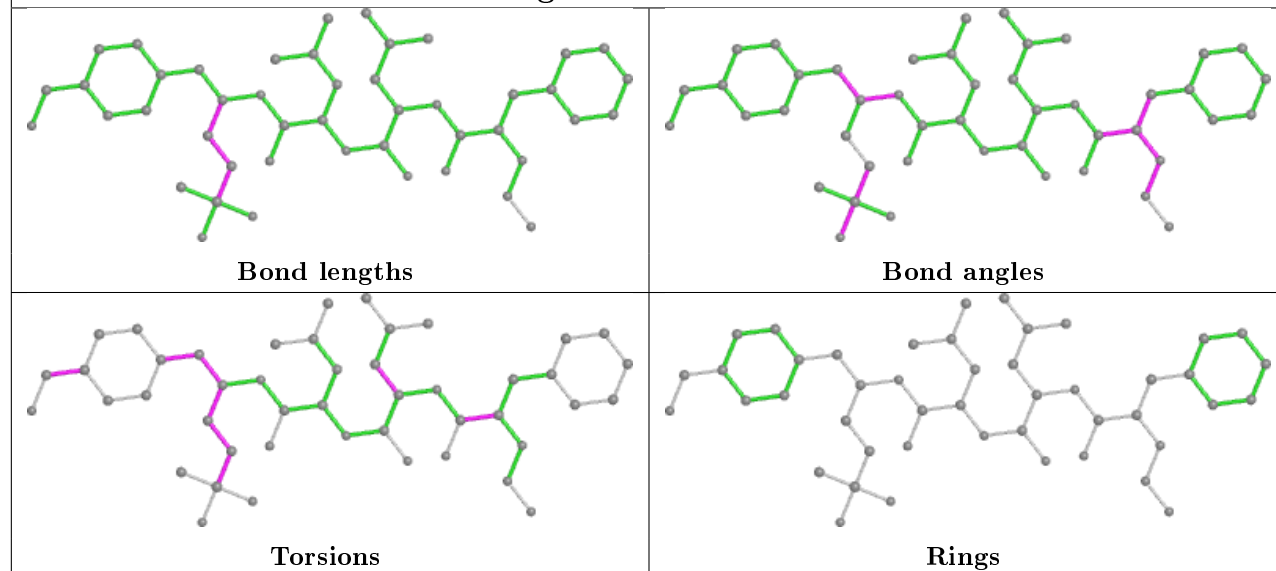
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	K	301	1G1	1	0
15	Y	301	1G1	6	0
15	H	301	1G1	1	0
15	V	301	1G1	4	0

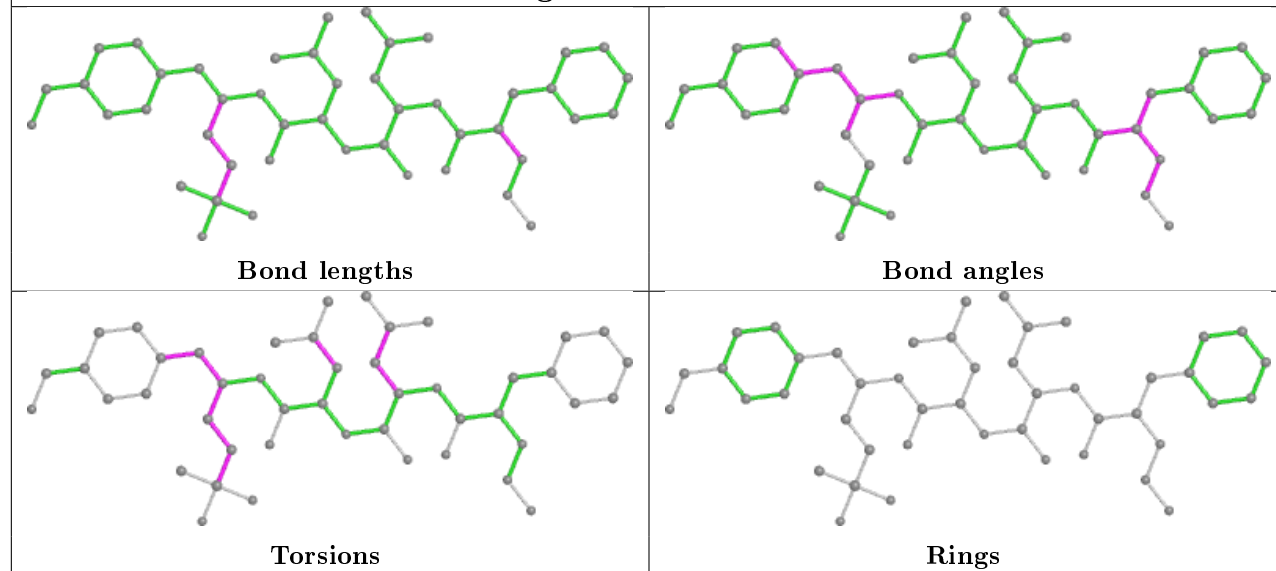
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

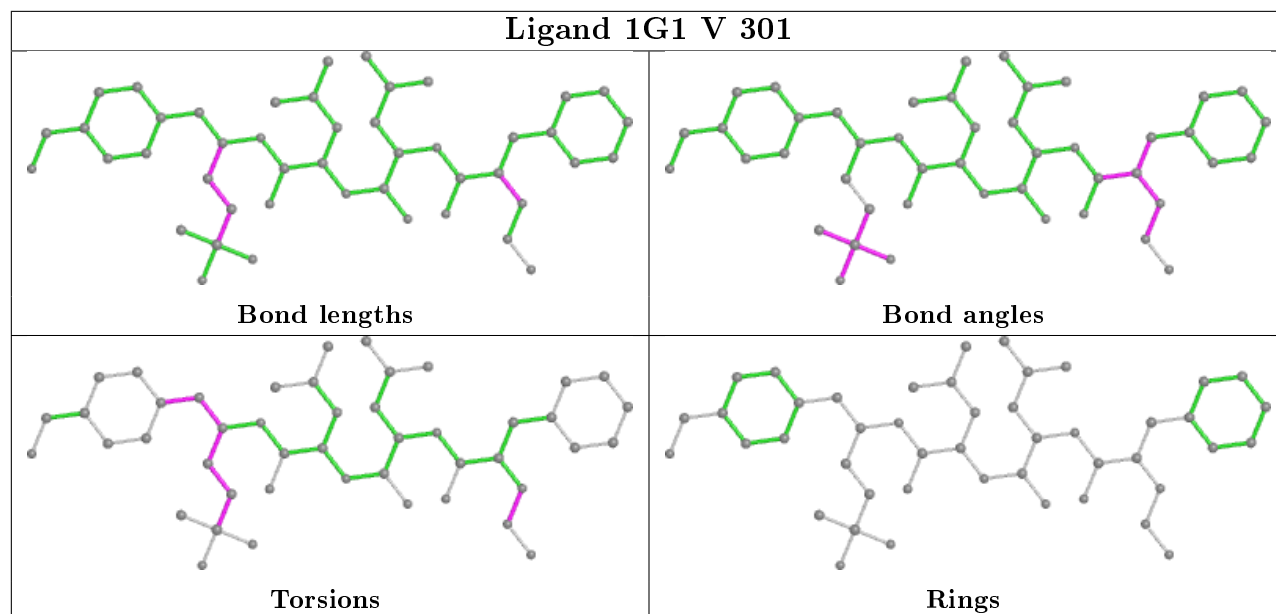


Ligand 1G1 Y 301



Ligand 1G1 H 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	0.13	7 (2%) 53 54	61, 76, 101, 119	0
1	O	250/250 (100%)	0.16	11 (4%) 34 33	63, 81, 106, 123	0
2	B	244/258 (94%)	0.44	22 (9%) 9 7	58, 80, 121, 136	0
2	P	244/258 (94%)	0.51	26 (10%) 6 4	62, 82, 117, 134	0
3	C	241/254 (94%)	0.43	28 (11%) 4 3	59, 82, 123, 156	0
3	Q	241/254 (94%)	0.75	41 (17%) 1 1	68, 97, 148, 191	0
4	D	242/260 (93%)	0.29	15 (6%) 20 19	61, 82, 108, 127	0
4	R	242/260 (93%)	0.45	21 (8%) 10 8	65, 89, 120, 138	0
5	E	233/234 (99%)	0.35	19 (8%) 11 9	66, 90, 117, 125	0
5	S	233/234 (99%)	0.46	25 (10%) 6 4	68, 94, 125, 135	0
6	F	244/288 (84%)	0.19	17 (6%) 16 14	63, 81, 113, 137	0
6	T	244/288 (84%)	0.20	18 (7%) 14 12	63, 82, 118, 140	0
7	G	243/252 (96%)	0.09	11 (4%) 33 31	60, 76, 99, 129	0
7	U	243/252 (96%)	0.14	11 (4%) 33 31	61, 75, 97, 129	0
8	H	222/232 (95%)	0.07	3 (1%) 75 77	59, 70, 86, 104	0
8	V	222/232 (95%)	0.05	4 (1%) 68 70	58, 69, 86, 109	0
9	I	204/205 (99%)	-0.19	2 (0%) 82 83	55, 67, 81, 88	0
9	W	204/205 (99%)	-0.09	5 (2%) 57 59	58, 67, 84, 94	0
10	J	198/198 (100%)	0.11	9 (4%) 33 31	54, 67, 87, 123	0
10	X	198/198 (100%)	0.12	10 (5%) 28 26	58, 68, 84, 124	0
11	K	212/212 (100%)	0.13	11 (5%) 27 25	54, 68, 89, 95	0
11	Y	212/212 (100%)	0.11	11 (5%) 27 25	57, 70, 92, 100	0
12	L	222/222 (100%)	-0.08	6 (2%) 54 55	55, 68, 96, 104	0
12	Z	222/222 (100%)	-0.01	8 (3%) 42 42	56, 70, 96, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/233 (100%)	-0.10	7 (3%) 50 51	53, 69, 86, 101	0
13	a	233/233 (100%)	-0.08	4 (1%) 70 72	55, 68, 82, 96	0
14	N	196/196 (100%)	-0.13	5 (2%) 56 57	57, 65, 82, 89	0
14	b	196/196 (100%)	-0.14	4 (2%) 65 67	55, 64, 82, 89	0
All	All	6368/6588 (96%)	0.17	361 (5%) 23 22	53, 74, 113, 191	0

All (361) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	J	197	ALA	10.0
10	X	198	GLN	9.7
2	P	220	ASN	9.7
4	R	119	ALA	9.6
4	D	120	SER	9.6
2	P	219	ALA	9.5
7	U	243	ASP	9.2
4	D	119	ALA	9.1
10	X	197	ALA	9.0
10	J	198	GLN	8.9
4	R	120	SER	8.9
7	G	1	ALA	8.8
2	P	51	VAL	8.6
3	C	49	THR	8.5
2	B	220	ASN	8.3
8	V	222	ASP	8.1
7	U	1	ALA	8.0
3	Q	240	GLU	7.9
2	B	219	ALA	7.8
4	D	118	GLY	7.7
3	Q	241	GLN	7.6
6	F	1	GLY	7.5
3	Q	49	THR	7.5
3	C	50	LEU	7.5
11	Y	104	TYR	7.4
3	Q	50	LEU	7.4
9	W	1	SER	7.4
4	D	121	GLY	7.2
4	R	121	GLY	7.2
2	B	51	VAL	7.0
8	H	222	ASP	7.0
3	Q	48	SER	6.8

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Mol	Chain	Res	Type	RSRZ
7	G	243	ASP	6.8
4	R	125	LEU	6.7
5	E	202	ASP	6.7
2	B	221	ASP	6.6
11	K	104	TYR	6.5
2	B	218	GLY	6.5
1	A	1	MET	6.3
8	V	221	CYS	6.2
3	Q	203	THR	6.2
2	P	221	ASP	6.1
11	Y	212	GLY	6.0
3	Q	205	ALA	6.0
3	Q	58	THR	5.9
5	E	1	PHE	5.9
8	H	221	CYS	5.9
5	S	1	PHE	5.9
4	R	124	ARG	5.8
1	A	250	LEU	5.7
3	C	241	GLN	5.7
2	P	225	TYR	5.7
13	M	233	ILE	5.7
4	R	118	GLY	5.6
4	R	1	ASP	5.5
5	S	2	ARG	5.4
9	I	1	SER	5.3
1	O	250	LEU	5.3
5	S	173	ARG	5.3
1	O	2	THR	5.2
5	S	52	ALA	5.1
1	O	249	ALA	5.1
4	D	122	GLU	5.1
5	S	54	GLU	5.1
2	P	218	GLY	5.0
5	E	2	ARG	5.0
12	L	173	LYS	4.9
10	J	1	MET	4.9
12	L	174	TYR	4.9
3	Q	239	GLN	4.9
2	B	50	LYS	4.8
5	S	202	ASP	4.8
1	A	2	THR	4.8
6	F	202	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
7	G	242	GLN	4.8
13	a	233	ILE	4.6
11	K	182	GLU	4.6
10	X	1	MET	4.6
2	P	59	ASP	4.5
2	B	240	LYS	4.5
4	D	124	ARG	4.5
2	P	60	THR	4.5
4	R	122	GLU	4.4
3	Q	52	LEU	4.4
12	Z	174	TYR	4.4
3	Q	59	PRO	4.4
10	X	194	ASP	4.4
3	Q	175	LYS	4.4
3	Q	202	GLN	4.4
11	K	212	GLY	4.4
5	E	233	ILE	4.3
2	P	223	GLU	4.3
3	C	203	THR	4.3
7	U	242	GLN	4.3
4	D	125	LEU	4.2
2	P	61	SER	4.2
1	O	1	MET	4.2
6	F	244	ASN	4.2
1	A	201	GLU	4.1
2	B	223	GLU	4.0
5	E	3	ASN	4.0
2	B	60	THR	4.0
2	P	50	LYS	4.0
11	K	209	ASN	4.0
5	S	201	ARG	3.9
12	L	163	GLY	3.9
13	M	1	THR	3.9
11	K	183	ASP	3.9
4	D	123	GLU	3.9
6	T	1	GLY	3.9
11	K	40	PHE	3.9
4	D	1	ASP	3.8
6	T	244	ASN	3.8
2	B	61	SER	3.8
3	Q	206	LYS	3.8
3	Q	237	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
6	T	53	LYS	3.8
4	R	2	ARG	3.7
5	S	58	TYR	3.7
5	E	30	GLN	3.7
3	C	240	GLU	3.7
3	Q	51	LYS	3.7
5	S	3	ASN	3.6
3	Q	187	GLU	3.6
4	R	230	GLU	3.6
12	Z	173	LYS	3.6
1	A	248	GLU	3.6
12	L	1	GLN	3.6
8	H	198	GLU	3.6
2	B	217	LYS	3.5
11	Y	182	GLU	3.5
6	F	205	GLU	3.5
4	R	239	GLU	3.5
6	F	241	LYS	3.5
11	K	208	ASN	3.5
5	E	203	GLU	3.4
2	B	244	THR	3.4
5	S	187	GLU	3.4
3	Q	236	GLN	3.4
11	Y	40	PHE	3.4
2	P	203	SER	3.4
3	C	181	GLU	3.4
3	Q	235	GLU	3.3
6	T	2	THR	3.3
10	X	196	GLN	3.3
2	P	52	THR	3.3
5	S	194	GLU	3.3
3	C	202	GLN	3.3
4	D	2	ARG	3.3
10	J	196	GLN	3.3
6	F	181	GLU	3.3
1	A	249	ALA	3.2
13	a	1	THR	3.2
3	C	48	SER	3.2
5	S	180	LYS	3.2
7	U	188	GLU	3.2
5	S	29	LYS	3.2
3	C	206	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	225	TYR	3.1
6	F	243	ILE	3.1
2	B	242	GLY	3.1
6	F	229	GLY	3.1
3	Q	60	SER	3.1
5	S	200	LEU	3.1
3	Q	204	GLY	3.1
13	a	232	LYS	3.1
3	C	175	LYS	3.1
5	S	227	GLU	3.1
3	C	51	LYS	3.0
3	Q	234	ILE	3.0
13	M	232	LYS	3.0
9	W	192	ASP	3.0
11	Y	209	ASN	3.0
10	X	95	ARG	3.0
3	C	141	ASP	3.0
6	T	177	ASP	3.0
4	R	241	ALA	3.0
5	S	51	ASN	3.0
7	G	222	ASP	3.0
2	P	243	ILE	3.0
2	P	19	TYR	3.0
3	Q	167	LYS	3.0
3	C	235	GLU	3.0
6	F	2	THR	3.0
2	P	222	GLY	2.9
3	Q	1	GLY	2.9
10	J	174	MET	2.9
3	C	167	LYS	2.9
6	F	53	LYS	2.9
13	M	47	ASP	2.9
6	F	182	GLY	2.9
6	T	228	LYS	2.9
10	J	139	TYR	2.9
2	B	235	LYS	2.9
2	P	241	THR	2.9
3	Q	55	THR	2.9
3	C	225	GLU	2.9
11	Y	147	ASP	2.9
10	X	139	TYR	2.9
11	Y	106	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
7	G	5	ARG	2.8
11	Y	208	ASN	2.8
10	J	193	ASP	2.8
5	E	54	GLU	2.8
5	E	201	ARG	2.8
2	B	58	GLN	2.8
2	B	180	LYS	2.8
6	F	204	LYS	2.8
14	N	105	LYS	2.8
3	Q	141	ASP	2.7
1	O	248	GLU	2.7
9	I	131	GLU	2.7
6	F	193	ALA	2.7
5	S	57	SER	2.7
2	P	184	LYS	2.7
14	b	107	LYS	2.7
5	E	165	GLN	2.7
2	P	242	GLY	2.7
6	T	205	GLU	2.7
3	Q	53	GLN	2.7
2	P	217	LYS	2.7
7	U	178	LYS	2.7
5	E	218	ASP	2.7
10	J	95	ARG	2.7
3	Q	216	ASP	2.7
5	E	207	VAL	2.7
11	K	106	ARG	2.7
2	P	180	LYS	2.7
6	T	230	ASP	2.7
10	J	194	ASP	2.7
3	C	59	PRO	2.6
5	E	173	ARG	2.6
6	T	206	LYS	2.6
7	G	181	LYS	2.6
3	C	239	GLN	2.6
4	D	242	GLU	2.6
4	R	117	GLU	2.6
6	T	181	GLU	2.6
5	E	210	LEU	2.6
4	R	242	GLU	2.6
1	O	201	GLU	2.6
2	P	182	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
5	S	233	ILE	2.5
6	T	229	GLY	2.5
2	B	203	SER	2.5
3	C	46	ARG	2.5
2	B	62	THR	2.5
3	Q	238	LYS	2.5
3	Q	225	GLU	2.5
4	R	240	ALA	2.5
7	U	219	ALA	2.5
3	C	139	ARG	2.5
3	Q	47	ARG	2.5
3	C	187	GLU	2.5
14	b	195	GLN	2.5
12	Z	163	GLY	2.4
2	P	113	ARG	2.4
3	Q	181	GLU	2.4
7	U	2	GLY	2.4
3	Q	39	CYS	2.4
6	T	217	LEU	2.4
4	R	157	TYR	2.4
3	Q	223	SER	2.4
11	K	147	ASP	2.4
1	O	4	ARG	2.4
12	Z	165	ASN	2.4
1	A	231	LYS	2.4
3	Q	26	LYS	2.4
5	E	194	GLU	2.4
12	Z	210	ASP	2.4
4	D	201	GLU	2.4
9	W	160	GLU	2.4
1	O	53	SER	2.3
2	P	235	LYS	2.3
3	C	27	ARG	2.3
6	T	166	GLN	2.3
2	B	59	ASP	2.3
5	E	227	GLU	2.3
3	Q	139	ARG	2.3
5	S	50	ARG	2.3
6	T	215	CYS	2.3
7	G	153	TYR	2.3
4	R	233	LYS	2.3
5	S	209	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
11	K	211	ILE	2.3
11	Y	151	GLU	2.3
7	U	222	ASP	2.3
4	D	238	LYS	2.3
6	T	204	LYS	2.3
10	X	174	MET	2.3
13	M	216	ASN	2.3
2	B	182	ASP	2.3
14	N	195	GLN	2.3
6	T	201	GLU	2.3
3	Q	56	ARG	2.3
11	Y	183	ASP	2.3
4	D	217	GLN	2.2
3	C	142	GLU	2.2
13	M	204	THR	2.2
14	b	105	LYS	2.2
4	R	169	GLU	2.2
9	W	191	LYS	2.2
5	E	122	TYR	2.2
4	R	201	GLU	2.2
6	T	243	ILE	2.2
11	Y	211	ILE	2.2
2	P	240	LYS	2.2
7	G	179	LYS	2.2
1	O	61	LEU	2.2
5	S	55	LEU	2.2
3	Q	221	ALA	2.2
2	B	222	GLY	2.2
10	X	151	ASP	2.2
5	E	180	LYS	2.2
6	T	202	ASP	2.2
14	N	104	ASP	2.2
6	F	203	ASN	2.1
12	Z	80	ASN	2.1
3	C	180	LYS	2.1
7	U	179	LYS	2.1
14	N	9	LYS	2.1
6	F	201	GLU	2.1
11	K	72	GLU	2.1
3	C	236	GLN	2.1
14	N	149	GLU	2.1
12	Z	1	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	52	SER	2.1
5	S	163	ARG	2.1
3	C	60	SER	2.1
5	S	217	LYS	2.1
4	R	123	GLU	2.1
7	G	208	GLU	2.1
2	P	230	LYS	2.1
9	W	133	LYS	2.1
12	L	80	ASN	2.1
6	F	207	ASP	2.1
3	Q	171	GLU	2.1
5	E	187	GLU	2.1
3	Q	44	CYS	2.1
7	U	124	TYR	2.1
10	X	193	ASP	2.1
13	a	47	ASP	2.1
5	S	59	GLN	2.1
3	C	165	ASN	2.1
3	C	1	GLY	2.1
14	b	104	ASP	2.1
6	F	180	PRO	2.0
8	V	215	GLU	2.0
12	L	165	ASN	2.0
3	Q	46	ARG	2.0
7	G	188	GLU	2.0
1	O	230	ASP	2.0
4	D	142	ASP	2.0
8	V	145	ASP	2.0
12	Z	167	LYS	2.0
13	M	46	GLY	2.0
5	S	165	GLN	2.0
7	U	58	THR	2.0
3	C	171	GLU	2.0
7	G	241	GLU	2.0
4	R	203	LYS	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

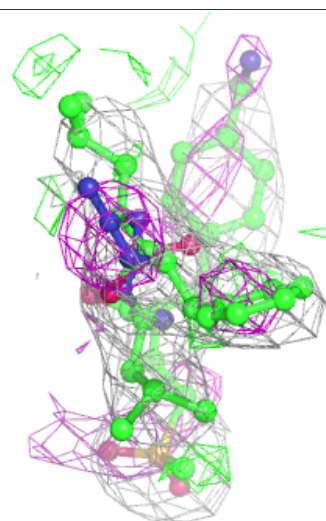
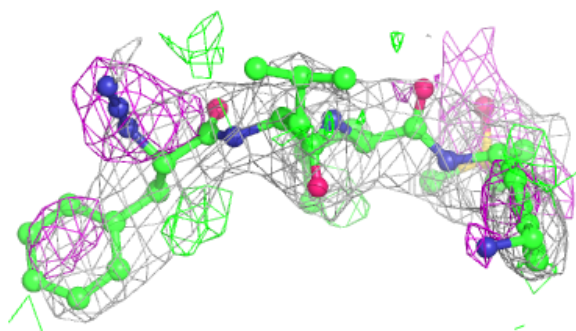
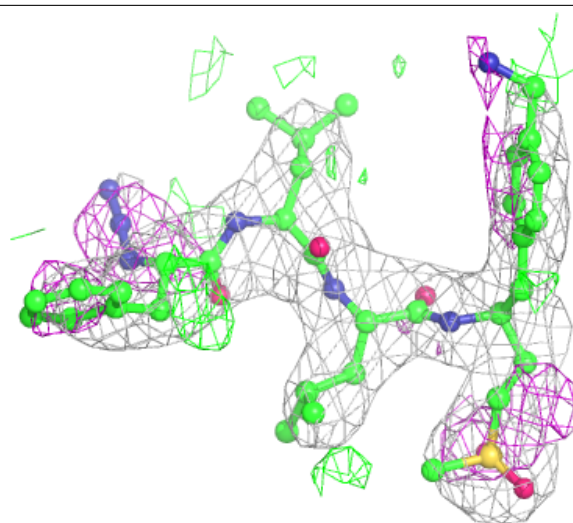
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	1G1	H	301	46/46	0.83	0.29	65,70,83,83	0
15	1G1	V	301	46/46	0.85	0.30	65,72,84,84	0
15	1G1	K	301	46/46	0.87	0.24	52,56,69,70	0
15	1G1	Y	301	46/46	0.87	0.26	55,58,65,65	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.

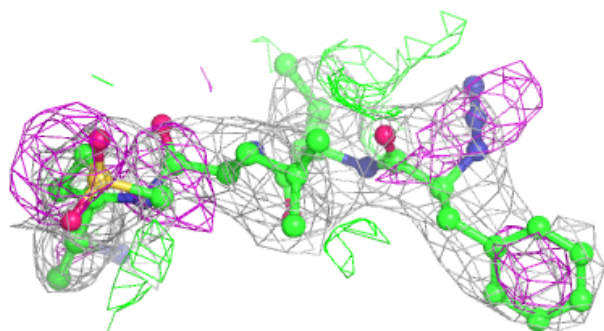
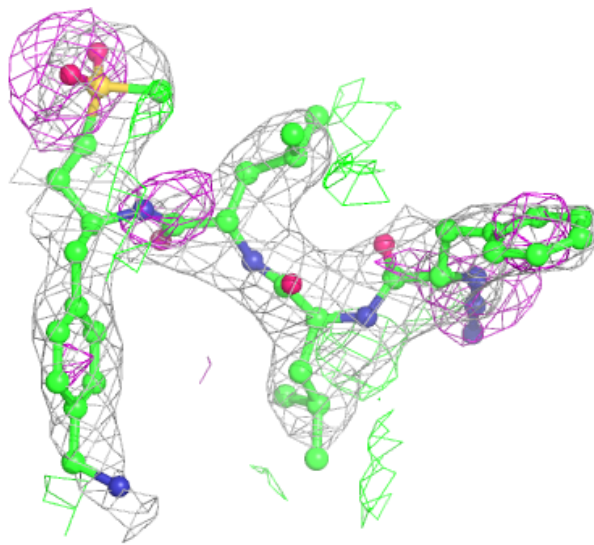
Electron density around 1G1 H 301:

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



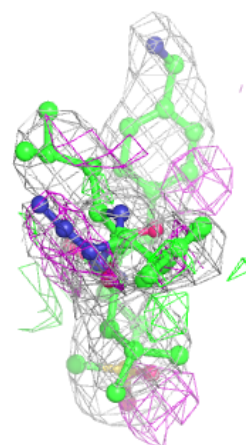
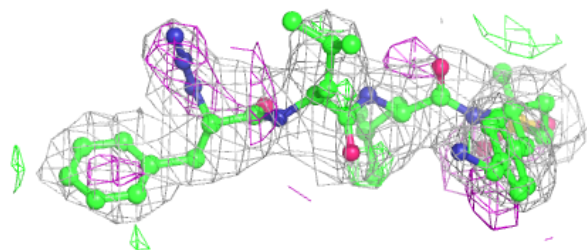
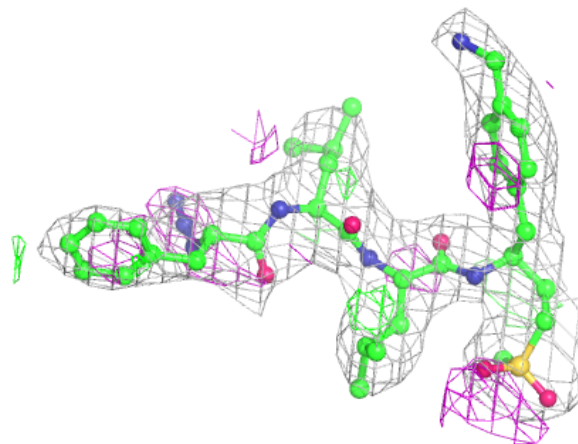
Electron density around 1G1 V 301:

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



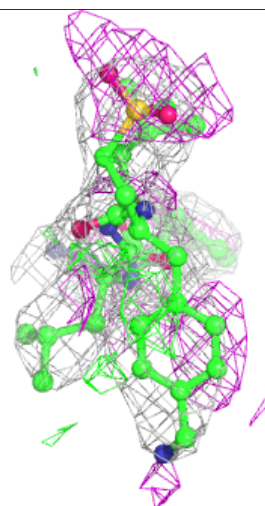
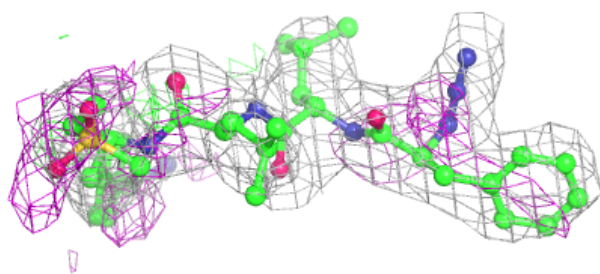
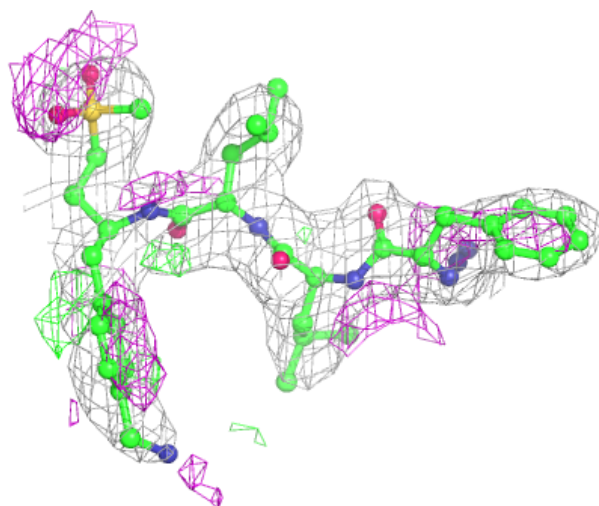
Electron density around 1G1 K 301:

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



Electron density around 1G1 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 [i](#)

There are no such residues in this entry.