Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2024 – 02:17 pm GMT

PDB ID	:	6HW4
Title	:	Yeast 20S proteasome in complex with 16
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2018-10-11
Resolution	:	2.90 Å(reported)

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

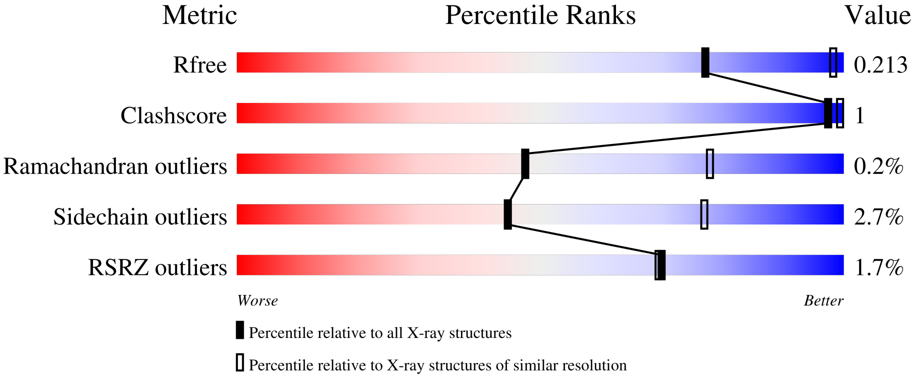
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

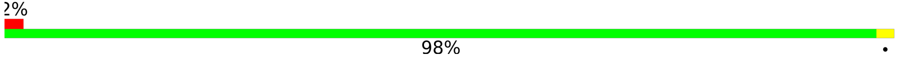
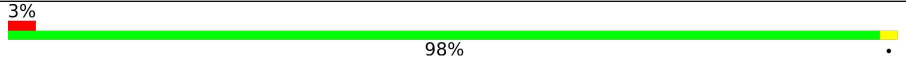
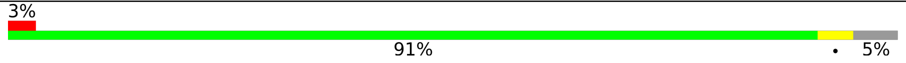
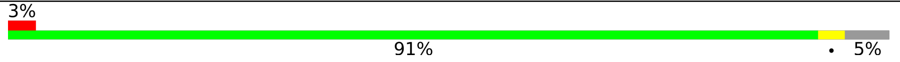
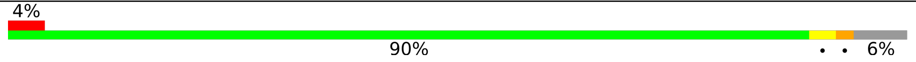
The reported resolution of this entry is 2.90 Å.

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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	250	
1	O	250	
2	B	258	
2	P	258	
3	C	254	

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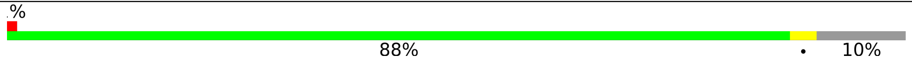
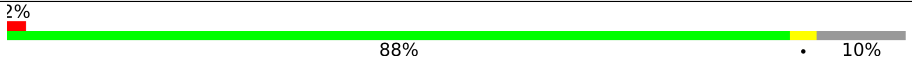
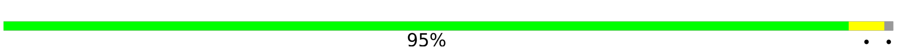
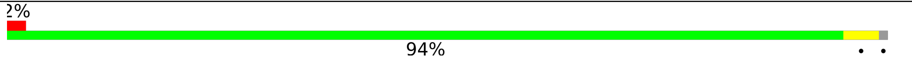
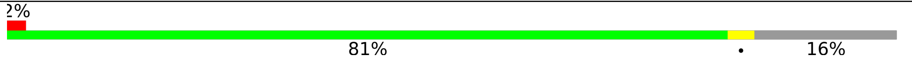
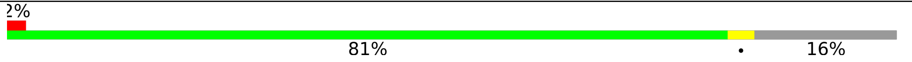
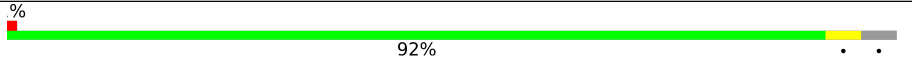
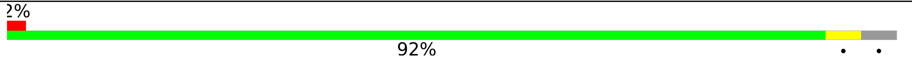
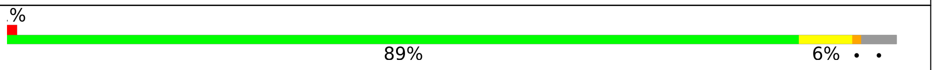
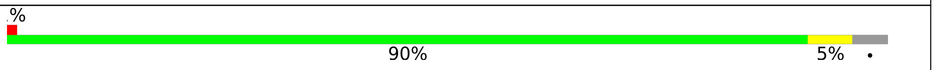
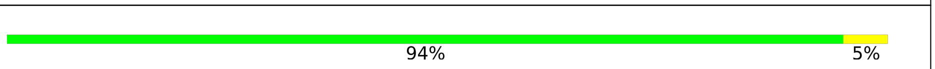
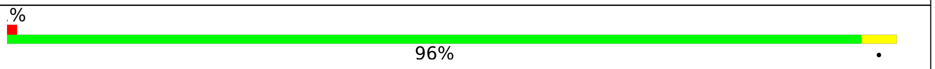
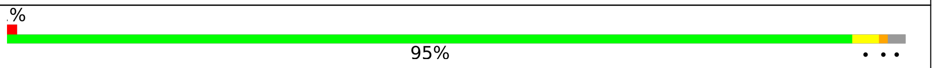
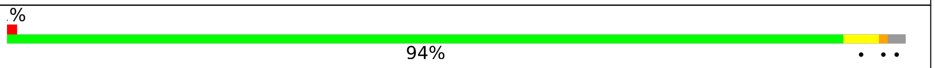
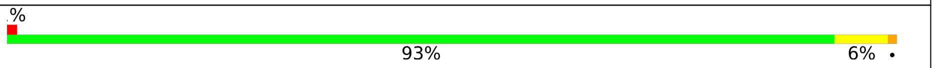
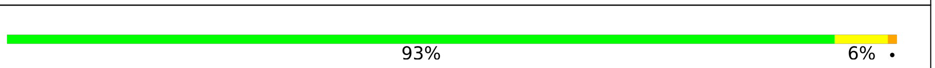
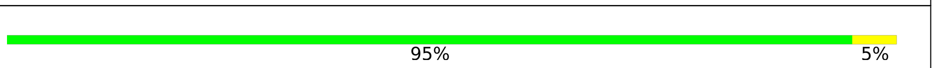
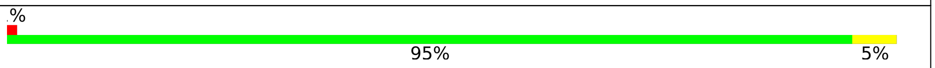
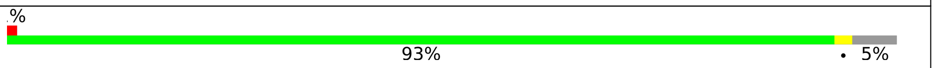
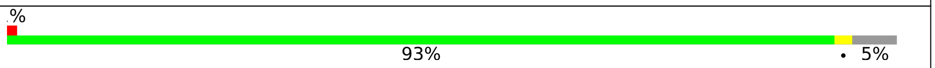
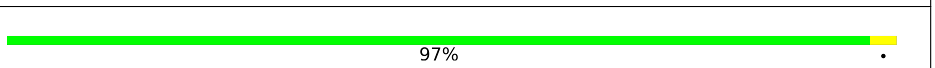
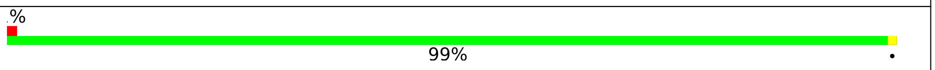
Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

2 Entry composition ⓘ

There are 18 unique types of molecules in this entry. The entry contains 49789 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total 1881	C 1176	N 329	O 372	S 4	0	0	0
3	Q	240	Total 1881	C 1176	N 329	O 372	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total 1813	C 1136	N 304	O 366	S 7	0	0	0
4	R	235	Total 1813	C 1136	N 304	O 366	S 7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	231	1773	1114	307	348	4	0	0	0
5	S	231	1773	1114	307	348	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	243	1892	1203	329	356	4	0	0	0
6	T	243	1892	1203	329	356	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	241	1907	1214	320	365	8	0	0	0
7	U	241	1907	1214	320	365	8	0	0	0

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

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

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

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

- Molecule 10 is a protein called Proteasome subunit beta type-4.

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

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

- Molecule 11 is a protein called PROTEASOME SUBUNIT BETA TYPE-5.

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

- Molecule 12 is a protein called Proteasome subunit beta type-6.

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

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

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

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

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0

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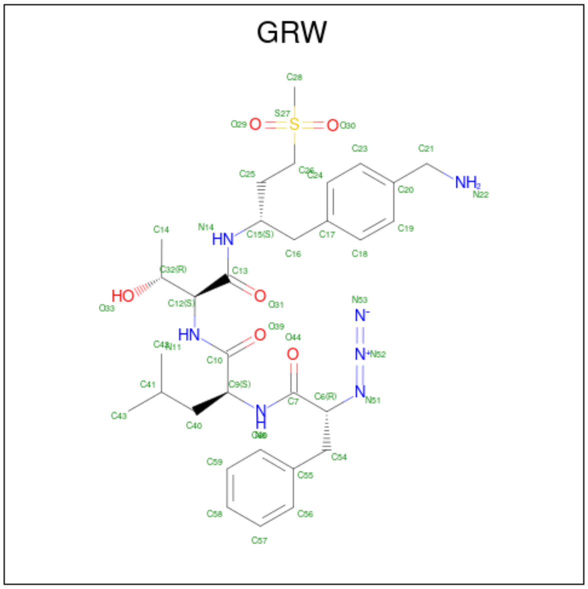
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	X	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is (2 {S})- {N}-[(2 {S},3 {R})-1-[[(2 {S})-1-[4-(aminomethyl)phenyl]-4-methylsulfonyl-butan-2-yl]amino]-3-oxidanyl-1-oxidanylidene-butan-2-yl]-2-[[(2 {R})-2-azido-3-phenyl-propanoyl]amino]-4-methyl-pentanamide (three-letter code: GRW) (formula: $C_{31}H_{45}N_7O_6S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	1	Total C N O S 45 31 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	K	1	Total C N O S 45 31 7 6 1	0	0
17	V	1	Total C N O S 45 31 7 6 1	0	0
17	Y	1	Total C N O S 45 31 7 6 1	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	17	Total O 17 17	0	0
18	B	17	Total O 17 17	0	0
18	C	14	Total O 14 14	0	0
18	D	6	Total O 6 6	0	0
18	E	8	Total O 8 8	0	0
18	F	15	Total O 15 15	0	0
18	G	14	Total O 14 14	0	0
18	H	12	Total O 12 12	0	0
18	I	4	Total O 4 4	0	0
18	J	12	Total O 12 12	0	0
18	K	13	Total O 13 13	0	0
18	L	9	Total O 9 9	0	0
18	M	8	Total O 8 8	0	0
18	N	11	Total O 11 11	0	0
18	O	8	Total O 8 8	0	0
18	P	7	Total O 7 7	0	0

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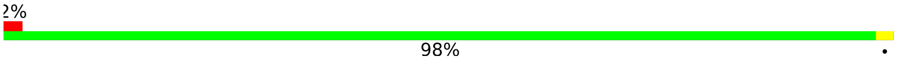
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	Q	9	Total O 9 9	0	0
18	R	7	Total O 7 7	0	0
18	S	8	Total O 8 8	0	0
18	T	10	Total O 10 10	0	0
18	U	18	Total O 18 18	0	0
18	V	9	Total O 9 9	0	0
18	W	4	Total O 4 4	0	0
18	X	14	Total O 14 14	0	0
18	Y	16	Total O 16 16	0	0
18	Z	11	Total O 11 11	0	0
18	a	13	Total O 13 13	0	0
18	b	9	Total O 9 9	0	0

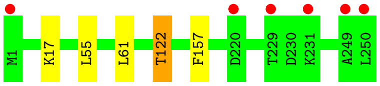
3 Residue-property plots ⓘ

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 subunit alpha type-2

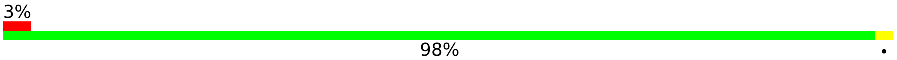
Chain A:

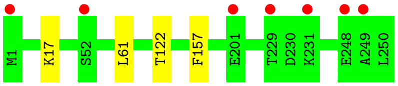




- Molecule 1: Proteasome subunit alpha type-2

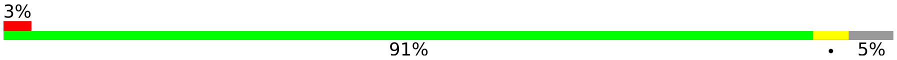
Chain O:

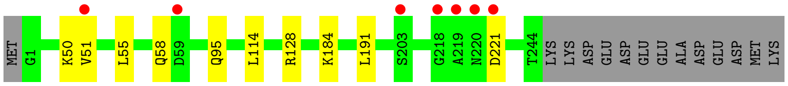




- Molecule 2: Proteasome subunit alpha type-3

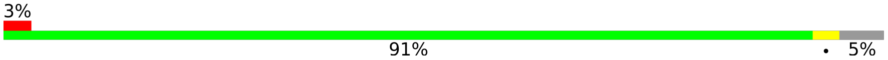
Chain B:

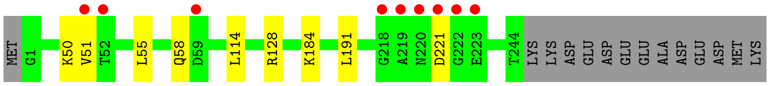




- Molecule 2: Proteasome subunit alpha type-3

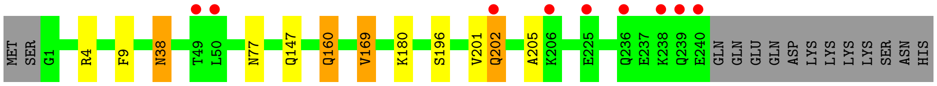
Chain P:





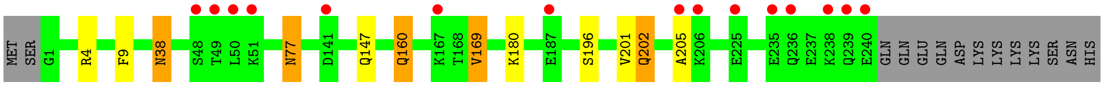
- Molecule 3: Proteasome subunit alpha type-4

Chain C:



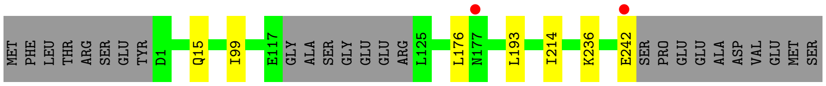
- Molecule 3: Proteasome subunit alpha type-4

Chain Q:



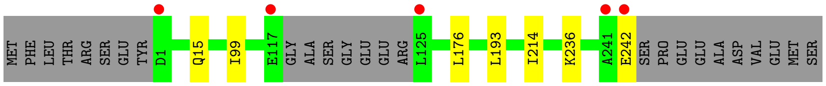
- Molecule 4: Proteasome subunit alpha type-5

Chain D:



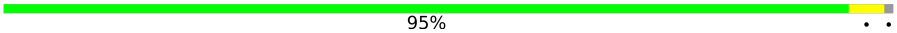
- Molecule 4: Proteasome subunit alpha type-5

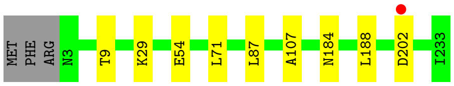
Chain R:



- Molecule 5: Proteasome subunit alpha type-6

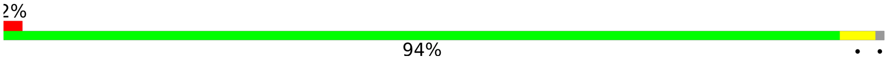
Chain E:

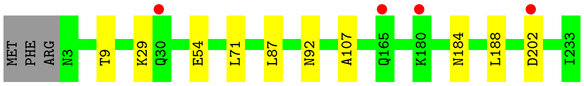




- Molecule 5: Proteasome subunit alpha type-6

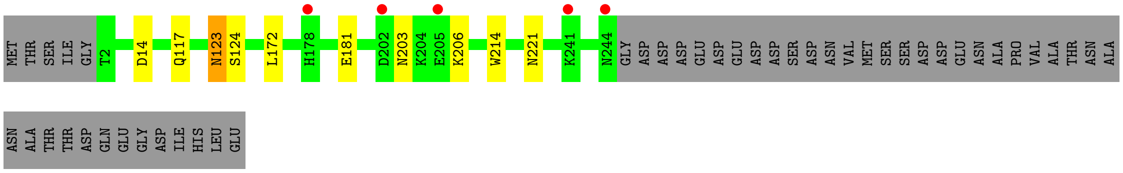
Chain S:





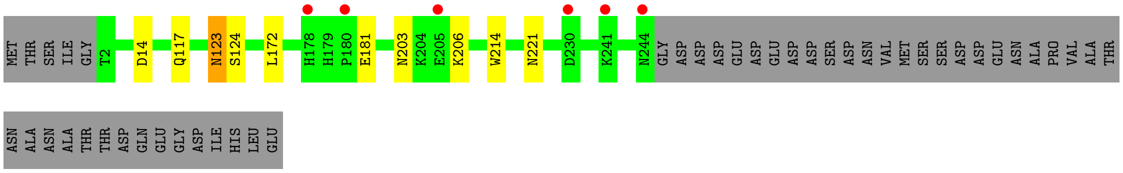
- Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



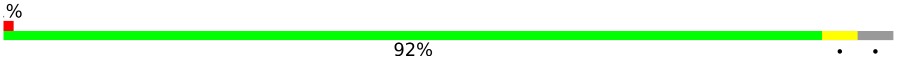
- Molecule 6: Probable proteasome subunit alpha type-7

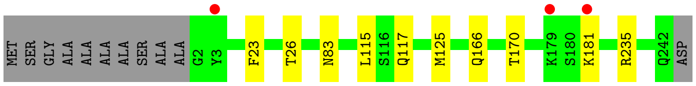
Chain T:



- Molecule 7: Proteasome subunit alpha type-1

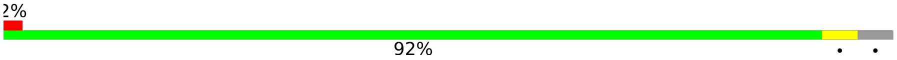
Chain G:

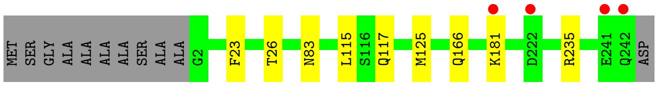




- Molecule 7: Proteasome subunit alpha type-1

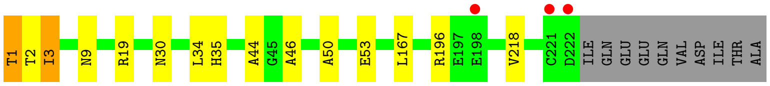
Chain U:





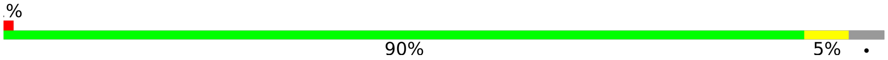
- Molecule 8: Proteasome subunit beta type-2

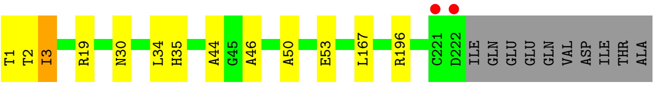
Chain H:



- Molecule 8: Proteasome subunit beta type-2

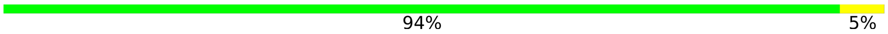
Chain V:

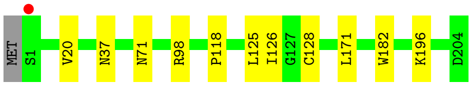




- Molecule 9: Proteasome subunit beta type-3

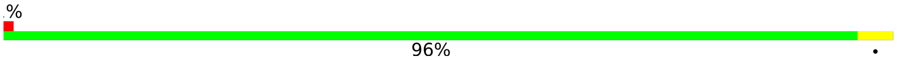
Chain I:

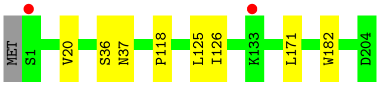




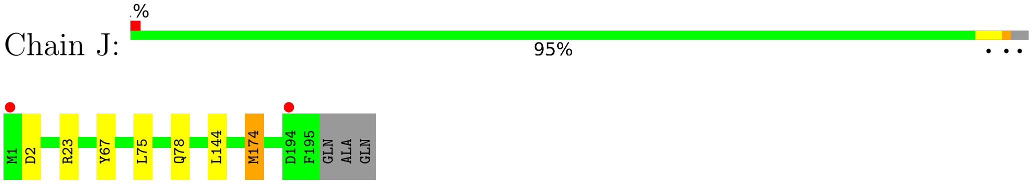
- Molecule 9: Proteasome subunit beta type-3

Chain W:

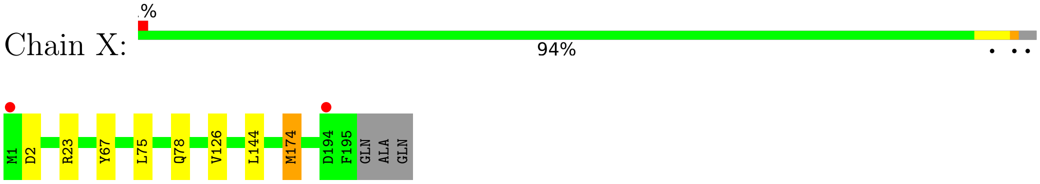




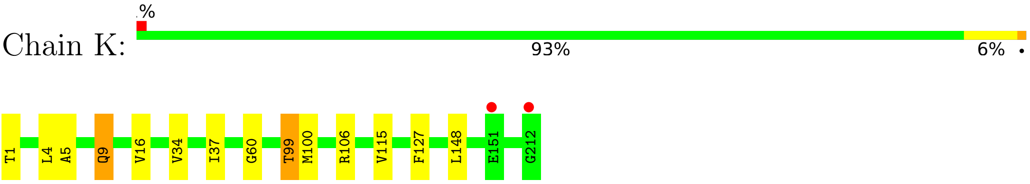
- Molecule 10: Proteasome subunit beta type-4



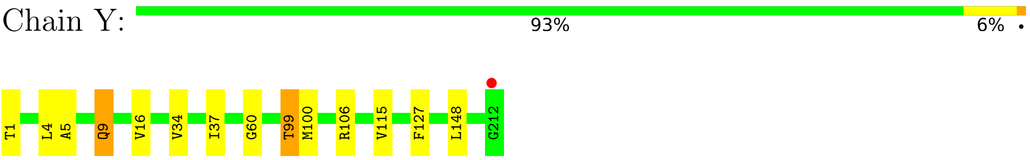
- Molecule 10: Proteasome subunit beta type-4



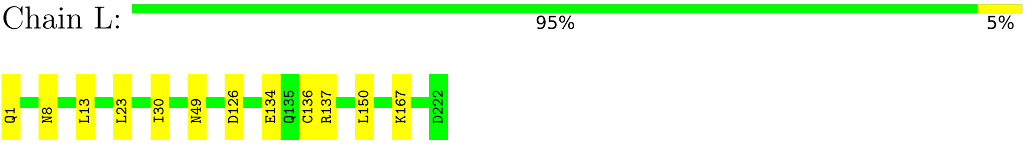
- Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5



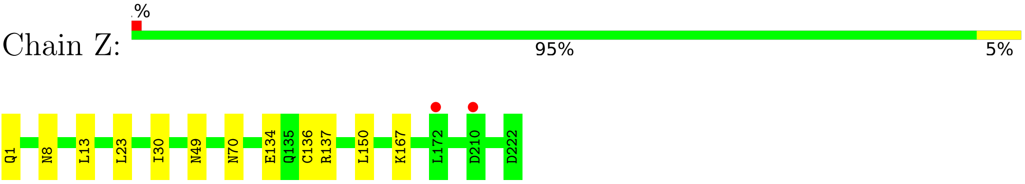
- Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5



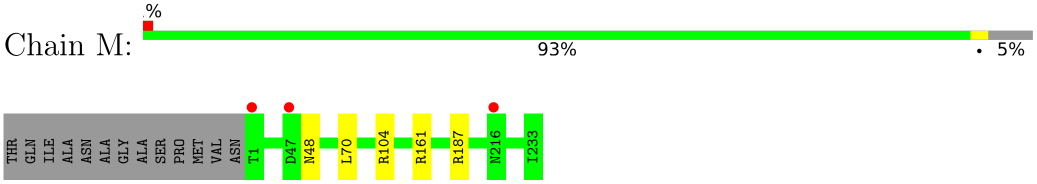
- Molecule 12: Proteasome subunit beta type-6



- Molecule 12: Proteasome subunit beta type-6

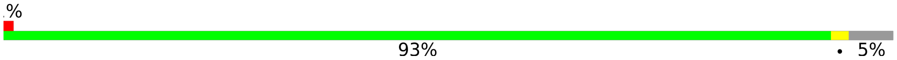


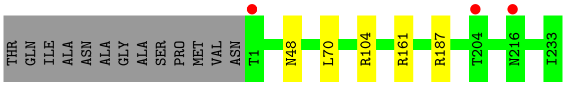
- Molecule 13: Proteasome subunit beta type-7



- Molecule 13: Proteasome subunit beta type-7

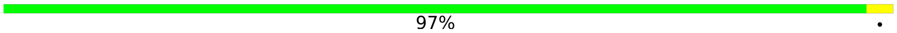
Chain a:

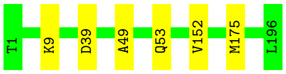




- Molecule 14: Proteasome subunit beta type-1

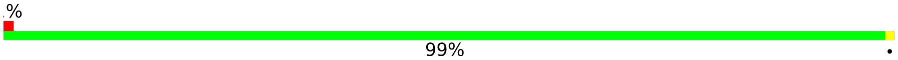
Chain N:

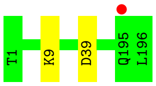




- Molecule 14: Proteasome subunit beta type-1

Chain b:





4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	137.01Å 299.28Å 145.57Å 90.00° 113.03° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.4 (15.00-2.90) 98.1 (15.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.173 , 0.210 0.178 , 0.213	Depositor DCC
R_{free} test set	11568 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	65.3	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 38.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	49789	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GRW, MG

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	0.37	0/1952	0.58	0/2642
1	O	0.37	0/1952	0.57	0/2642
2	B	0.37	0/1934	0.59	0/2618
2	P	0.37	0/1934	0.59	0/2618
3	C	0.37	0/1910	0.63	0/2586
3	Q	0.37	0/1910	0.63	0/2586
4	D	0.37	0/1837	0.58	0/2475
4	R	0.36	0/1837	0.58	0/2475
5	E	0.36	0/1800	0.57	0/2433
5	S	0.37	0/1800	0.58	0/2433
6	F	0.37	0/1932	0.55	0/2609
6	T	0.36	0/1932	0.55	0/2609
7	G	0.37	0/1945	0.57	0/2634
7	U	0.37	0/1945	0.57	0/2634
8	H	0.35	0/1715	0.60	1/2326 (0.0%)
8	V	0.35	0/1715	0.60	0/2326
9	I	0.37	0/1611	0.59	0/2174
9	W	0.36	0/1611	0.59	0/2174
10	J	0.36	0/1589	0.60	0/2142
10	X	0.36	0/1589	0.61	0/2142
11	K	0.36	0/1681	0.64	1/2274 (0.0%)
11	Y	0.37	0/1681	0.64	1/2274 (0.0%)
12	L	0.36	0/1795	0.58	0/2420
12	Z	0.37	0/1795	0.58	0/2420
13	M	0.37	0/1855	0.63	0/2514
13	a	0.37	0/1855	0.63	0/2514
14	N	0.34	0/1541	0.57	0/2087
14	b	0.34	0/1541	0.57	0/2087
All	All	0.36	0/50194	0.59	3/67868 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Y	4	LEU	CD1-CG-CD2	-12.54	72.87	110.50
11	K	4	LEU	CD1-CG-CD2	-12.47	73.09	110.50
8	H	1	THR	CA-CB-OG1	5.17	119.87	109.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	2	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	2	0
2	P	1904	0	1904	1	0
3	C	1881	0	1895	5	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	1	0
4	R	1813	0	1797	1	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	2	0
7	U	1907	0	1901	1	0
8	H	1684	0	1687	11	0
8	V	1684	0	1687	8	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	4	0
10	J	1561	0	1569	2	0
10	X	1561	0	1569	3	0
11	K	1644	0	1594	8	0
11	Y	1644	0	1594	9	0
12	L	1757	0	1711	3	0
12	Z	1757	0	1711	4	0
13	M	1824	0	1832	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	a	1824	0	1832	0	0
14	N	1512	0	1481	2	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	X	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	H	45	0	0	3	0
17	K	45	0	0	1	0
17	V	45	0	0	2	0
17	Y	45	0	0	1	0
18	A	17	0	0	0	0
18	B	17	0	0	0	0
18	C	14	0	0	0	0
18	D	6	0	0	0	0
18	E	8	0	0	0	0
18	F	15	0	0	0	0
18	G	14	0	0	0	0
18	H	12	0	0	0	0
18	I	4	0	0	0	0
18	J	12	0	0	0	0
18	K	13	0	0	0	0
18	L	9	0	0	0	0
18	M	8	0	0	0	0
18	N	11	0	0	0	0
18	O	8	0	0	0	0
18	P	7	0	0	0	0
18	Q	9	0	0	0	0
18	R	7	0	0	0	0
18	S	8	0	0	0	0
18	T	10	0	0	0	0
18	U	18	0	0	0	0
18	V	9	0	0	0	0
18	W	4	0	0	0	0
18	X	14	0	0	0	0
18	Y	16	0	0	0	0
18	Z	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	a	13	0	0	0	0
18	b	9	0	0	0	0
All	All	49789	0	49064	78	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 1.

All (78) 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)
8:H:3:ILE:HG21	8:H:44:ALA:HB1	1.63	0.79
8:V:3:ILE:HG21	8:V:44:ALA:HB1	1.65	0.77
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.78	0.66
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.80	0.64
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.64	0.62
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.64	0.60
17:H:301:GRW:C57	9:I:125:LEU:HD21	2.33	0.59
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.89	0.55
11:K:1:THR:HB	17:K:301:GRW:O30	2.07	0.55
17:H:301:GRW:C10	17:H:301:GRW:C14	2.85	0.54
8:V:35:HIS:NE2	8:V:53:GLU:OE1	2.41	0.53
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.90	0.53
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.89	0.53
14:N:152:VAL:HA	14:N:175:MET:HE1	1.90	0.53
8:H:35:HIS:NE2	8:H:53:GLU:OE1	2.41	0.53
8:V:19:ARG:NH1	8:V:167:LEU:O	2.42	0.52
12:L:134:GLU:OE1	12:L:137:ARG:NH2	2.43	0.52
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.92	0.52
8:V:1:THR:HG22	8:V:2:THR:N	2.26	0.51
8:H:3:ILE:CG2	8:H:44:ALA:HB1	2.39	0.51
17:V:301:GRW:C57	9:W:125:LEU:HD21	2.41	0.51
6:T:123:ASN:HD22	6:T:124:SER:N	2.09	0.51
11:K:5:ALA:HB3	11:K:100:MET:CE	2.41	0.51
8:H:1:THR:HG22	8:H:2:THR:N	2.24	0.51
12:Z:134:GLU:OE1	12:Z:137:ARG:NH2	2.43	0.51
8:H:19:ARG:NH1	8:H:167:LEU:O	2.44	0.50
11:Y:1:THR:HB	17:Y:301:GRW:O30	2.11	0.50
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.41	0.50
11:K:99:THR:HG22	11:K:115:VAL:HB	1.93	0.49
14:N:49:ALA:O	14:N:53:GLN:HB2	2.12	0.49
6:F:123:ASN:HD22	6:F:124:SER:N	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.48	0.49
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.43	0.49
11:Y:9:GLN:NE2	11:Y:148:LEU:O	2.46	0.48
11:Y:99:THR:HG22	11:Y:115:VAL:HB	1.94	0.48
8:V:3:ILE:CG2	8:V:44:ALA:HB1	2.41	0.48
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.49	0.47
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.11	0.47
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.62	0.47
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	1.97	0.47
8:V:3:ILE:HD11	8:V:46:ALA:HB2	1.97	0.47
11:K:16:VAL:HG21	11:K:34:VAL:HG23	1.98	0.46
8:H:1:THR:CG2	8:H:2:THR:N	2.78	0.46
1:A:55:LEU:HD12	7:G:170:THR:HG23	1.98	0.46
17:V:301:GRW:C10	17:V:301:GRW:C14	2.94	0.45
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.98	0.45
11:K:9:GLN:NE2	11:K:148:LEU:O	2.49	0.45
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.99	0.45
8:V:50:ALA:CB	9:W:126:ILE:HG23	2.47	0.45
8:H:1:THR:HB	17:H:301:GRW:O30	2.17	0.45
10:J:174:MET:HA	10:X:174:MET:HA	1.99	0.45
3:C:38:ASN:C	3:C:38:ASN:HD22	2.20	0.45
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.99	0.44
8:V:1:THR:CG2	8:V:2:THR:N	2.80	0.44
8:H:3:ILE:HD11	8:H:46:ALA:HB2	2.00	0.44
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.83	0.44
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.00	0.44
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.17	0.44
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.01	0.43
3:C:9:PHE:H	4:D:15:GLN:HE22	1.67	0.43
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.99	0.43
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.99	0.43
12:L:8:ASN:HA	12:L:30:ILE:O	2.19	0.43
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.00	0.42
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.01	0.42
3:Q:38:ASN:HD22	3:Q:38:ASN:C	2.22	0.42
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.84	0.42
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.67	0.42
7:U:23:PHE:O	7:U:26:THR:HB	2.20	0.42
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.68	0.42
6:T:123:ASN:HD22	6:T:123:ASN:C	2.24	0.41
3:C:201:VAL:O	3:C:202:GLN:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:218:VAL:CG2	9:I:196:LYS:HB2	2.51	0.41
8:H:50:ALA:HB2	9:I:128:CYS:HB2	2.03	0.41
7:G:23:PHE:O	7:G:26:THR:HB	2.21	0.40
3:Q:77:ASN:HD22	3:Q:77:ASN:N	2.19	0.40
9:I:98:ARG:O	9:I:126:ILE:HD11	2.21	0.40
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.51	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%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
2	B	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	19	51
2	P	242/258 (94%)	232 (96%)	8 (3%)	2 (1%)	19	51
3	C	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	19	51
3	Q	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	19	51
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	220/232 (95%)	214 (97%)	5 (2%)	1 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	V	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	61
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	61
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
13	a	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
All	All	6276/6614 (95%)	6104 (97%)	161 (3%)	11 (0%)	47	78

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
10	J	2	ASP
10	X	2	ASP
3	C	205	ALA
3	Q	205	ALA
2	B	221	ASP
2	P	221	ASP
8	H	9	ASN

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%)	57	84
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	89
2	B	203/216 (94%)	197 (97%)	6 (3%)	41	75
2	P	203/216 (94%)	197 (97%)	6 (3%)	41	75
3	C	212/226 (94%)	205 (97%)	7 (3%)	38	72
3	Q	212/226 (94%)	205 (97%)	7 (3%)	38	72
4	D	194/215 (90%)	188 (97%)	6 (3%)	40	74
4	R	194/215 (90%)	188 (97%)	6 (3%)	40	74
5	E	190/193 (98%)	183 (96%)	7 (4%)	34	68
5	S	190/193 (98%)	183 (96%)	7 (4%)	34	68
6	F	201/239 (84%)	192 (96%)	9 (4%)	27	61
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	61
7	G	206/210 (98%)	199 (97%)	7 (3%)	37	71
7	U	206/210 (98%)	199 (97%)	7 (3%)	37	71
8	H	181/190 (95%)	177 (98%)	4 (2%)	52	81
8	V	181/190 (95%)	177 (98%)	4 (2%)	52	81
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	86
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	86
10	J	173/175 (99%)	169 (98%)	4 (2%)	50	80
10	X	173/175 (99%)	169 (98%)	4 (2%)	50	80
11	K	169/169 (100%)	166 (98%)	3 (2%)	59	85
11	Y	169/169 (100%)	166 (98%)	3 (2%)	59	85
12	L	185/185 (100%)	179 (97%)	6 (3%)	39	73
12	Z	185/185 (100%)	180 (97%)	5 (3%)	44	77
13	M	199/208 (96%)	194 (98%)	5 (2%)	47	78
13	a	199/208 (96%)	194 (98%)	5 (2%)	47	78
14	N	162/162 (100%)	160 (99%)	2 (1%)	71	91
14	b	162/162 (100%)	160 (99%)	2 (1%)	71	91
All	All	5312/5540 (96%)	5168 (97%)	144 (3%)	44	77

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
2	B	50	LYS
2	B	55	LEU
2	B	58	GLN
2	B	114	LEU
2	B	184	LYS
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
4	D	99	ILE
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP
6	F	117	GLN
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	125	MET

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Mol	Chain	Res	Type
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
8	H	3	ILE
8	H	30	ASN
8	H	34	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	23	ARG
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	9	GLN
11	K	99	THR
11	K	106	ARG
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	126	ASP
12	L	136	CYS
12	L	167	LYS
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	39	ASP
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	55	LEU
2	P	58	GLN
2	P	114	LEU
2	P	184	LYS
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	77	ASN

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Mol	Chain	Res	Type
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
4	R	99	ILE
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	14	ASP
6	T	117	GLN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
8	V	3	ILE
8	V	30	ASN
8	V	34	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	23	ARG
10	X	78	GLN

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Mol	Chain	Res	Type
10	X	144	LEU
10	X	174	MET
11	Y	9	GLN
11	Y	99	THR
11	Y	106	ARG
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	136	CYS
12	Z	167	LYS
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	39	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	160	ASN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN

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Mol	Chain	Res	Type
5	E	120	GLN
5	E	147	GLN
5	E	184	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
8	H	165	ASN
8	H	172	ASN
10	J	55	GLN
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN

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Mol	Chain	Res	Type
4	R	15	GLN
4	R	91	HIS
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	175	ASN
8	V	22	GLN
8	V	165	ASN
8	V	172	ASN
10	X	55	GLN
10	X	118	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	158	ASN
12	Z	159	GLN
13	a	18	ASN
13	a	26	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
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 monosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
17	GRW	V	301	8	45,46,46	1.76	6 (13%)	58,62,62	7.65	15 (25%)
17	GRW	H	301	8	45,46,46	1.77	4 (8%)	58,62,62	7.96	11 (18%)
17	GRW	Y	301	11	45,46,46	1.52	6 (13%)	58,62,62	8.08	10 (17%)
17	GRW	K	301	11	45,46,46	1.45	5 (11%)	58,62,62	8.04	12 (20%)

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
17	GRW	V	301	8	-	10/51/51/51	0/2/2/2
17	GRW	H	301	8	-	7/51/51/51	0/2/2/2
17	GRW	Y	301	11	-	13/51/51/51	0/2/2/2
17	GRW	K	301	11	-	13/51/51/51	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	GRW	N52-N51	-7.19	1.04	1.23
17	V	301	GRW	C54-C55	-5.88	1.37	1.51
17	V	301	GRW	N52-N51	-5.72	1.08	1.23
17	H	301	GRW	C54-C55	-5.54	1.38	1.51
17	Y	301	GRW	C16-C17	-5.27	1.38	1.51
17	K	301	GRW	C16-C17	-5.14	1.38	1.51
17	H	301	GRW	C16-C17	-4.97	1.39	1.51
17	V	301	GRW	C16-C17	-4.92	1.39	1.51
17	Y	301	GRW	O29-S27	4.03	1.53	1.44
17	K	301	GRW	O29-S27	3.86	1.52	1.44
17	K	301	GRW	O30-S27	3.76	1.52	1.44
17	V	301	GRW	C21-C20	-3.75	1.38	1.51
17	H	301	GRW	C21-C20	-3.74	1.38	1.51
17	Y	301	GRW	O30-S27	3.69	1.52	1.44
17	Y	301	GRW	C21-C20	-3.59	1.38	1.51
17	K	301	GRW	C54-C55	-3.54	1.42	1.51
17	Y	301	GRW	C54-C55	-3.50	1.42	1.51
17	K	301	GRW	C21-C20	-3.46	1.39	1.51
17	Y	301	GRW	C26-S27	2.51	1.81	1.78
17	V	301	GRW	C6-N51	-2.36	1.45	1.48
17	V	301	GRW	C54-C6	-2.25	1.50	1.53

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	301	GRW	C6-N51-N52	60.53	178.92	115.24
17	K	301	GRW	C6-N51-N52	60.26	178.63	115.24
17	H	301	GRW	C6-N51-N52	59.60	177.94	115.24
17	V	301	GRW	C6-N51-N52	56.56	174.74	115.24
17	V	301	GRW	O30-S27-C26	6.63	112.99	108.34
17	V	301	GRW	O29-S27-O30	-4.74	106.97	117.09
17	V	301	GRW	C25-C15-N14	-3.96	104.96	110.54
17	H	301	GRW	O29-S27-O30	-3.96	108.64	117.09
17	K	301	GRW	O29-S27-C26	-3.78	105.69	108.34
17	V	301	GRW	O30-S27-C28	3.68	112.60	108.91
17	Y	301	GRW	O29-S27-O30	-3.65	109.28	117.09
17	K	301	GRW	O29-S27-O30	-3.57	109.46	117.09
17	Y	301	GRW	O30-S27-C26	3.50	110.80	108.34
17	Y	301	GRW	O29-S27-C26	-3.46	105.92	108.34
17	H	301	GRW	C10-C9-N8	-3.42	101.84	111.16
17	Y	301	GRW	C16-C17-C18	-2.96	115.03	120.91
17	V	301	GRW	C15-N14-C13	2.93	127.86	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	301	GRW	C25-C15-N14	-2.90	106.46	110.54
17	V	301	GRW	O29-S27-C28	-2.88	106.01	108.91
17	V	301	GRW	C54-C6-C7	-2.85	103.49	109.55
17	Y	301	GRW	C16-C17-C24	2.78	126.42	120.91
17	K	301	GRW	C16-C17-C18	-2.76	115.43	120.91
17	K	301	GRW	C16-C17-C24	2.62	126.12	120.91
17	H	301	GRW	C15-N14-C13	2.57	127.29	123.20
17	V	301	GRW	C10-C9-N8	-2.56	104.20	111.16
17	V	301	GRW	C32-C12-C13	-2.55	105.67	111.28
17	H	301	GRW	C16-C15-N14	-2.55	105.49	110.39
17	V	301	GRW	C16-C15-N14	-2.50	105.58	110.39
17	V	301	GRW	C7-C6-N51	-2.43	103.09	108.85
17	H	301	GRW	C40-C9-C10	-2.41	104.84	110.57
17	H	301	GRW	O30-S27-C28	2.39	111.31	108.91
17	H	301	GRW	C54-C6-C7	-2.35	104.56	109.55
17	Y	301	GRW	C54-C55-C60	2.34	125.56	120.91
17	Y	301	GRW	C40-C9-C10	-2.33	105.02	110.57
17	K	301	GRW	O30-S27-C26	2.32	109.97	108.34
17	H	301	GRW	C32-C12-C13	-2.31	106.19	111.28
17	K	301	GRW	C28-S27-C26	2.29	114.04	105.21
17	K	301	GRW	C9-C10-N11	-2.22	111.83	116.70
17	K	301	GRW	C54-C55-C60	2.21	125.30	120.91
17	V	301	GRW	C40-C9-C10	-2.19	105.36	110.57
17	Y	301	GRW	C9-C10-N11	-2.17	111.94	116.70
17	H	301	GRW	C32-C12-N11	-2.13	106.28	111.72
17	K	301	GRW	C40-C9-C10	-2.12	105.52	110.57
17	V	301	GRW	C25-C15-C16	2.10	114.56	111.14
17	K	301	GRW	O39-C10-N11	2.10	126.81	122.93
17	K	301	GRW	C25-C15-N14	-2.06	107.64	110.54
17	V	301	GRW	C54-C6-N51	2.04	112.67	109.30
17	Y	301	GRW	C54-C55-C56	-2.03	116.88	120.91

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	GRW	N51-C6-C7-N8
17	K	301	GRW	N51-C6-C7-N8
17	K	301	GRW	N51-C6-C7-O44
17	V	301	GRW	N51-C6-C7-N8
17	V	301	GRW	C6-N51-N52-N53
17	Y	301	GRW	N51-C6-C7-N8

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Mol	Chain	Res	Type	Atoms
17	Y	301	GRW	N51-C6-C7-O44
17	H	301	GRW	C54-C6-C7-O44
17	Y	301	GRW	C6-C54-C55-C60
17	K	301	GRW	C6-C54-C55-C60
17	V	301	GRW	C15-C16-C17-C24
17	V	301	GRW	C15-C16-C17-C18
17	Y	301	GRW	C6-C54-C55-C56
17	K	301	GRW	C6-C54-C55-C56
17	H	301	GRW	C15-C16-C17-C18
17	H	301	GRW	C15-C16-C17-C24
17	K	301	GRW	C54-C6-C7-O44
17	V	301	GRW	C54-C6-C7-O44
17	K	301	GRW	C15-C16-C17-C24
17	K	301	GRW	C15-C16-C17-C18
17	Y	301	GRW	C15-C16-C17-C24
17	Y	301	GRW	C15-C16-C17-C18
17	K	301	GRW	C25-C26-S27-C28
17	Y	301	GRW	C25-C26-S27-C28
17	Y	301	GRW	C54-C6-C7-O44
17	H	301	GRW	C54-C6-C7-N8
17	Y	301	GRW	C6-N51-N52-N53
17	V	301	GRW	N14-C15-C25-C26
17	V	301	GRW	C54-C6-C7-N8
17	K	301	GRW	C7-C6-N51-N52
17	V	301	GRW	C7-C6-N51-N52
17	K	301	GRW	C25-C26-S27-O30
17	K	301	GRW	C25-C26-S27-O29
17	Y	301	GRW	C25-C26-S27-O30
17	Y	301	GRW	C25-C26-S27-O29
17	V	301	GRW	C13-C12-N11-C10
17	H	301	GRW	C13-C12-N11-C10
17	V	301	GRW	C25-C26-S27-C28
17	H	301	GRW	C6-N51-N52-N53
17	K	301	GRW	C54-C6-C7-N8
17	K	301	GRW	C15-C25-C26-S27
17	Y	301	GRW	C54-C6-C7-N8
17	Y	301	GRW	C15-C25-C26-S27

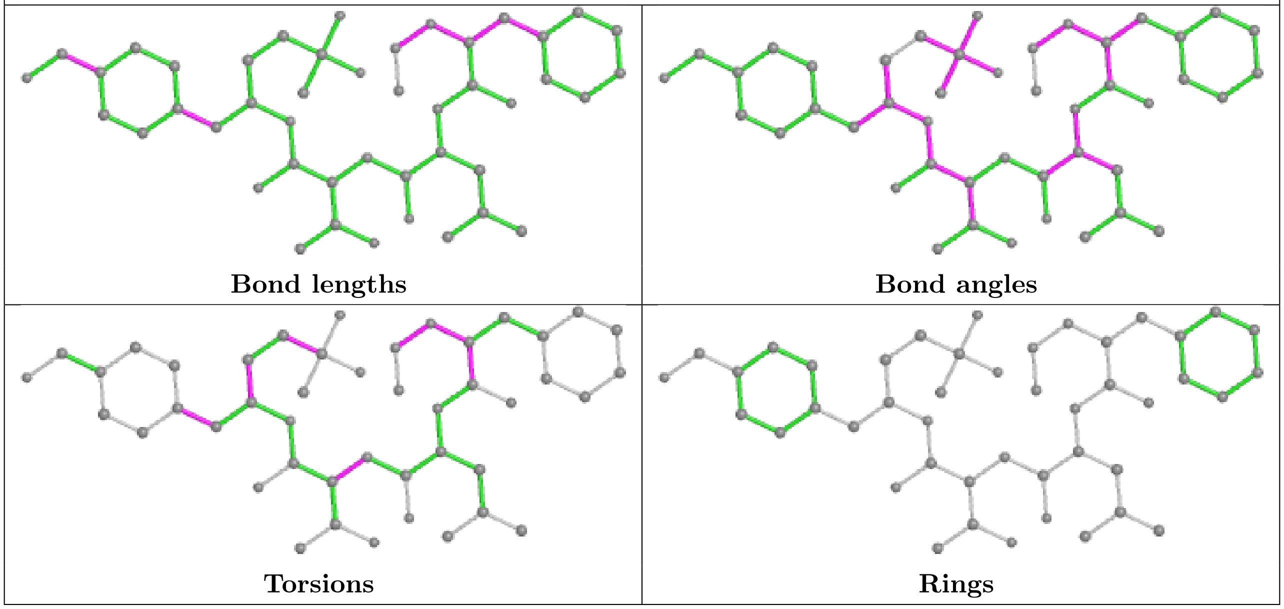
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	V	301	GRW	2	0
17	H	301	GRW	3	0
17	Y	301	GRW	1	0
17	K	301	GRW	1	0

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

Ligand GRW V 301



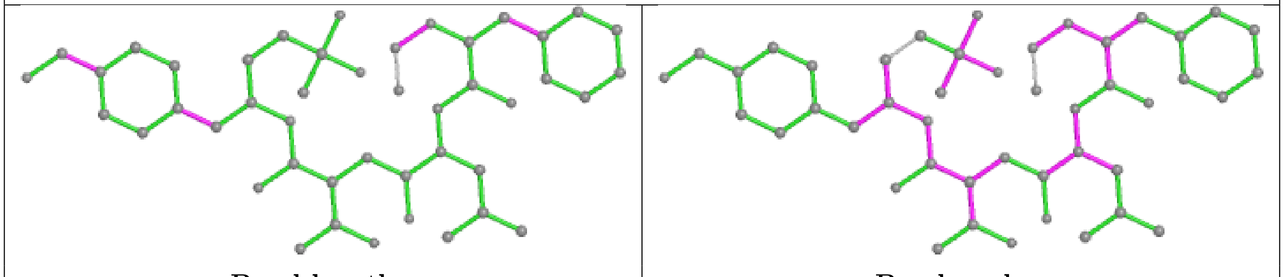
Bond lengths

Bond angles

Torsions

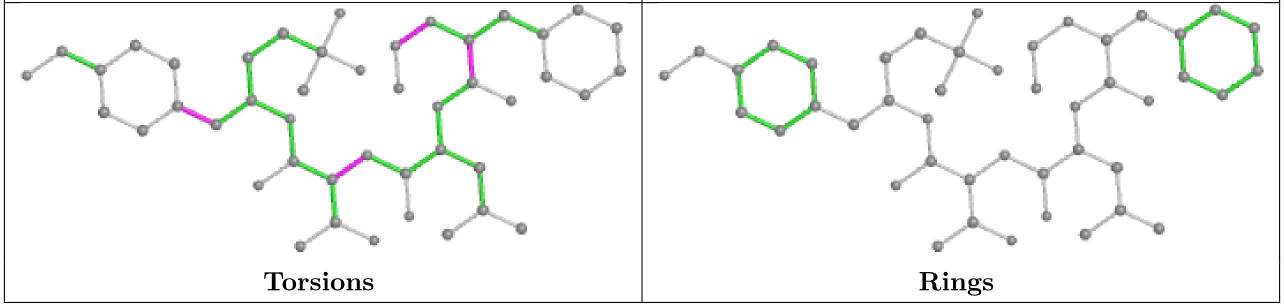
Rings

Ligand GRW H 301



Bond lengths

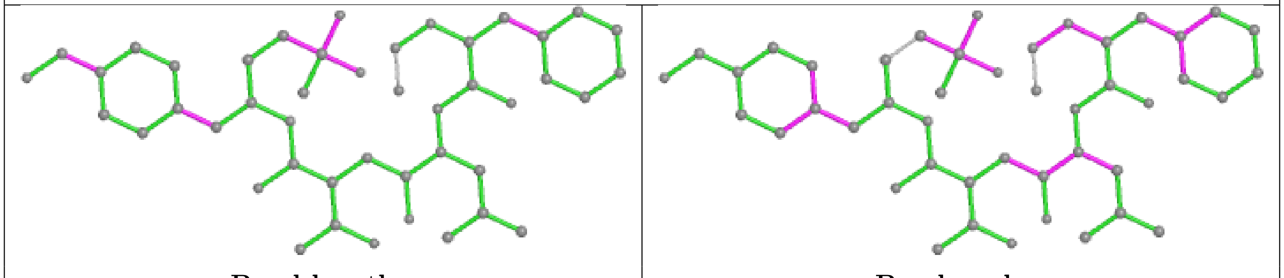
Bond angles



Torsions

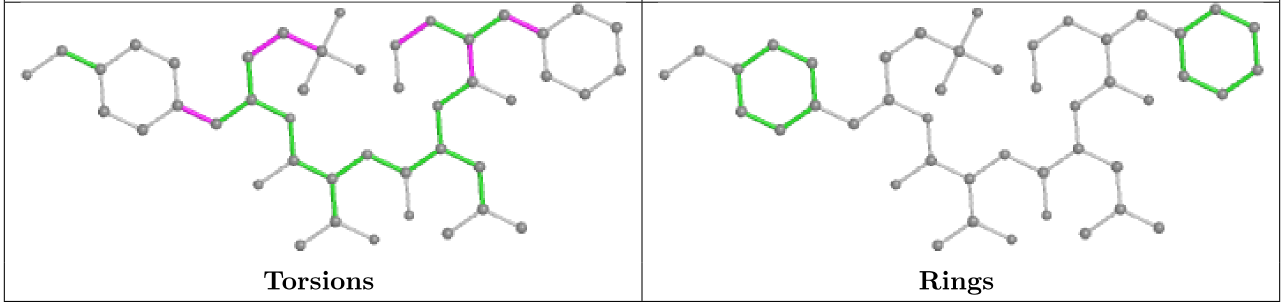
Rings

Ligand GRW Y 301



Bond lengths

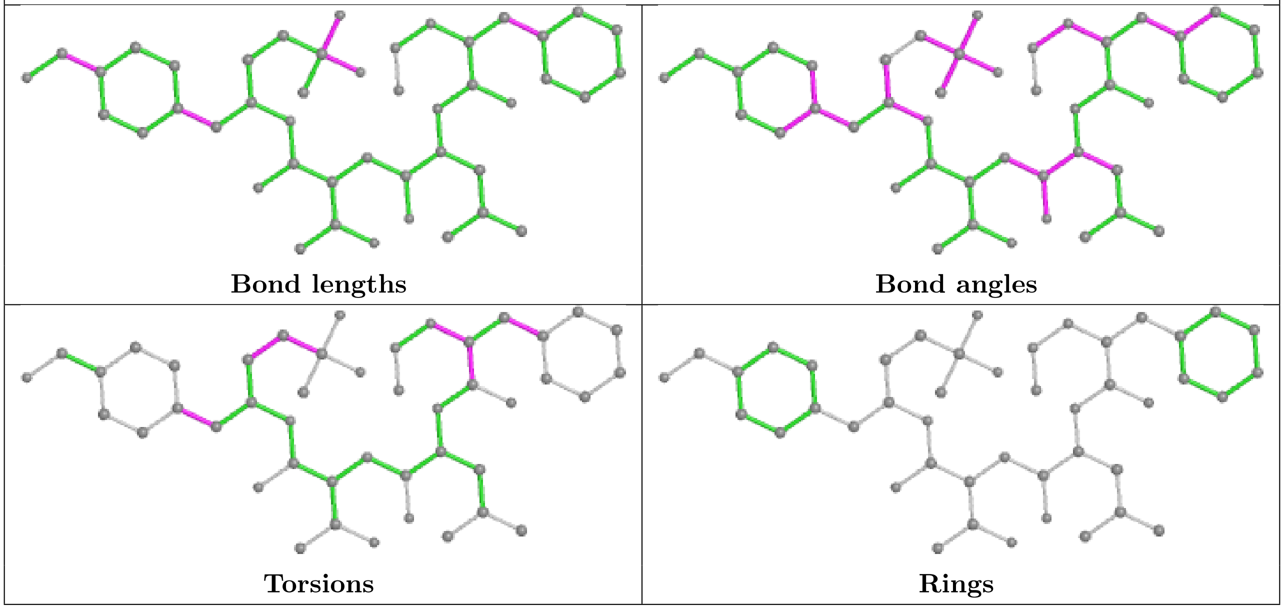
Bond angles



Torsions

Rings

Ligand GRW K 301



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.41	6 (2%)	59	56	44, 64, 106, 156	0
1	O	250/250 (100%)	-0.32	7 (2%)	53	49	51, 72, 114, 153	0
2	B	244/258 (94%)	-0.34	7 (2%)	51	47	48, 69, 117, 167	0
2	P	244/258 (94%)	-0.30	9 (3%)	41	37	52, 73, 121, 167	0
3	C	240/254 (94%)	-0.28	9 (3%)	40	36	51, 75, 136, 160	0
3	Q	240/254 (94%)	-0.02	15 (6%)	20	16	56, 86, 167, 189	0
4	D	235/260 (90%)	-0.40	2 (0%)	84	84	52, 75, 108, 148	0
4	R	235/260 (90%)	-0.36	5 (2%)	63	61	54, 77, 116, 156	0
5	E	231/234 (98%)	-0.34	1 (0%)	92	93	55, 80, 115, 155	0
5	S	231/234 (98%)	-0.29	4 (1%)	70	69	53, 80, 122, 154	0
6	F	243/288 (84%)	-0.45	5 (2%)	63	61	47, 71, 118, 150	0
6	T	243/288 (84%)	-0.40	6 (2%)	57	55	46, 72, 124, 158	0
7	G	241/252 (95%)	-0.46	3 (1%)	79	79	45, 65, 109, 152	0
7	U	241/252 (95%)	-0.51	4 (1%)	70	69	48, 65, 101, 132	0
8	H	222/232 (95%)	-0.44	3 (1%)	75	75	50, 65, 102, 138	0
8	V	222/232 (95%)	-0.40	2 (0%)	84	84	53, 69, 109, 145	0
9	I	204/205 (99%)	-0.72	1 (0%)	91	91	44, 60, 87, 112	0
9	W	204/205 (99%)	-0.66	2 (0%)	82	82	46, 65, 94, 125	0
10	J	195/198 (98%)	-0.56	2 (1%)	82	82	46, 63, 93, 134	0
10	X	195/198 (98%)	-0.57	2 (1%)	82	82	47, 66, 95, 148	0
11	K	212/212 (100%)	-0.62	2 (0%)	84	84	45, 65, 95, 123	0
11	Y	212/212 (100%)	-0.63	1 (0%)	91	91	44, 63, 95, 122	0
12	L	222/222 (100%)	-0.57	0	100	100	46, 66, 103, 119	0
12	Z	222/222 (100%)	-0.62	2 (0%)	84	84	35, 62, 96, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.63	3 (1%)	77	77	38, 64, 91, 100	0
13	a	233/246 (94%)	-0.62	3 (1%)	77	77	43, 61, 88, 107	0
14	N	196/196 (100%)	-0.64	0	100	100	37, 59, 87, 115	0
14	b	196/196 (100%)	-0.62	1 (0%)	91	91	40, 60, 91, 114	0
All	All	6336/6614 (95%)	-0.46	107 (1%)	70	69	35, 68, 113, 189	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	8.7
3	C	206	LYS	7.2
2	B	220	ASN	6.3
3	Q	206	LYS	6.3
2	P	219	ALA	6.1
1	O	231	LYS	5.7
3	Q	50	LEU	5.6
1	O	1	MET	5.3
8	V	222	ASP	5.2
5	E	202	ASP	4.8
1	A	1	MET	4.7
10	J	1	MET	4.7
3	Q	48	SER	4.7
10	X	1	MET	4.7
5	S	202	ASP	4.6
3	Q	239	GLN	4.6
2	P	221	ASP	4.6
2	P	220	ASN	4.3
8	V	221	CYS	3.9
10	J	194	ASP	3.9
2	B	51	VAL	3.9
2	B	221	ASP	3.9
10	X	194	ASP	3.9
3	Q	240	GLU	3.8
3	Q	236	GLN	3.7
8	H	221	CYS	3.7
8	H	222	ASP	3.6
3	C	239	GLN	3.6
9	W	1	SER	3.6
1	A	231	LYS	3.4
6	T	241	LYS	3.4
11	K	212	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
4	D	242	GLU	3.3
3	Q	238	LYS	3.3
1	O	249	ALA	3.3
6	F	202	ASP	3.2
3	Q	205	ALA	3.2
1	O	229	THR	3.1
3	C	49	THR	3.1
2	P	222	GLY	3.1
2	B	218	GLY	3.0
4	R	241	ALA	3.0
2	P	218	GLY	3.0
3	C	50	LEU	2.9
3	Q	141	ASP	2.9
1	A	229	THR	2.9
13	a	1	THR	2.9
3	C	202	GLN	2.9
4	R	242	GLU	2.9
2	B	219	ALA	2.8
1	A	249	ALA	2.8
13	M	1	THR	2.8
2	B	59	ASP	2.7
13	a	216	ASN	2.7
7	G	179	LYS	2.6
2	P	59	ASP	2.6
11	Y	212	GLY	2.6
6	F	241	LYS	2.6
5	S	180	LYS	2.6
13	M	216	ASN	2.6
13	M	47	ASP	2.5
1	A	250	LEU	2.5
2	P	51	VAL	2.5
4	R	117	GLU	2.5
6	T	178	HIS	2.5
7	G	3	TYR	2.5
7	U	222	ASP	2.5
6	T	244	ASN	2.4
1	O	201	GLU	2.4
3	C	225	GLU	2.4
3	C	240	GLU	2.4
12	Z	210	ASP	2.4
3	Q	167	LYS	2.4
1	O	52	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	238	LYS	2.4
7	U	181	LYS	2.3
11	K	151	GLU	2.3
3	Q	225	GLU	2.3
7	G	181	LYS	2.3
3	Q	51	LYS	2.3
5	S	30	GLN	2.3
7	U	242	GLN	2.3
6	T	230	ASP	2.3
5	S	165	GLN	2.3
13	a	204	THR	2.2
4	R	1	ASP	2.2
2	P	223	GLU	2.2
6	T	180	PRO	2.2
7	U	241	GLU	2.2
9	I	1	SER	2.2
3	Q	235	GLU	2.2
9	W	133	LYS	2.2
2	P	52	THR	2.2
6	F	178	HIS	2.2
3	C	236	GLN	2.2
2	B	203	SER	2.2
4	R	125	LEU	2.1
3	Q	187	GLU	2.1
6	T	205	GLU	2.1
4	D	177	ASN	2.1
1	O	248	GLU	2.1
12	Z	172	LEU	2.0
8	H	198	GLU	2.0
1	A	220	ASP	2.0
6	F	205	GLU	2.0
6	F	244	ASN	2.0
14	b	195	GLN	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 monosaccharides in this entry.

6.4 Ligands

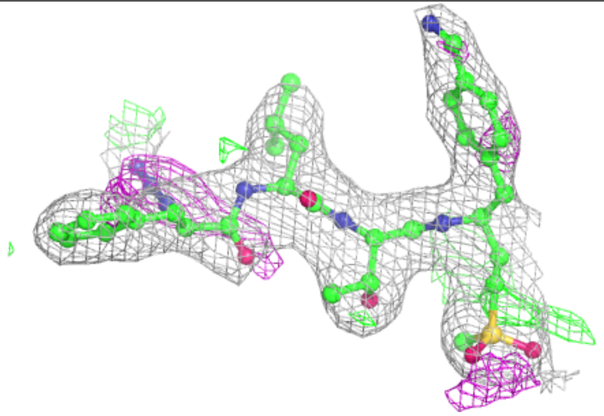
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’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

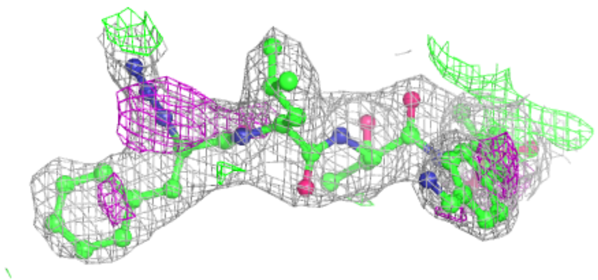
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
15	MG	G	301	1/1	0.92	0.27	65,65,65,65	0
17	GRW	K	301	45/45	0.92	0.21	42,51,71,86	0
17	GRW	V	301	45/45	0.93	0.24	57,72,99,111	0
17	GRW	H	301	45/45	0.94	0.23	53,65,96,96	0
15	MG	I	301	1/1	0.94	0.44	79,79,79,79	0
15	MG	X	201	1/1	0.94	0.26	47,47,47,47	0
17	GRW	Y	301	45/45	0.94	0.20	41,53,67,87	0
16	CL	G	302	1/1	0.98	0.13	54,54,54,54	0
15	MG	K	302	1/1	0.99	0.07	70,70,70,70	0
16	CL	U	301	1/1	0.99	0.18	55,55,55,55	0
15	MG	L	301	1/1	0.99	0.06	77,77,77,77	0
15	MG	N	201	1/1	0.99	0.08	46,46,46,46	0
15	MG	I	302	1/1	0.99	0.09	56,56,56,56	0
15	MG	Z	301	1/1	0.99	0.19	59,59,59,59	0

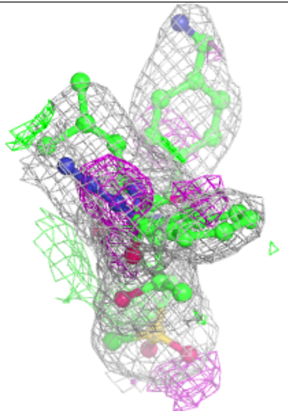
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GRW 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)

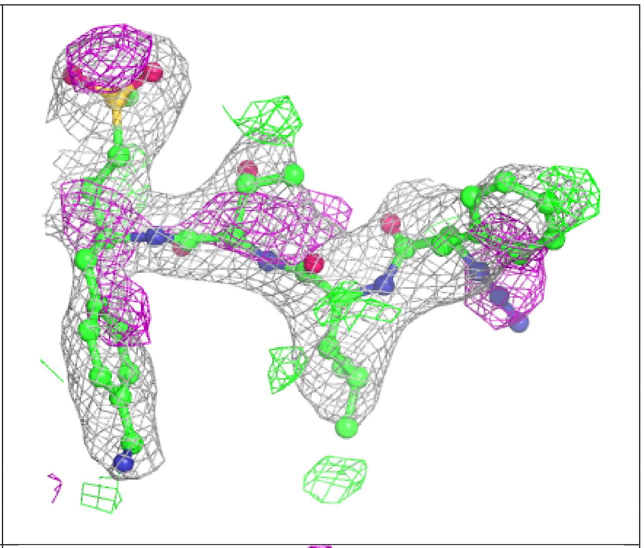


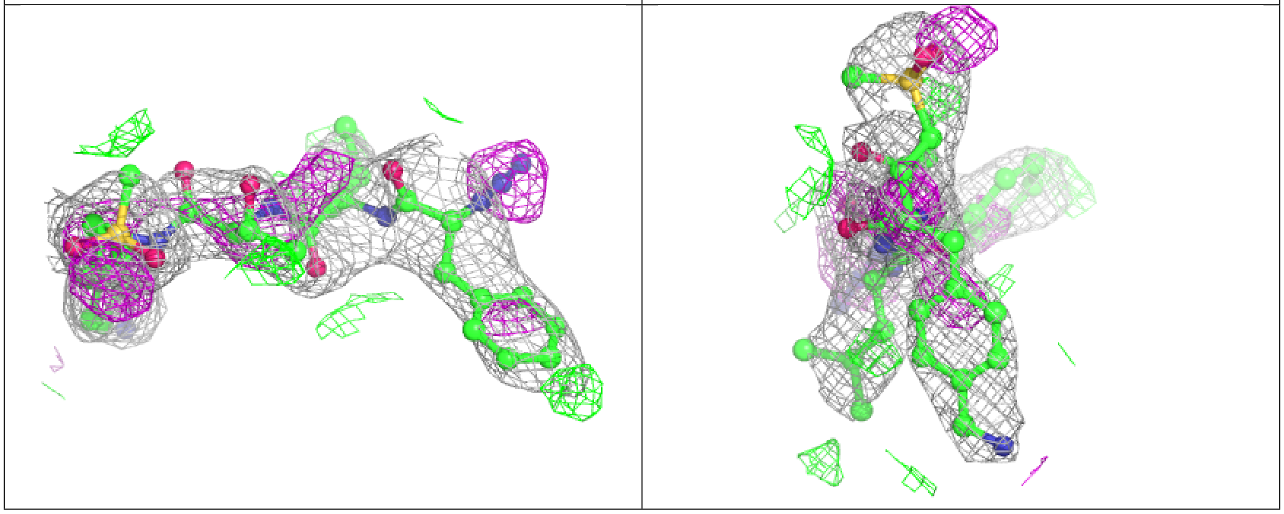




Electron density around GRW V 301:

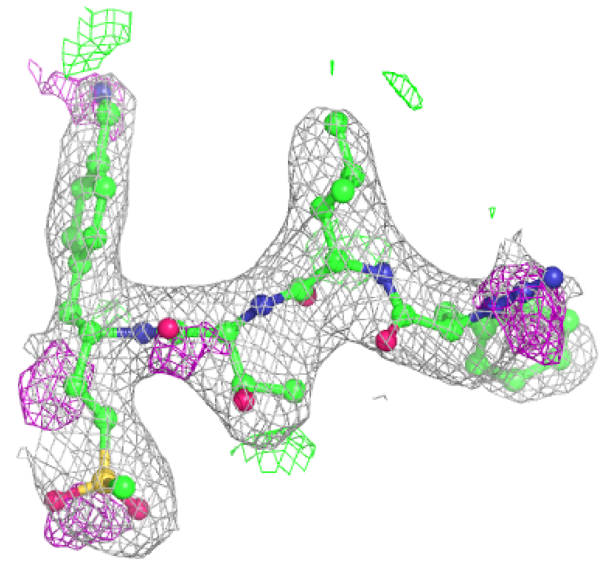
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

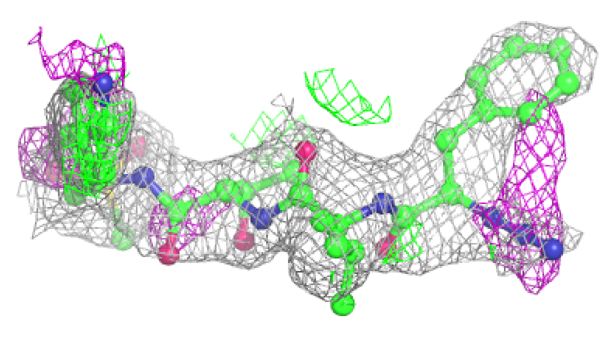


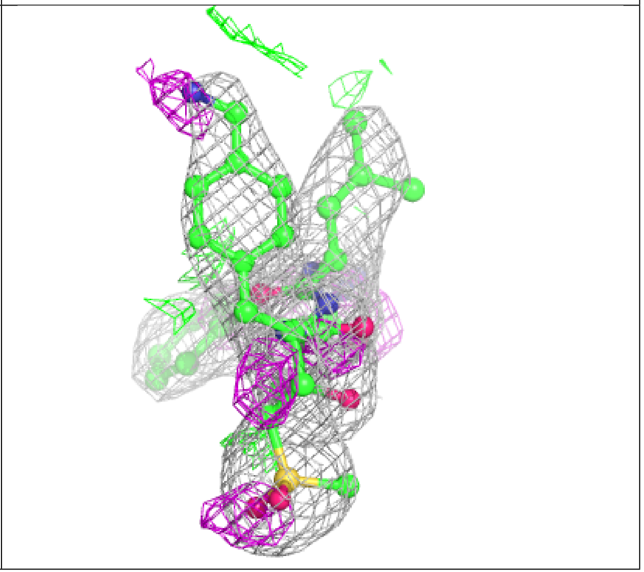


Electron density around GRW H 301:

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

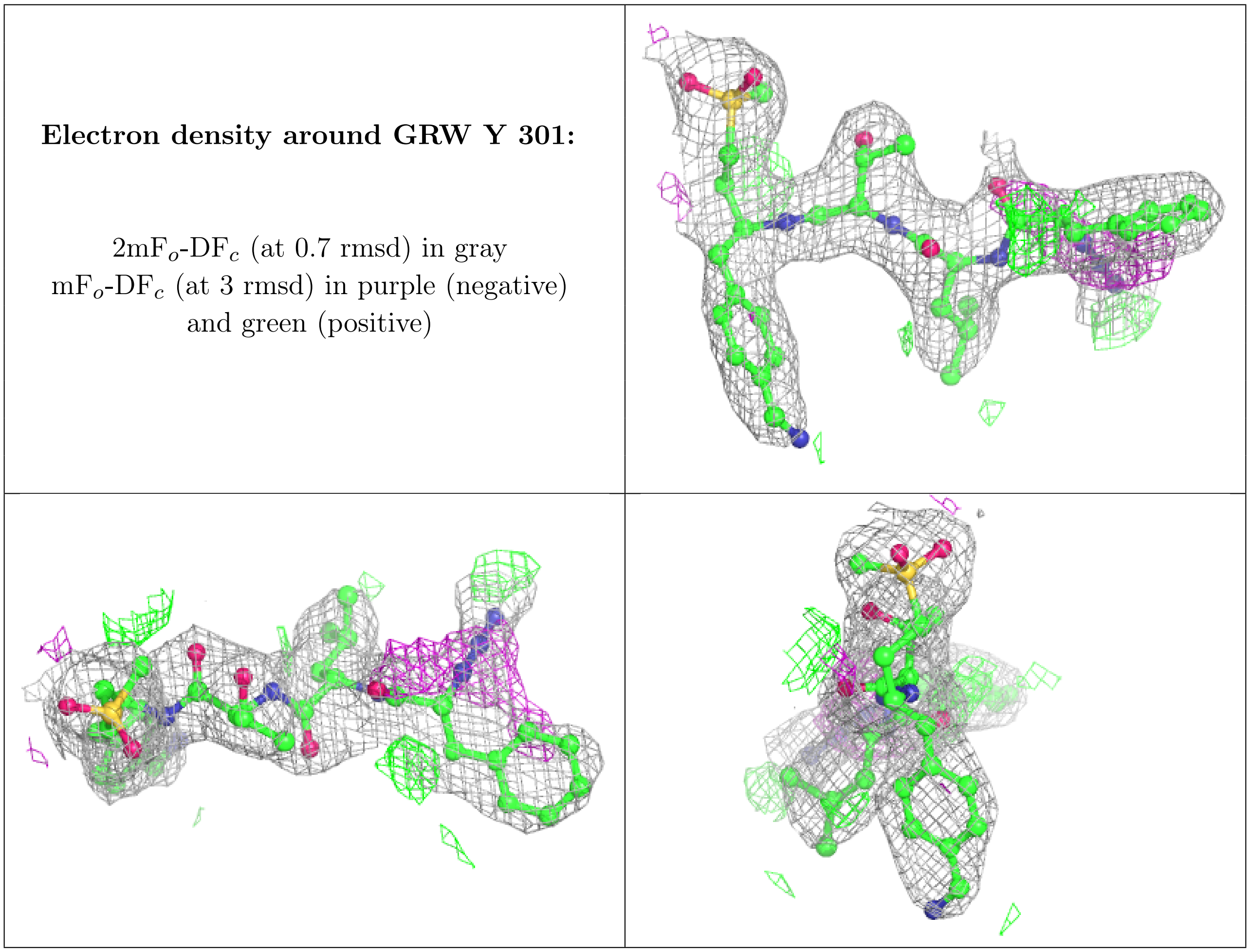






Electron density around GRW Y 301:

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



6.5 Other polymers

There are no such residues in this entry.