Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 03:54 pm GMT

PDB ID	:	6HW6
Title	:	Yeast 20S proteasome in complex with 20
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2018-10-11
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 (i) symbol.

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

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

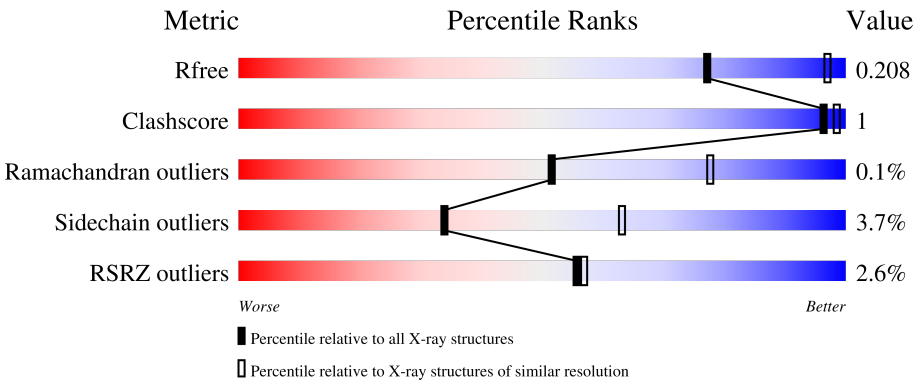
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.70 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 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	4% 97% •
1	O	250	3% 97% •
2	B	258	4% 89% 5% 5%
2	P	258	5% 90% • 5%
3	C	254	7% 88% 5% • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	8% 89% 6%
4	D	260	86% 10%
4	R	260	2% 85% 5% 10%
5	E	234	4% 92% 6%
5	S	234	3% 91% 7%
6	F	288	3% 80% 16%
6	T	288	3% 80% 16%
7	G	252	2% 92%
7	U	252	2% 92%
8	H	232	2% 92%
8	V	232	93%
9	I	205	93% 6%
9	W	205	2% 93% 5%
10	J	198	93% 5%
10	X	198	2% 93% 5%
11	K	212	94% 6%
11	Y	212	94% 6%
12	L	222	93% 6%
12	Z	222	2% 93% 6%
13	M	246	91% 5%
13	a	246	92% 5%
14	N	196	96%
14	b	196	2% 97%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MG	H	302	-	-	-	X

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 49859 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
			Total	C	N	O	S			
1	A	250	1915	1219	315	377	4	0	0	0
1	O	250	1915	1219	315	377	4	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	235	1813	1136	304	366	7	0	0	0
4	R	235	1813	1136	304	366	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
			Total	C	N	O	S			
10	X	195	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
			Total	C	N	O	S			
11	K	212	1644	1045	280	312	7	0	0	0
			Total	C	N	O	S			
11	Y	212	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
			Total	C	N	O	S			
12	L	222	1757	1115	303	335	4	0	0	0
			Total	C	N	O	S			
12	Z	222	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
			Total	C	N	O	S			
13	M	233	1824	1154	312	351	7	0	0	0
			Total	C	N	O	S			
13	a	233	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
			Total	C	N	O	S			
14	N	196	1512	955	250	300	7	0	0	0
			Total	C	N	O	S			
14	b	196	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
			Total	Mg		
15	G	1	1	1	0	0
			Total	Mg		
15	H	1	1	1	0	0

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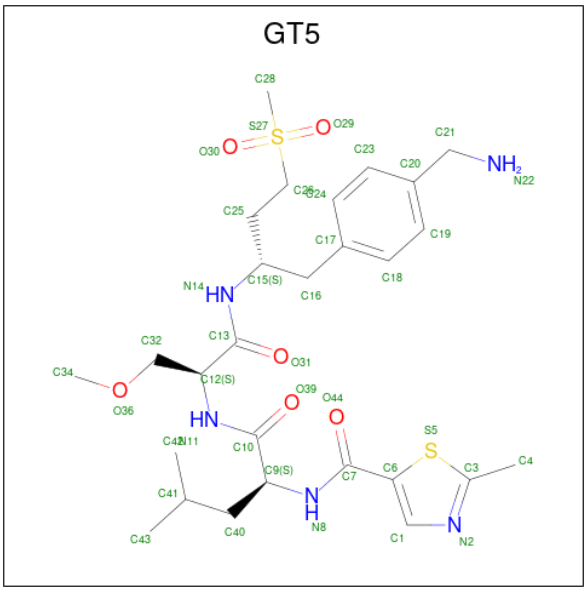
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
15	I	2	2	2	0	0
			Total	Mg		
15	K	1	1	1	0	0
			Total	Mg		
15	L	1	1	1	0	0
			Total	Mg		
15	N	1	1	1	0	0
			Total	Mg		
15	Z	1	1	1	0	0

- Molecule 16 is {N}-[(2 {S})-1-[[(2 {S})-1-[[(2 {S})-1-[4-(aminomethyl)phenyl]-4-methylsulfonyl-butan-2-yl]amino]-3-methoxy-1-oxidanylidene-propan-2-yl]amino]-4-methyl-1-oxidanylidene-pentan-2-yl]-2-methyl-1,3-thiazole-5-carboxamide (three-letter code: GT5) (formula: $C_{27}H_{41}N_5O_6S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
16	H	1	40	27	5	6	2	0	0
			Total	C	N	O	S		
16	K	1	40	27	5	6	2	0	0
			Total	C	N	O	S		
16	V	1	40	27	5	6	2	0	0
			Total	C	N	O	S		
16	Y	1	40	27	5	6	2	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
17	A	13	13	13	0	0
			Total	O		
17	B	21	21	21	0	0
			Total	O		
17	C	18	18	18	0	0
			Total	O		
17	D	13	13	13	0	0
			Total	O		
17	E	8	8	8	0	0
			Total	O		
17	F	11	11	11	0	0
			Total	O		
17	G	14	14	14	0	0
			Total	O		
17	H	17	17	17	0	0
			Total	O		
17	I	14	14	14	0	0
			Total	O		
17	J	19	19	19	0	0
			Total	O		
17	K	24	24	24	0	0
			Total	O		
17	L	21	21	21	0	0
			Total	O		
17	M	21	21	21	0	0
			Total	O		
17	N	10	10	10	0	0
			Total	O		
17	O	11	11	11	0	0
			Total	O		
17	P	15	15	15	0	0
			Total	O		
17	Q	16	16	16	0	0
			Total	O		
17	R	8	8	8	0	0
			Total	O		
17	S	4	4	4	0	0
			Total	O		
17	T	11	11	11	0	0
			Total	O		
17	U	11	11	11	0	0
			Total	O		
17	V	12	12	12	0	0

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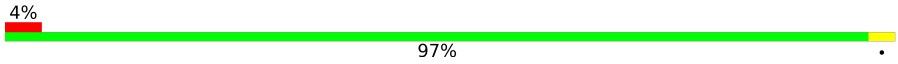
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
17	Y	20	20	20	0	0
			Total	O		
17	W	6	6	6	0	0
			Total	O		
17	X	12	12	12	0	0
			Total	O		
17	Z	11	11	11	0	0
			Total	O		
17	a	17	17	17	0	0
			Total	O		
17	b	17	17	17	0	0

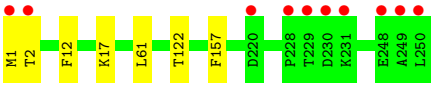
3 Residue-property plots (i)

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

• Molecule 1: Proteasome subunit alpha type-2

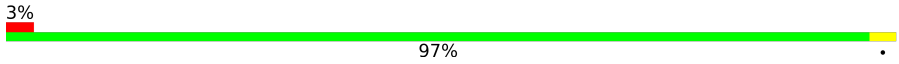
Chain A:





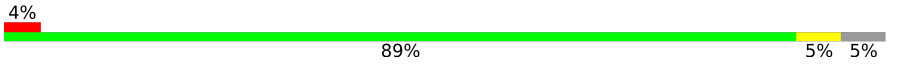
• Molecule 1: Proteasome subunit alpha type-2

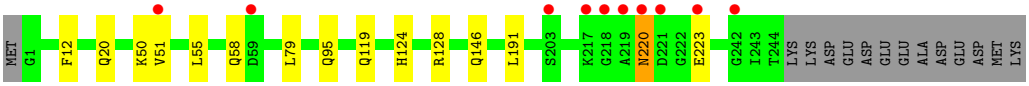
Chain O:



• Molecule 2: Proteasome subunit alpha type-3

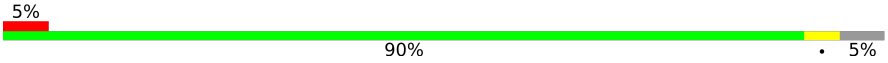
Chain B:

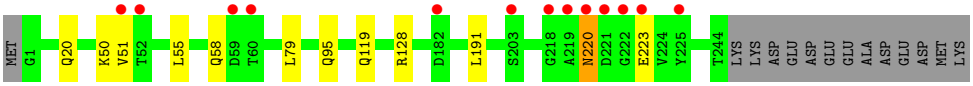




• Molecule 2: Proteasome subunit alpha type-3

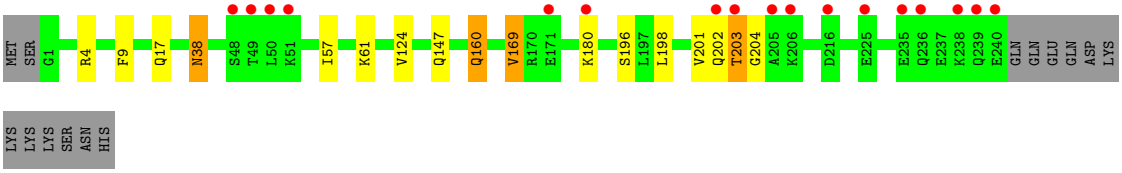
Chain P:





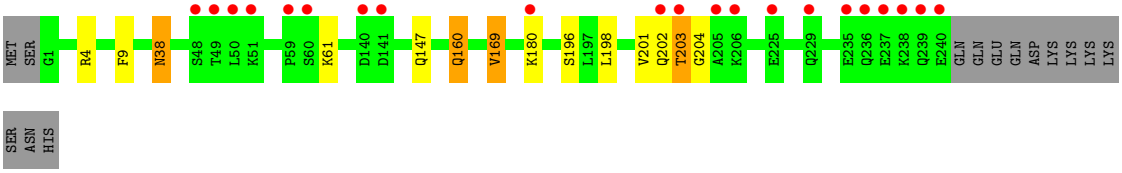
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



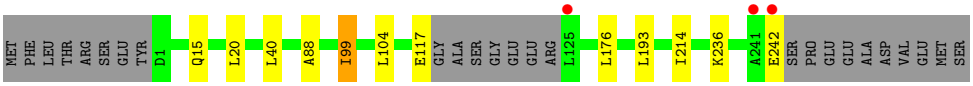
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



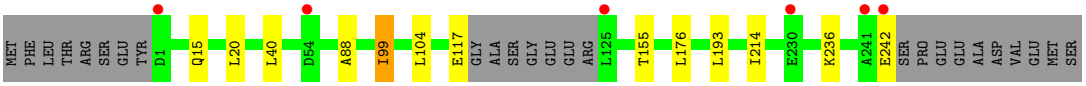
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



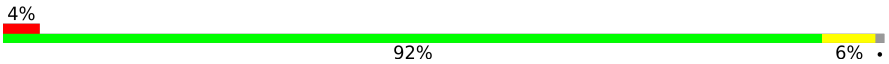
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



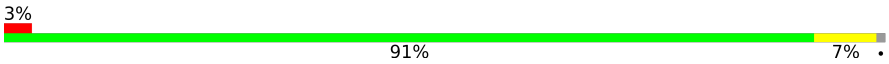
• Molecule 5: Proteasome subunit alpha type-6

Chain E:



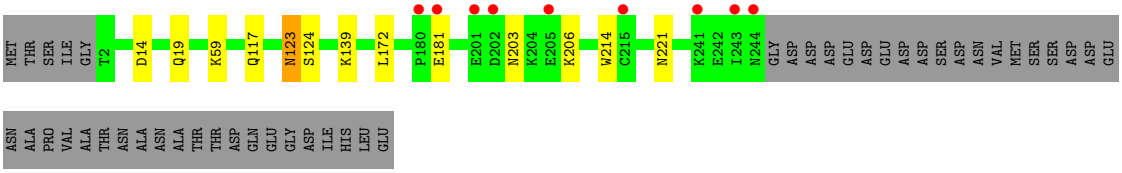
• Molecule 5: Proteasome subunit alpha type-6

Chain S:



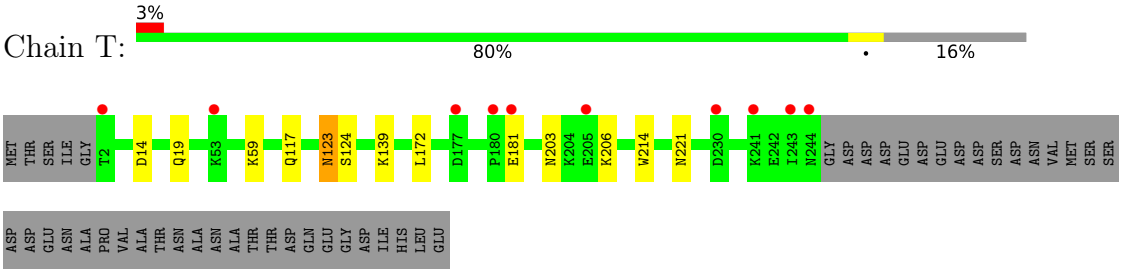
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



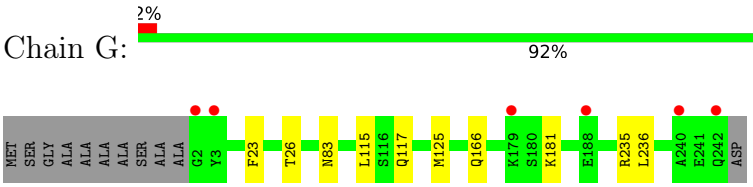
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



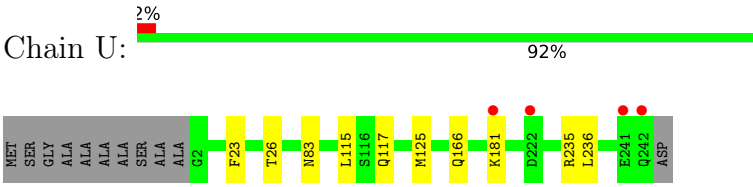
- Molecule 7: Proteasome subunit alpha type-1

Chain G:



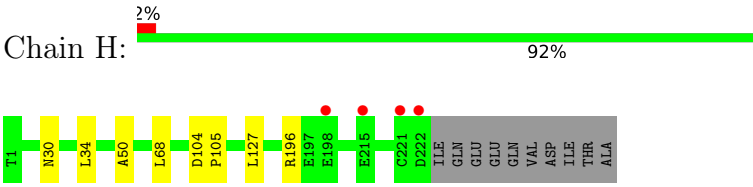
- Molecule 7: Proteasome subunit alpha type-1

Chain U:



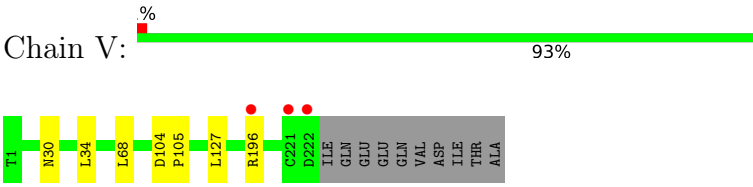
- Molecule 8: Proteasome subunit beta type-2

Chain H:



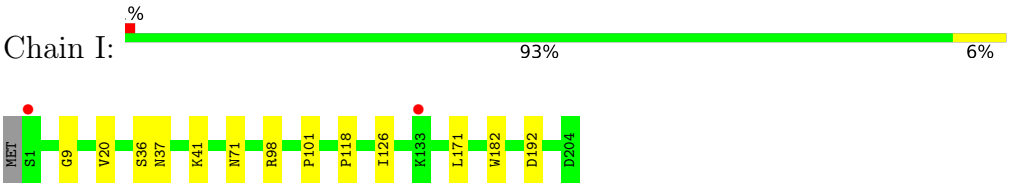
- Molecule 8: Proteasome subunit beta type-2

Chain V:



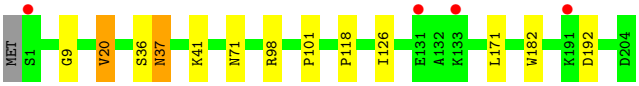
- Molecule 9: Proteasome subunit beta type-3

Chain I:

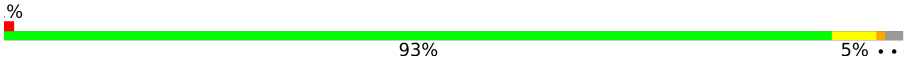


- Molecule 9: Proteasome subunit beta type-3

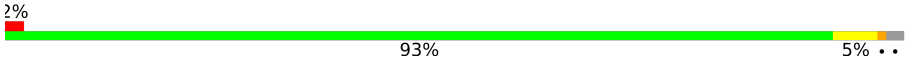
Chain W:

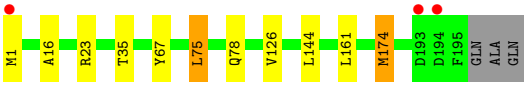


• Molecule 10: Proteasome subunit beta type-4

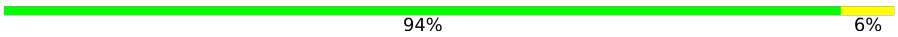
Chain J: 

• Molecule 10: Proteasome subunit beta type-4

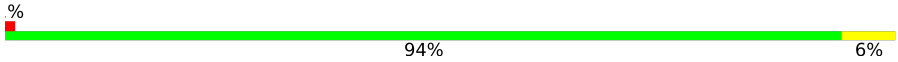
Chain X: 



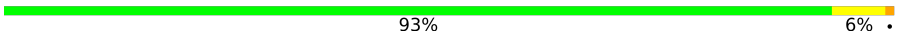
• Molecule 11: Proteasome subunit beta type-5

Chain K: 

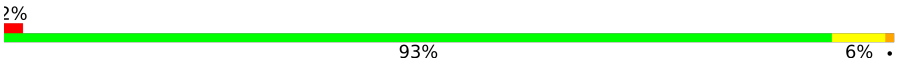
• Molecule 11: Proteasome subunit beta type-5

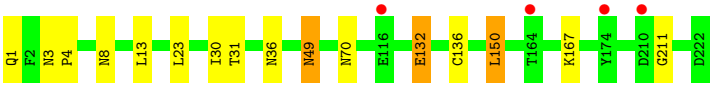
Chain Y: 

• Molecule 12: Proteasome subunit beta type-6

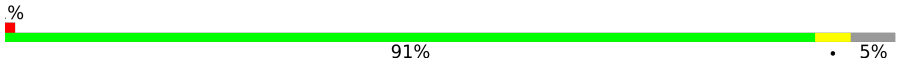
Chain L: 

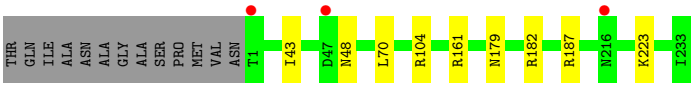
• Molecule 12: Proteasome subunit beta type-6

Chain Z: 



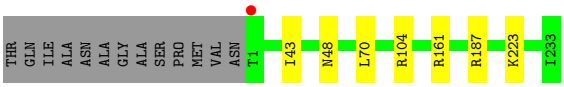
• Molecule 13: Proteasome subunit beta type-7

Chain M: 

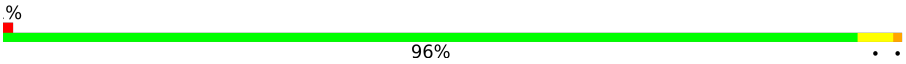


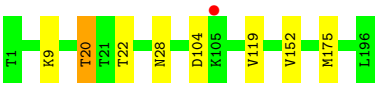
• Molecule 13: Proteasome subunit beta type-7

Chain a:

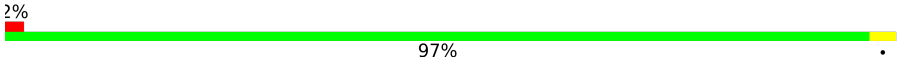


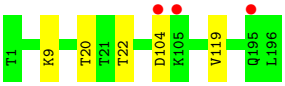
• Molecule 14: Proteasome subunit beta type-1

Chain N: 



• Molecule 14: Proteasome subunit beta type-1

Chain b: 



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.99Å 299.93Å 145.50Å 90.00° 113.23° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (15.00-2.70) 98.8 (15.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.175 , 0.206 0.180 , 0.208	Depositor DCC
R_{free} test set	14449 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	58.7	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	49859	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GT5, 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	0.38	0/1952	0.59	0/2642
1	O	0.38	0/1952	0.59	0/2642
2	B	0.37	0/1934	0.62	0/2618
2	P	0.37	0/1934	0.62	0/2618
3	C	0.39	0/1910	0.66	0/2586
3	Q	0.39	0/1910	0.66	0/2586
4	D	0.38	0/1837	0.60	0/2475
4	R	0.38	0/1837	0.60	0/2475
5	E	0.38	0/1800	0.59	1/2433 (0.0%)
5	S	0.38	0/1800	0.60	1/2433 (0.0%)
6	F	0.37	0/1932	0.57	0/2609
6	T	0.37	0/1932	0.57	0/2609
7	G	0.38	0/1945	0.58	0/2634
7	U	0.38	0/1945	0.58	0/2634
8	H	0.35	0/1715	0.58	0/2326
8	V	0.35	0/1715	0.58	0/2326
9	I	0.37	0/1611	0.59	0/2174
9	W	0.37	0/1611	0.59	0/2174
10	J	0.36	0/1589	0.61	0/2142
10	X	0.36	0/1589	0.61	0/2142
11	K	0.36	0/1681	0.59	0/2274
11	Y	0.35	0/1681	0.60	0/2274
12	L	0.38	0/1795	0.60	0/2420
12	Z	0.38	0/1795	0.60	0/2420
13	M	0.38	0/1855	0.65	0/2514
13	a	0.38	0/1855	0.65	0/2514
14	N	0.35	0/1541	0.58	0/2087
14	b	0.35	0/1541	0.57	0/2087
All	All	0.37	0/50194	0.60	2/67868 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	71	LEU	CA-CB-CG	5.12	127.08	115.30
5	S	71	LEU	CA-CB-CG	5.02	126.85	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	2	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	8	0
2	P	1904	0	1904	5	0
3	C	1881	0	1895	10	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	6	0
5	S	1773	0	1775	6	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	1	0
7	U	1907	0	1901	1	0
8	H	1684	0	1687	2	0
8	V	1684	0	1687	1	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	8	0
10	J	1561	0	1569	4	0
10	X	1561	0	1569	4	0
11	K	1644	0	1594	8	0
11	Y	1644	0	1594	7	0
12	L	1757	0	1711	9	0
12	Z	1757	0	1711	9	0
13	M	1824	0	1832	1	0
13	a	1824	0	1832	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1512	0	1481	2	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	H	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	Z	1	0	0	0	0
16	H	40	0	0	0	0
16	K	40	0	0	1	0
16	V	40	0	0	0	0
16	Y	40	0	0	1	0
17	A	13	0	0	0	0
17	B	21	0	0	0	0
17	C	18	0	0	0	0
17	D	13	0	0	0	0
17	E	8	0	0	0	0
17	F	11	0	0	0	0
17	G	14	0	0	0	0
17	H	17	0	0	0	0
17	I	14	0	0	0	0
17	J	19	0	0	0	0
17	K	24	0	0	0	0
17	L	21	0	0	0	0
17	M	21	0	0	0	0
17	N	10	0	0	0	0
17	O	11	0	0	0	0
17	P	15	0	0	0	0
17	Q	16	0	0	0	0
17	R	8	0	0	0	0
17	S	4	0	0	0	0
17	T	11	0	0	0	0
17	U	11	0	0	0	0
17	V	12	0	0	0	0
17	W	6	0	0	0	0
17	X	12	0	0	0	0
17	Y	20	0	0	0	0
17	Z	11	0	0	0	0
17	a	17	0	0	0	0
17	b	17	0	0	0	0
All	All	49859	0	49064	95	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 (95) 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)
11:K:31:VAL:HA	12:L:132:GLU:OE1	1.69	0.91
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.57	0.69
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.58	0.68
11:Y:31:VAL:HA	12:Z:132:GLU:OE1	1.97	0.65
3:C:202:GLN:O	3:C:203:THR:OG1	2.15	0.65
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.47	0.63
3:Q:202:GLN:O	3:Q:203:THR:OG1	2.15	0.62
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.65	0.62
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.65	0.61
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.84	0.60
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.83	0.59
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.84	0.59
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.50	0.58
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.50	0.57
5:S:12:PHE:H	6:T:19:GLN:HE22	1.50	0.57
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.86	0.57
3:C:198:LEU:HA	3:C:201:VAL:HG12	1.88	0.56
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.52	0.56
5:E:12:PHE:H	6:F:19:GLN:HE22	1.52	0.55
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.89	0.55
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.05	0.54
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.90	0.53
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.91	0.53
7:G:23:PHE:O	7:G:26:THR:HB	2.09	0.53
6:T:123:ASN:HD22	6:T:124:SER:N	2.06	0.52
6:F:123:ASN:HD22	6:F:124:SER:N	2.07	0.52
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.58	0.52
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.10	0.51
3:C:9:PHE:H	4:D:15:GLN:HE22	1.57	0.51
11:K:31:VAL:HG11	16:K:301:GT5:C23	2.40	0.51
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.51
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.93	0.51
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.09	0.51
10:J:174:MET:HA	10:X:174:MET:HA	1.93	0.50
3:C:201:VAL:O	3:C:202:GLN:HB2	2.10	0.50
11:Y:31:VAL:HG11	16:Y:301:GT5:C23	2.41	0.50
2:B:12:PHE:H	3:C:17:GLN:HE22	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.11	0.49
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.77	0.49
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.79	0.48
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.11	0.48
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.79	0.48
14:N:152:VAL:HA	14:N:175:MET:HE1	1.95	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.97	0.47
11:K:176:ASN:ND2	11:K:190:ASN:HD22	2.13	0.47
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.46	0.46
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.98	0.46
11:K:100:MET:CE	11:K:127:PHE:HB2	2.47	0.45
11:Y:176:ASN:ND2	11:Y:190:ASN:HD22	2.15	0.45
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.45
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.99	0.45
9:I:98:ARG:O	9:I:126:ILE:HD11	2.17	0.45
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.46	0.45
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.98	0.45
9:W:98:ARG:O	9:W:126:ILE:HD11	2.17	0.45
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.82	0.45
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.98	0.44
12:L:8:ASN:HA	12:L:30:ILE:O	2.17	0.44
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.18	0.44
6:F:123:ASN:HD22	6:F:123:ASN:C	2.20	0.44
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.99	0.44
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.16	0.44
6:T:123:ASN:HD22	6:T:123:ASN:C	2.19	0.43
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.53	0.43
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.00	0.43
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.15	0.43
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.53	0.43
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.01	0.43
1:A:12:PHE:H	2:B:20:GLN:HE22	1.65	0.43
3:C:38:ASN:C	3:C:38:ASN:HD22	2.21	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.01	0.42
1:O:12:PHE:H	2:P:20:GLN:HE22	1.68	0.42
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.02	0.42
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.85	0.42
3:Q:38:ASN:HD22	3:Q:38:ASN:C	2.23	0.42
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.85	0.42
11:K:37:ILE:HG23	11:K:60:GLY:HA2	2.02	0.41
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:ASN:OD1	2:B:220:ASN:N	2.53	0.41
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.02	0.41
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.01	0.41
9:I:101:PRO:HB3	9:I:126:ILE:HD12	2.03	0.41
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.02	0.41
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.02	0.41
5:E:118:ASN:HD22	5:E:118:ASN:N	2.18	0.41
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.01	0.41
4:R:155:THR:HG23	5:S:59:GLN:HE22	1.86	0.41
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.02	0.41
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.02	0.41
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	2.02	0.41
14:N:20:THR:CG2	14:N:28:ASN:HB3	2.51	0.40
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.03	0.40
2:P:220:ASN:OD1	2:P:220:ASN:N	2.54	0.40
9:W:101:PRO:HB3	9:W:126:ILE:HD12	2.03	0.40
11:K:209:ASN:O	9:W:37:ASN:ND2	2.54	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%)	243 (98%)	5 (2%)	0	100	100
1	O	248/250 (99%)	243 (98%)	5 (2%)	0	100	100
2	B	242/258 (94%)	235 (97%)	6 (2%)	1 (0%)	34	60
2	P	242/258 (94%)	235 (97%)	6 (2%)	1 (0%)	34	60
3	C	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	19	43
3	Q	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	19	43
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (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%)	6 (3%)	0	100	100
8	V	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
10	X	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
13	a	231/246 (94%)	224 (97%)	7 (3%)	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%)	6131 (98%)	139 (2%)	6 (0%)	51	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	203	THR
3	Q	203	THR
2	B	51	VAL
2	P	51	VAL
3	C	204	GLY
3	Q	204	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	204 (98%)	5 (2%)	49	77
1	O	209/209 (100%)	204 (98%)	5 (2%)	49	77
2	B	203/216 (94%)	195 (96%)	8 (4%)	32	61
2	P	203/216 (94%)	195 (96%)	8 (4%)	32	61
3	C	212/226 (94%)	205 (97%)	7 (3%)	38	67
3	Q	212/226 (94%)	205 (97%)	7 (3%)	38	67
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	54
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	54
5	E	190/193 (98%)	179 (94%)	11 (6%)	20	43
5	S	190/193 (98%)	178 (94%)	12 (6%)	18	40
6	F	201/239 (84%)	190 (94%)	11 (6%)	21	46
6	T	201/239 (84%)	190 (94%)	11 (6%)	21	46
7	G	206/210 (98%)	198 (96%)	8 (4%)	32	61
7	U	206/210 (98%)	198 (96%)	8 (4%)	32	61
8	H	181/190 (95%)	176 (97%)	5 (3%)	43	73
8	V	181/190 (95%)	176 (97%)	5 (3%)	43	73
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	78
9	W	172/173 (99%)	167 (97%)	5 (3%)	42	71
10	J	173/175 (99%)	166 (96%)	7 (4%)	31	60
10	X	173/175 (99%)	166 (96%)	7 (4%)	31	60
11	K	169/169 (100%)	165 (98%)	4 (2%)	49	77
11	Y	169/169 (100%)	165 (98%)	4 (2%)	49	77
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	62
12	Z	185/185 (100%)	178 (96%)	7 (4%)	33	62
13	M	199/208 (96%)	192 (96%)	7 (4%)	36	65
13	a	199/208 (96%)	192 (96%)	7 (4%)	36	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	69
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	69
All	All	5312/5540 (96%)	5114 (96%)	198 (4%)	34	63

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	THR
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
2	B	50	LYS
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	119	GLN
2	B	191	LEU
2	B	220	ASN
2	B	223	GLU
3	C	4	ARG
3	C	38	ASN
3	C	61	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
4	D	20	LEU
4	D	40	LEU
4	D	99	ILE
4	D	117	GLU
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	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU

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Mol	Chain	Res	Type
5	E	71	LEU
5	E	99	ASN
5	E	116	GLN
5	E	174	THR
5	E	184	ASN
5	E	188	LEU
6	F	14	ASP
6	F	59	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
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
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	34	LEU
8	H	68	LEU
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
9	I	192	ASP
10	J	1	MET
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	9	GLN

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Mol	Chain	Res	Type
11	K	35	ILE
11	K	106	ARG
11	K	118	ASP
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	132	GLU
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	223	LYS
14	N	9	LYS
14	N	20	THR
14	N	22	THR
14	N	104	ASP
14	N	119	VAL
1	O	1	MET
1	O	2	THR
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	79	LEU
2	P	119	GLN
2	P	191	LEU
2	P	220	ASN
2	P	223	GLU
3	Q	4	ARG
3	Q	38	ASN
3	Q	61	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS

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Mol	Chain	Res	Type
4	R	20	LEU
4	R	40	LEU
4	R	99	ILE
4	R	117	GLU
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	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	99	ASN
5	S	116	GLN
5	S	174	THR
5	S	184	ASN
5	S	188	LEU
5	S	207	VAL
6	T	14	ASP
6	T	59	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
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
7	U	236	LEU
8	V	30	ASN
8	V	34	LEU

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Mol	Chain	Res	Type
8	V	68	LEU
8	V	127	LEU
8	V	196	ARG
11	Y	9	GLN
11	Y	35	ILE
11	Y	106	ARG
11	Y	118	ASP
9	W	20	VAL
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
9	W	192	ASP
10	X	1	MET
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	78	GLN
10	X	144	LEU
10	X	174	MET
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	132	GLU
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
13	a	223	LYS
14	b	9	LYS
14	b	20	THR
14	b	22	THR
14	b	104	ASP
14	b	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) 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	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	146	GLN
4	D	160	ASN
4	D	225	ASN
5	E	59	GLN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	147	GLN
5	E	184	ASN
6	F	19	GLN
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	167	GLN
7	G	175	ASN
8	H	30	ASN
8	H	57	GLN
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
10	J	55	GLN

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Mol	Chain	Res	Type
10	J	118	GLN
10	J	191	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	159	GLN
12	L	165	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
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
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	146	GLN
4	R	160	ASN
4	R	225	ASN
5	S	59	GLN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN

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Mol	Chain	Res	Type
5	S	120	GLN
5	S	147	GLN
5	S	184	ASN
6	T	19	GLN
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	167	GLN
7	U	175	ASN
8	V	30	ASN
8	V	57	GLN
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
11	Y	85	ASN
11	Y	176	ASN
10	X	55	GLN
10	X	86	GLN
10	X	118	GLN
10	X	191	GLN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	158	ASN
12	Z	159	GLN
12	Z	165	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	194	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
16	GT5	K	301	11	38,41,41	1.61	6 (15%)	48,56,56	1.48	8 (16%)
16	GT5	Y	301	11	38,41,41	1.68	8 (21%)	48,56,56	1.44	9 (18%)
16	GT5	V	301	8	38,41,41	1.73	7 (18%)	48,56,56	1.64	13 (27%)
16	GT5	H	301	8	38,41,41	1.74	7 (18%)	48,56,56	1.60	13 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	GT5	K	301	11	-	7/39/43/43	0/2/2/2
16	GT5	Y	301	11	-	7/39/43/43	0/2/2/2
16	GT5	V	301	8	-	3/39/43/43	0/2/2/2
16	GT5	H	301	8	-	3/39/43/43	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	301	GT5	C3-S5	-4.64	1.59	1.73
16	Y	301	GT5	C16-C17	-4.50	1.40	1.51
16	K	301	GT5	C3-S5	-4.44	1.59	1.73
16	K	301	GT5	C16-C17	-4.35	1.40	1.51
16	H	301	GT5	C16-C17	-4.25	1.41	1.51
16	V	301	GT5	C16-C17	-4.23	1.41	1.51
16	H	301	GT5	C3-S5	-4.22	1.60	1.73
16	V	301	GT5	C3-S5	-4.15	1.60	1.73
16	H	301	GT5	C26-S27	3.98	1.83	1.78
16	V	301	GT5	C26-S27	3.94	1.83	1.78
16	H	301	GT5	O29-S27	3.85	1.52	1.44
16	V	301	GT5	O29-S27	3.81	1.52	1.44
16	K	301	GT5	O29-S27	3.79	1.52	1.44
16	V	301	GT5	O30-S27	3.75	1.52	1.44
16	Y	301	GT5	O30-S27	3.72	1.52	1.44
16	H	301	GT5	O30-S27	3.72	1.52	1.44
16	Y	301	GT5	O29-S27	3.70	1.52	1.44
16	K	301	GT5	O30-S27	3.69	1.52	1.44
16	H	301	GT5	C25-C26	3.34	1.56	1.52
16	V	301	GT5	C25-C26	3.21	1.55	1.52
16	V	301	GT5	C21-C20	-3.07	1.40	1.51
16	H	301	GT5	C21-C20	-3.04	1.40	1.51
16	Y	301	GT5	C21-C20	-3.00	1.41	1.51
16	K	301	GT5	C21-C20	-2.93	1.41	1.51
16	Y	301	GT5	C26-S27	2.70	1.82	1.78
16	Y	301	GT5	C25-C26	2.39	1.55	1.52
16	K	301	GT5	C26-S27	2.34	1.81	1.78
16	Y	301	GT5	C1-C6	-2.28	1.34	1.37

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	K	301	GT5	O29-S27-C26	-4.20	105.40	108.34
16	H	301	GT5	O30-S27-C26	4.15	111.25	108.34
16	V	301	GT5	O30-S27-O29	-4.06	108.42	117.09
16	V	301	GT5	O30-S27-C26	4.05	111.18	108.34
16	H	301	GT5	O30-S27-O29	-3.96	108.63	117.09
16	Y	301	GT5	O30-S27-O29	-3.67	109.25	117.09
16	Y	301	GT5	O29-S27-C26	-3.42	105.95	108.34
16	K	301	GT5	O30-S27-O29	-3.35	109.93	117.09
16	V	301	GT5	C12-C13-N14	-3.28	109.52	116.70
16	H	301	GT5	C12-C13-N14	-3.17	109.75	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	301	GT5	C32-C12-C13	-3.17	102.88	110.32
16	H	301	GT5	C32-C12-C13	-3.11	103.01	110.32
16	V	301	GT5	C4-C3-S5	2.72	123.78	120.12
16	Y	301	GT5	C40-C9-C10	-2.70	104.14	110.57
16	K	301	GT5	C32-C12-C13	-2.68	104.03	110.32
16	K	301	GT5	C40-C9-C10	-2.66	104.24	110.57
16	Y	301	GT5	C32-C12-C13	-2.62	104.16	110.32
16	K	301	GT5	C4-C3-S5	2.60	123.62	120.12
16	K	301	GT5	C28-S27-C26	2.60	115.23	105.21
16	V	301	GT5	C40-C9-N8	-2.57	104.65	110.58
16	H	301	GT5	C40-C9-N8	-2.54	104.71	110.58
16	Y	301	GT5	C28-S27-C26	2.47	114.72	105.21
16	H	301	GT5	C10-C9-N8	-2.46	104.45	111.16
16	Y	301	GT5	C12-C13-N14	-2.44	111.35	116.70
16	V	301	GT5	C10-C9-N8	-2.44	104.52	111.16
16	V	301	GT5	C16-C17-C24	2.42	125.70	120.91
16	V	301	GT5	C16-C17-C18	-2.41	116.13	120.91
16	H	301	GT5	C4-C3-S5	2.39	123.33	120.12
16	Y	301	GT5	C4-C3-S5	2.37	123.31	120.12
16	H	301	GT5	O29-S27-C26	-2.34	106.70	108.34
16	H	301	GT5	C16-C17-C24	2.32	125.51	120.91
16	K	301	GT5	C12-C13-N14	-2.31	111.63	116.70
16	H	301	GT5	C16-C17-C18	-2.29	116.35	120.91
16	V	301	GT5	C28-S27-C26	2.24	113.86	105.21
16	V	301	GT5	O31-C13-N14	2.18	126.96	122.93
16	H	301	GT5	C28-S27-C26	2.17	113.58	105.21
16	H	301	GT5	O31-C13-N14	2.16	126.94	122.93
16	K	301	GT5	O29-S27-C28	-2.16	106.73	108.91
16	V	301	GT5	O29-S27-C28	-2.15	106.74	108.91
16	V	301	GT5	C6-C1-N2	2.10	113.31	109.09
16	H	301	GT5	C6-C1-N2	2.05	113.20	109.09
16	Y	301	GT5	C6-C1-N2	2.00	113.11	109.09
16	Y	301	GT5	C16-C15-N14	-2.00	106.54	110.39

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	K	301	GT5	C25-C26-S27-O29
16	K	301	GT5	C25-C26-S27-O30
16	Y	301	GT5	C25-C26-S27-O29
16	Y	301	GT5	C25-C26-S27-O30

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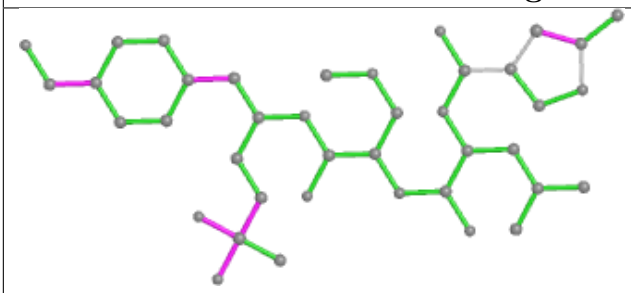
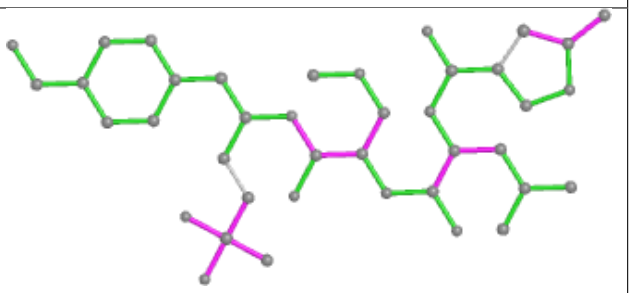
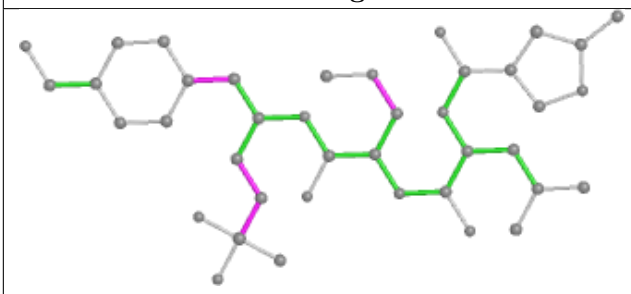
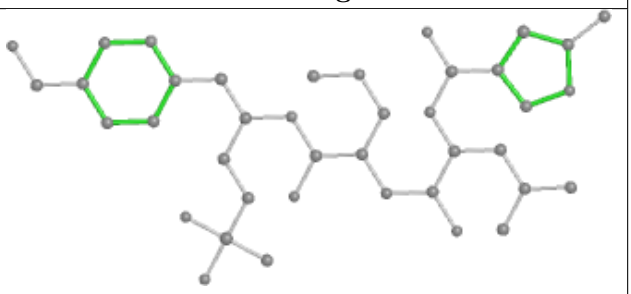
Mol	Chain	Res	Type	Atoms
16	V	301	GT5	C15-C16-C17-C24
16	H	301	GT5	C15-C16-C17-C24
16	V	301	GT5	C15-C16-C17-C18
16	H	301	GT5	C15-C16-C17-C18
16	Y	301	GT5	C15-C16-C17-C24
16	K	301	GT5	C15-C16-C17-C24
16	Y	301	GT5	C15-C16-C17-C18
16	K	301	GT5	C15-C16-C17-C18
16	H	301	GT5	C25-C26-S27-C28
16	K	301	GT5	C25-C26-S27-C28
16	V	301	GT5	C25-C26-S27-C28
16	Y	301	GT5	C25-C26-S27-C28
16	K	301	GT5	C12-C32-O36-C34
16	Y	301	GT5	C12-C32-O36-C34
16	K	301	GT5	C15-C25-C26-S27
16	Y	301	GT5	C15-C25-C26-S27

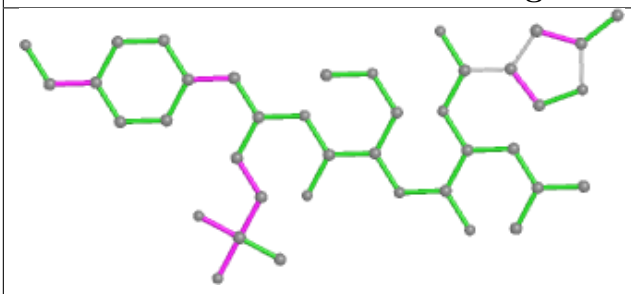
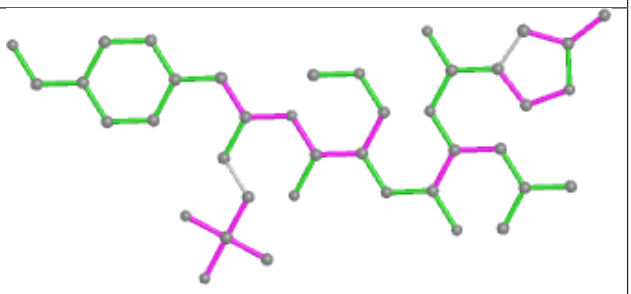
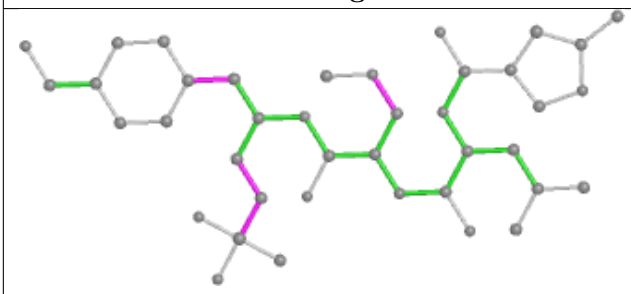
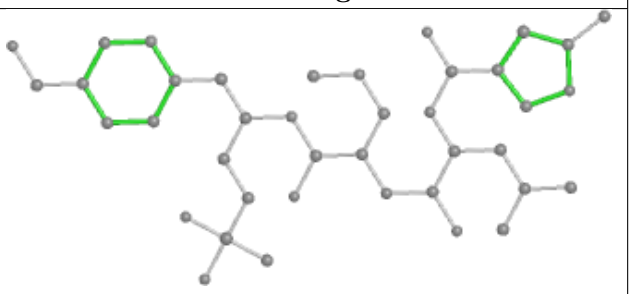
There are no ring outliers.

2 monomers are involved in 2 short contacts:

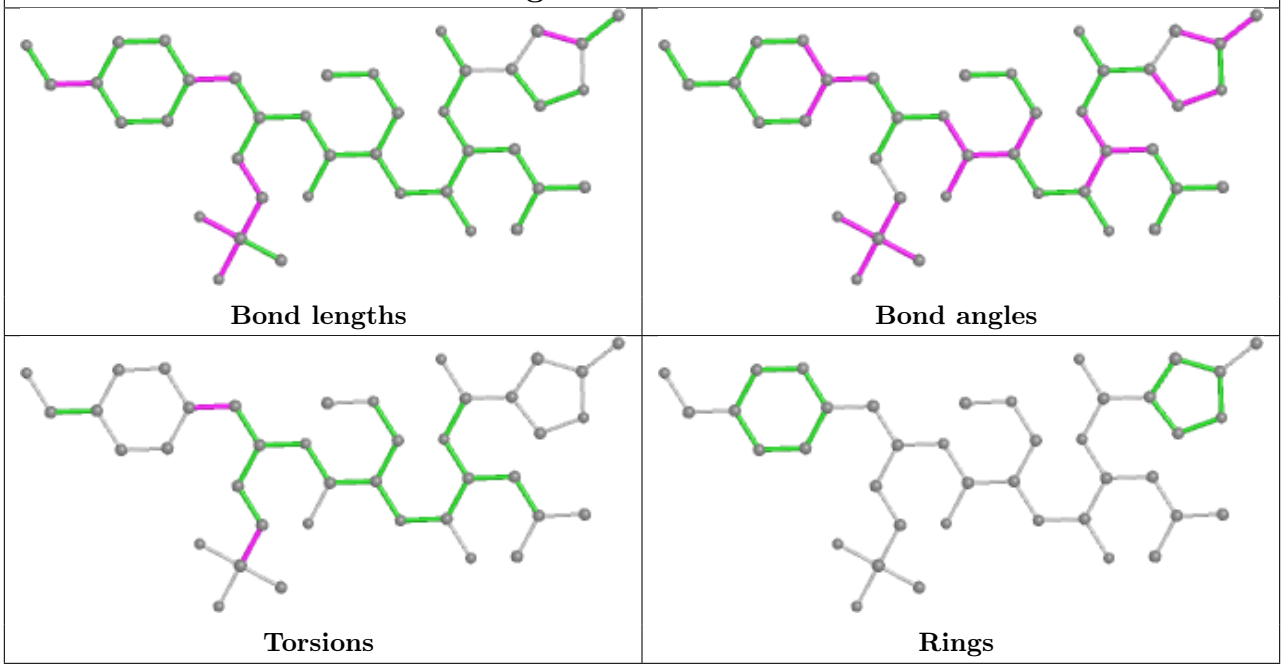
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	301	GT5	1	0
16	Y	301	GT5	1	0

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.

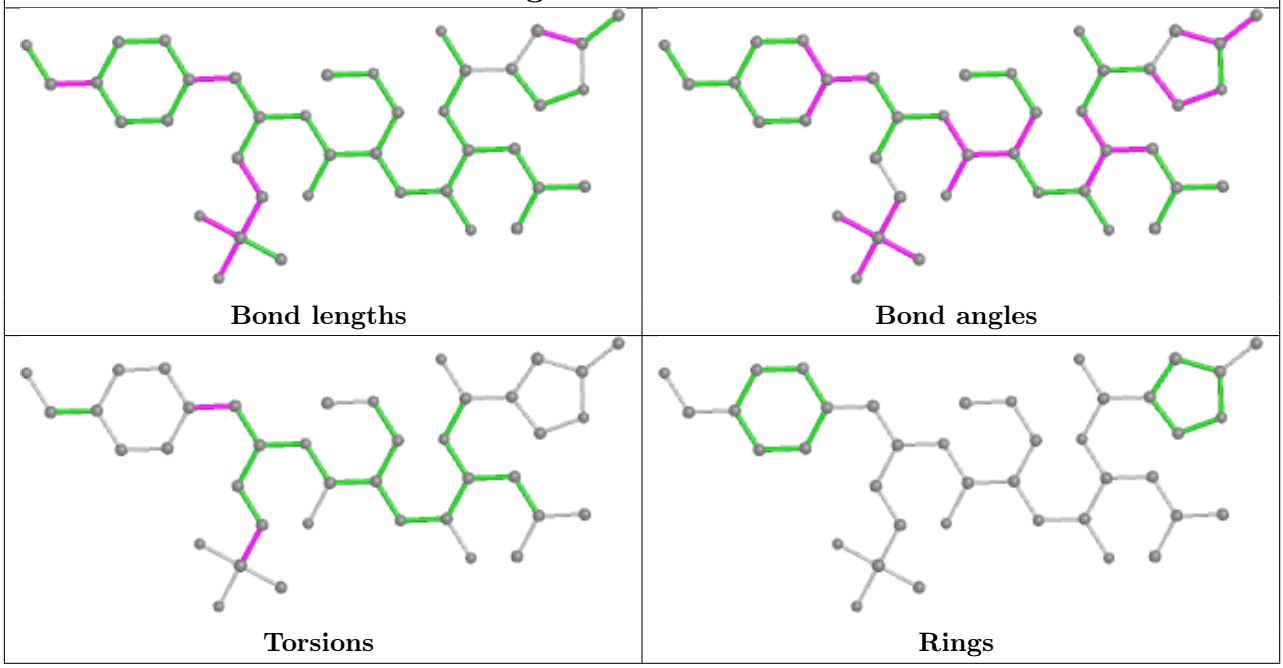
Ligand GT5 K 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GT5 Y 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GT5 V 301



Ligand GT5 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.27	10 (4%)	38	37	47, 62, 100, 137	0
1	O	250/250 (100%)	-0.24	8 (3%)	47	48	49, 67, 109, 140	0
2	B	244/258 (94%)	-0.18	10 (4%)	37	36	47, 63, 112, 175	0
2	P	244/258 (94%)	-0.16	13 (5%)	26	25	50, 67, 115, 177	0
3	C	240/254 (94%)	-0.10	17 (7%)	16	14	47, 66, 129, 160	0
3	Q	240/254 (94%)	0.10	21 (8%)	10	8	54, 81, 157, 196	0
4	D	235/260 (90%)	-0.35	3 (1%)	77	78	49, 69, 102, 145	0
4	R	235/260 (90%)	-0.24	6 (2%)	56	57	52, 73, 108, 151	0
5	E	231/234 (98%)	-0.19	9 (3%)	39	38	55, 74, 108, 149	0
5	S	231/234 (98%)	-0.12	7 (3%)	50	51	53, 77, 116, 150	0
6	F	243/288 (84%)	-0.33	9 (3%)	41	41	48, 68, 117, 145	0
6	T	243/288 (84%)	-0.26	10 (4%)	37	36	45, 71, 120, 153	0
7	G	241/252 (95%)	-0.29	6 (2%)	57	59	46, 62, 102, 151	0
7	U	241/252 (95%)	-0.38	4 (1%)	70	72	46, 62, 94, 136	0
8	H	222/232 (95%)	-0.26	4 (1%)	68	70	48, 60, 93, 135	0
8	V	222/232 (95%)	-0.26	3 (1%)	75	77	48, 63, 92, 141	0
9	I	204/205 (99%)	-0.58	2 (0%)	82	83	42, 56, 83, 107	0
9	W	204/205 (99%)	-0.54	4 (1%)	65	67	43, 57, 86, 110	0
10	J	195/198 (98%)	-0.51	2 (1%)	82	83	43, 56, 79, 128	0
10	X	195/198 (98%)	-0.50	3 (1%)	73	76	45, 57, 81, 134	0
11	K	212/212 (100%)	-0.54	1 (0%)	91	92	44, 56, 79, 105	0
11	Y	212/212 (100%)	-0.54	2 (0%)	84	85	45, 57, 86, 107	0
12	L	222/222 (100%)	-0.47	1 (0%)	91	92	43, 59, 86, 108	0
12	Z	222/222 (100%)	-0.45	4 (1%)	68	70	43, 59, 89, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.51	3 (1%)	77	78	42, 59, 80, 94	0
13	a	233/246 (94%)	-0.53	1 (0%)	92	93	41, 57, 78, 92	0
14	N	196/196 (100%)	-0.49	1 (0%)	91	92	45, 54, 81, 107	0
14	b	196/196 (100%)	-0.52	3 (1%)	73	76	45, 55, 81, 100	0
All	All	6336/6614 (95%)	-0.34	167 (2%)	56	57	41, 62, 106, 196	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	7.5
2	P	219	ALA	7.3
8	V	221	CYS	6.4
5	S	202	ASP	6.4
2	B	219	ALA	6.3
3	C	206	LYS	6.0
2	B	220	ASN	6.0
3	Q	50	LEU	5.8
3	Q	206	LYS	5.8
8	H	221	CYS	5.8
2	B	221	ASP	5.7
8	V	222	ASP	5.5
3	Q	239	GLN	5.3
2	P	221	ASP	5.3
5	E	202	ASP	5.2
1	O	249	ALA	5.2
2	P	222	GLY	4.7
3	Q	238	LYS	4.5
3	Q	202	GLN	4.5
2	P	51	VAL	4.5
8	H	222	ASP	4.4
2	B	51	VAL	4.3
3	Q	48	SER	4.3
2	B	218	GLY	4.2
4	D	242	GLU	4.2
5	S	54	GLU	4.2
3	C	49	THR	4.2
1	A	231	LYS	4.1
3	Q	236	GLN	4.1
3	Q	240	GLU	4.1
10	X	194	ASP	4.0
2	P	220	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.9
4	R	242	GLU	3.8
3	C	202	GLN	3.8
1	A	250	LEU	3.8
5	S	233	ILE	3.7
5	E	233	ILE	3.6
11	Y	212	GLY	3.6
11	K	212	GLY	3.5
1	A	249	ALA	3.5
7	G	179	LYS	3.5
4	R	241	ALA	3.5
6	T	244	ASN	3.5
2	P	59	ASP	3.4
6	F	202	ASP	3.4
4	R	125	LEU	3.4
1	O	201	GLU	3.4
2	P	223	GLU	3.4
3	Q	51	LYS	3.3
10	J	1	MET	3.3
3	C	238	LYS	3.3
9	W	133	LYS	3.2
3	C	240	GLU	3.2
6	T	241	LYS	3.2
7	U	181	LYS	3.2
1	A	229	THR	3.2
2	P	218	GLY	3.1
4	D	241	ALA	3.1
6	F	244	ASN	3.1
5	S	225	ASP	3.1
10	J	194	ASP	3.1
6	F	205	GLU	3.1
1	O	229	THR	3.1
3	C	239	GLN	3.1
3	Q	205	ALA	3.0
13	a	1	THR	3.0
5	S	180	LYS	2.9
13	M	1	THR	2.9
10	X	193	ASP	2.9
9	W	1	SER	2.9
6	T	53	LYS	2.8
8	H	198	GLU	2.8
3	C	48	SER	2.8

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Mol	Chain	Res	Type	RSRZ
5	E	54	GLU	2.8
6	F	181	GLU	2.8
1	O	231	LYS	2.8
3	C	225	GLU	2.8
1	O	250	LEU	2.8
5	E	201	ARG	2.7
3	C	50	LEU	2.7
3	Q	203	THR	2.7
7	G	2	GLY	2.7
3	Q	59	PRO	2.7
3	C	216	ASP	2.7
7	U	241	GLU	2.7
6	F	241	LYS	2.7
3	Q	225	GLU	2.6
3	Q	141	ASP	2.6
3	C	203	THR	2.6
14	N	105	LYS	2.6
1	A	2	THR	2.6
4	D	125	LEU	2.6
2	P	60	THR	2.6
7	U	222	ASP	2.6
6	T	230	ASP	2.6
7	U	242	GLN	2.6
2	B	59	ASP	2.6
9	I	1	SER	2.6
1	A	228	PRO	2.5
3	C	236	GLN	2.5
6	T	180	PRO	2.5
2	B	203	SER	2.5
2	B	242	GLY	2.5
10	X	1	MET	2.5
1	A	248	GLU	2.5
9	I	133	LYS	2.5
11	Y	202	GLU	2.5
4	R	230	GLU	2.5
2	B	217	LYS	2.5
8	V	196	ARG	2.5
4	R	54	ASP	2.5
12	L	172	LEU	2.4
13	M	47	ASP	2.4
12	Z	174	TYR	2.4
2	P	182	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
5	E	218	ASP	2.4
3	Q	235	GLU	2.4
3	Q	180	LYS	2.4
5	E	123	GLY	2.4
1	O	52	SER	2.3
1	O	248	GLU	2.3
14	b	195	GLN	2.3
5	E	225	ASP	2.3
7	G	3	TYR	2.3
1	O	230	ASP	2.3
6	T	205	GLU	2.3
1	A	220	ASP	2.3
7	G	240	ALA	2.2
13	M	216	ASN	2.2
6	T	2	THR	2.2
14	b	104	ASP	2.2
3	Q	60	SER	2.2
5	S	204	SER	2.2
6	F	215	CYS	2.2
7	G	188	GLU	2.2
2	P	52	THR	2.2
2	P	225	TYR	2.2
3	C	235	GLU	2.2
6	F	201	GLU	2.2
7	G	242	GLN	2.2
8	H	215	GLU	2.1
5	E	176	ASP	2.1
12	Z	164	THR	2.1
2	P	203	SER	2.1
12	Z	210	ASP	2.1
5	S	3	ASN	2.1
6	T	243	ILE	2.1
5	E	227	GLU	2.1
9	W	131	GLU	2.1
3	C	180	LYS	2.1
3	Q	140	ASP	2.1
6	F	243	ILE	2.1
4	R	1	ASP	2.1
9	W	191	LYS	2.1
2	B	223	GLU	2.1
3	C	205	ALA	2.1
3	Q	237	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
6	T	181	GLU	2.1
3	C	51	LYS	2.0
3	Q	229	GLN	2.0
6	F	180	PRO	2.0
3	C	171	GLU	2.0
1	A	230	ASP	2.0
6	T	177	ASP	2.0
12	Z	116	GLU	2.0
14	b	105	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

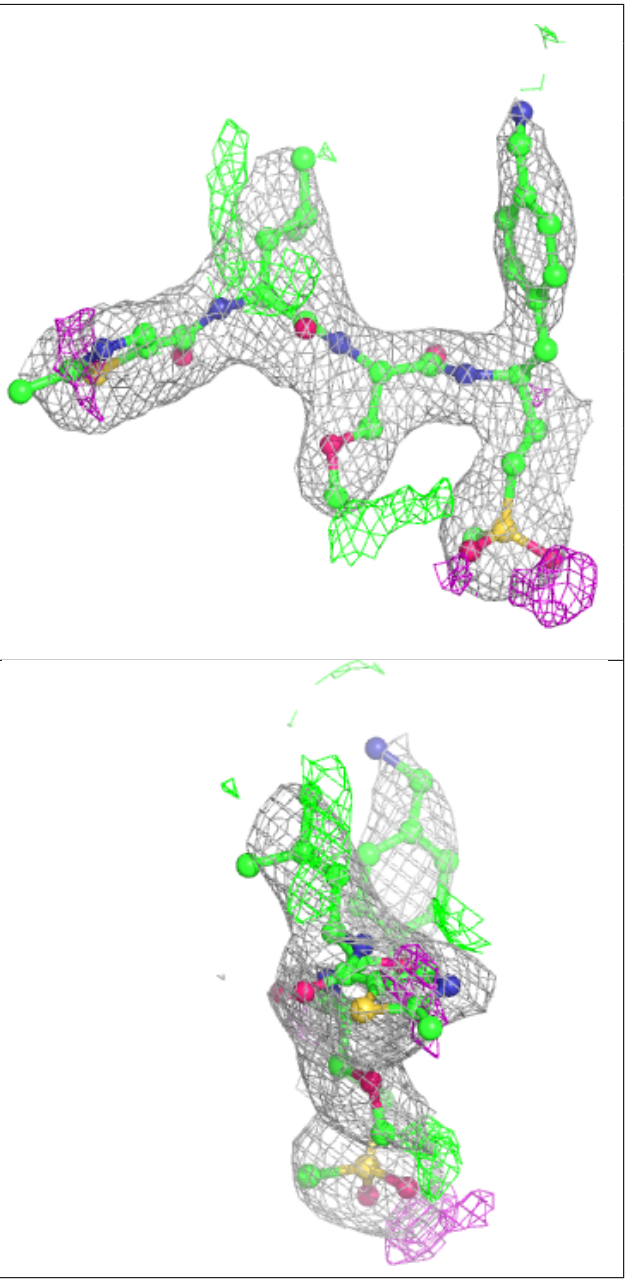
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	H	302	1/1	0.70	0.56	93,93,93,93	0
16	GT5	H	301	40/40	0.90	0.21	54,91,106,109	0
16	GT5	V	301	40/40	0.90	0.21	58,86,100,105	0
16	GT5	K	301	40/40	0.94	0.15	40,62,75,78	0
15	MG	I	301	1/1	0.94	0.12	69,69,69,69	0
16	GT5	Y	301	40/40	0.95	0.14	42,60,68,70	0
15	MG	Z	301	1/1	0.96	0.40	69,69,69,69	0
15	MG	N	201	1/1	0.97	0.14	50,50,50,50	0
15	MG	G	301	1/1	0.97	0.07	61,61,61,61	0
15	MG	I	302	1/1	0.98	0.10	64,64,64,64	0
15	MG	L	301	1/1	0.98	0.12	107,107,107,107	0
15	MG	K	302	1/1	0.99	0.06	69,69,69,69	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.

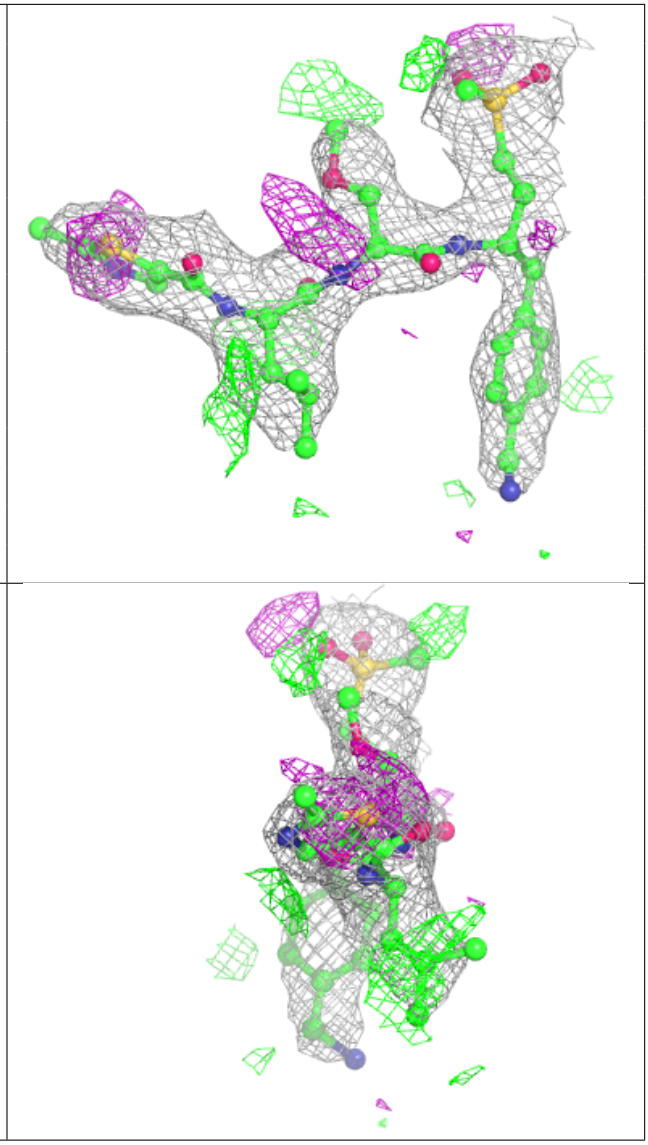
Electron density around GT5 H 301:

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



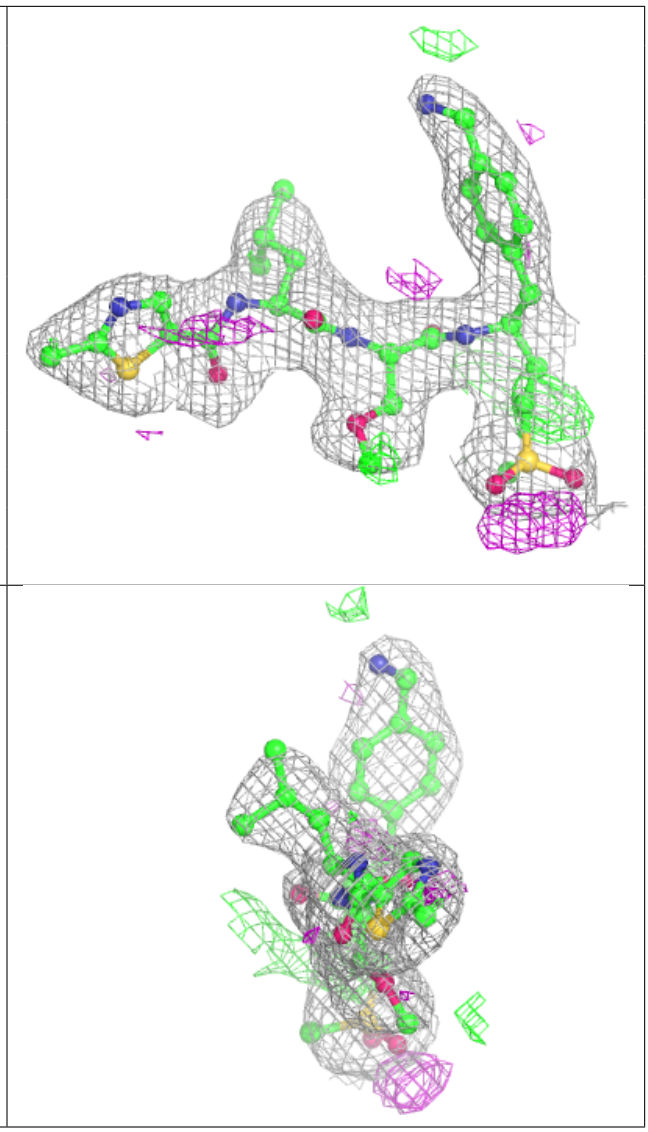
Electron density around GT5 V 301:

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



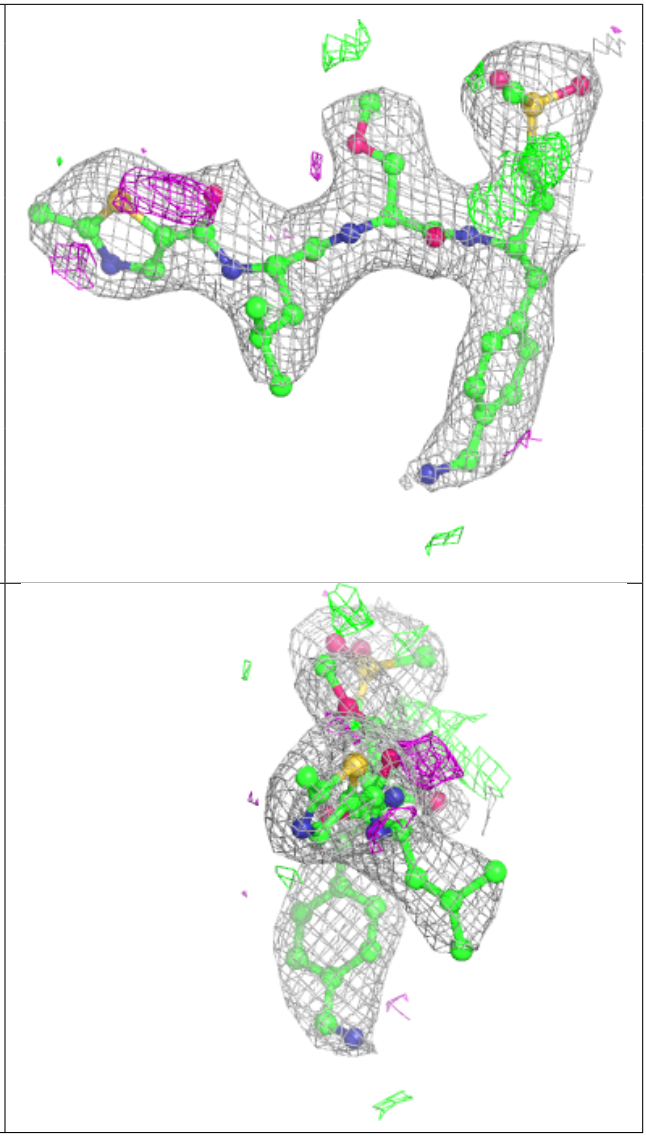
Electron density around GT5 K 301:

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



Electron density around GT5 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.