Full wwPDB X-ray Structure Validation Report (i)

Jan 2, 2024 – 08:57 pm GMT

PDB ID	:	5JHS
Title	:	Yeast 20S proteasome in complex with the peptidic epoxyketone inhibitor 15
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2016-04-21
Resolution	:	3.00 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:

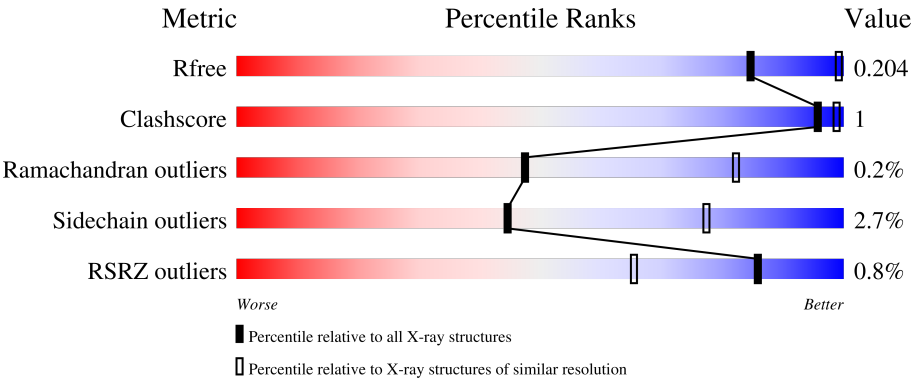
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	98%
1	O	250	98%
2	B	258	89% 5%
2	P	258	90% 5%
3	C	254	90% 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	4% 91% 6%
4	D	260	87% 10%
4	R	260	87% 10%
5	E	234	95%
5	S	234	93% 6%
6	F	288	81% 16%
6	T	288	81% 16%
7	G	252	91% 5%
7	U	252	% 91% 5%
8	H	232	% 92%
8	V	232	% 93%
9	I	205	95% 5%
9	W	205	96%
10	J	198	% 92% 5%
10	X	198	2% 92% 5%
11	K	212	94% 6%
11	Y	212	93% 6%
12	L	222	94% 5%
12	Z	222	94% 5%
13	M	246	90% 5%
13	a	246	92% 5%
14	N	196	98%
14	b	196	99%

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
17	6KG	H	301	-	-	-	X

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 49501 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	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	241	Total	C	N	O	S	0	0	0
			1906	1214	320	364	8			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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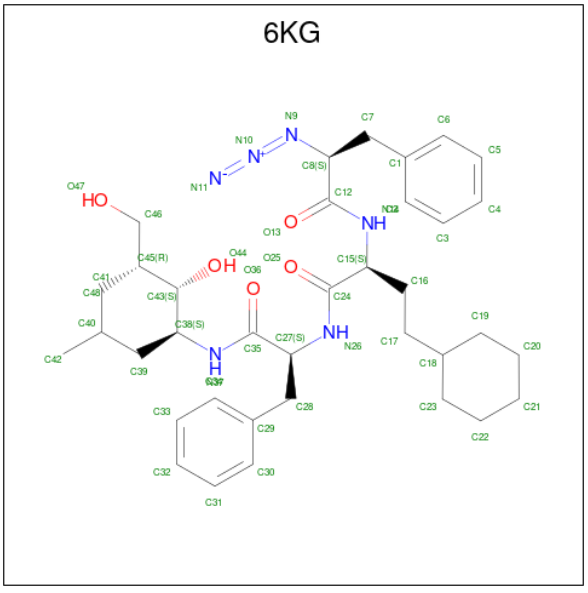
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

- 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 Nalpha-[(2S)-2-{[(2S)-2-azido-3-phenylpropanoyl]amino}-4-cyclohexylbutanoyl]-N-[(2R,3S,4S)-1,3-dihydroxy-2,6-dimethylheptan-4-yl]-L-phenylalaninamide (three-letter code: 6KG) (formula: $C_{37}H_{54}N_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	1	Total C N O 48 37 6 5	0	0
17	K	1	Total C N O 48 37 6 5	0	0

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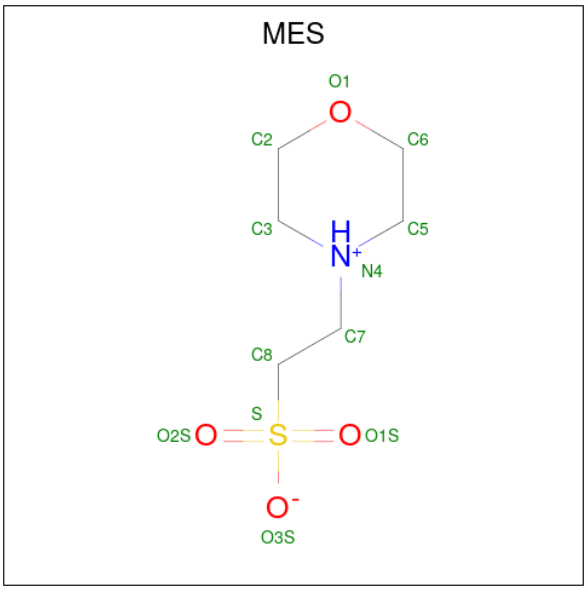
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	Y	1	Total C N O 48 37 6 5	0	0

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	H	1	Total C N O S 12 6 1 4 1	0	0
18	K	1	Total C N O S 12 6 1 4 1	0	0
18	V	1	Total C N O S 12 6 1 4 1	0	0
18	Y	1	Total C N O S 12 6 1 4 1	0	0

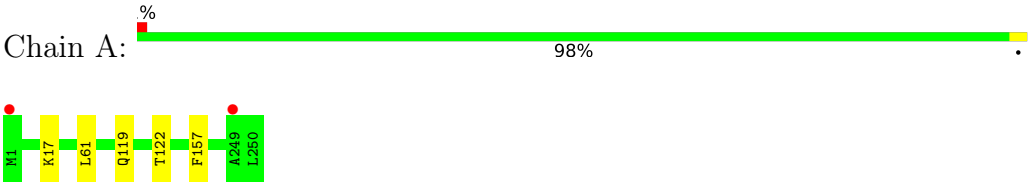
- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	N	1	Total O 1 1	0	0
19	V	1	Total O 1 1	0	0
19	W	2	Total O 2 2	0	0
19	b	1	Total O 1 1	0	0

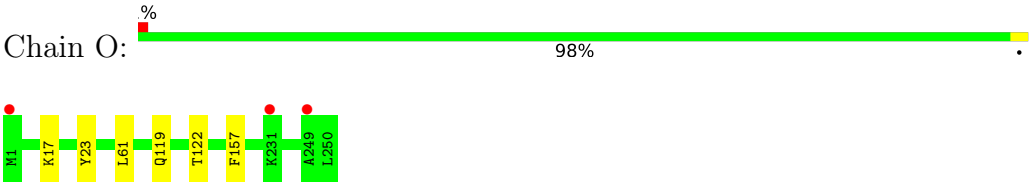
3 Residue-property plots (i)

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.

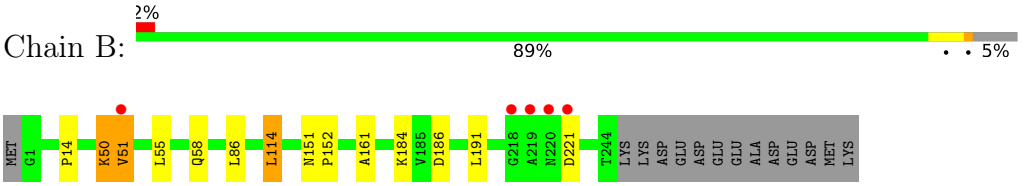
• Molecule 1: Proteasome subunit alpha type-2



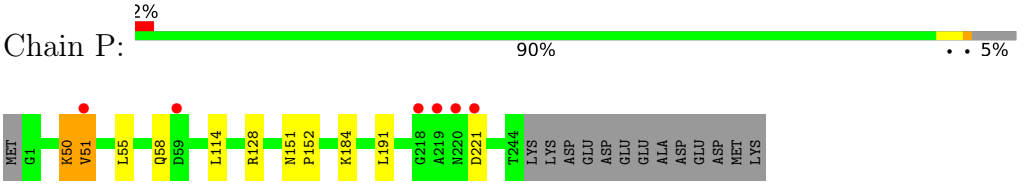
• Molecule 1: Proteasome subunit alpha type-2



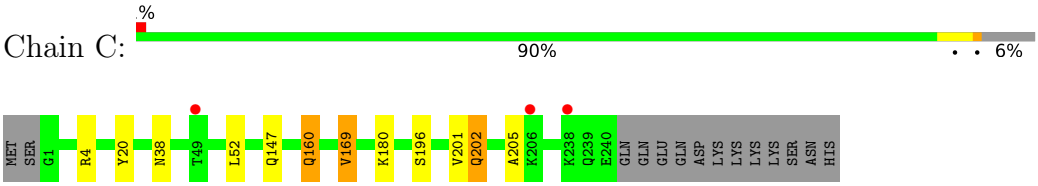
• Molecule 2: Proteasome subunit alpha type-3



• Molecule 2: Proteasome subunit alpha type-3

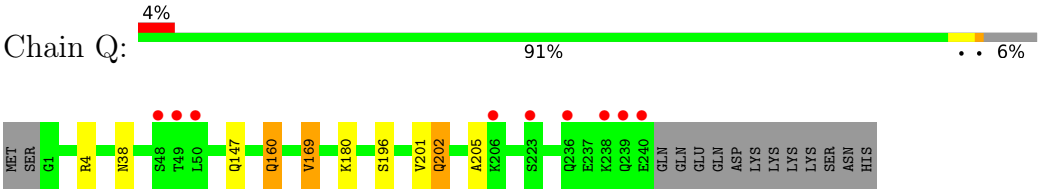


• Molecule 3: Proteasome subunit alpha type-4



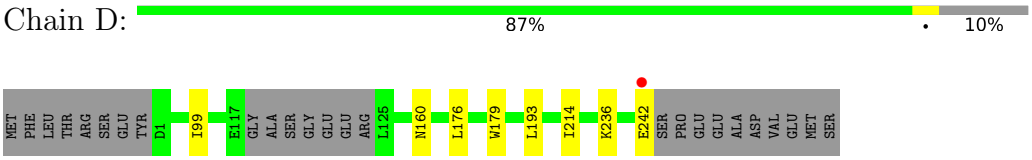
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



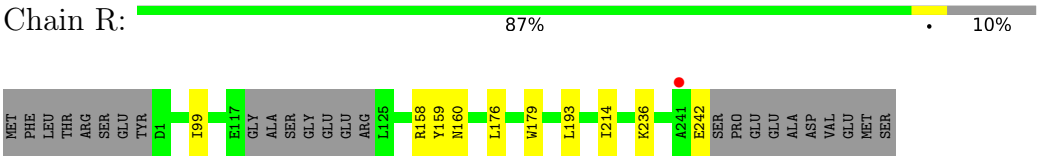
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



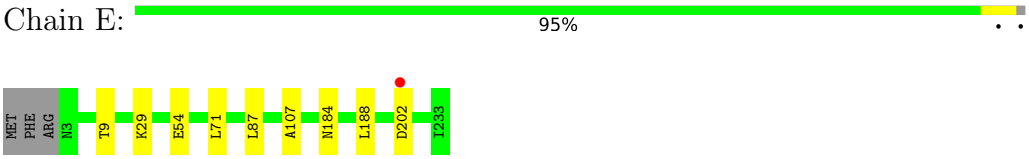
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



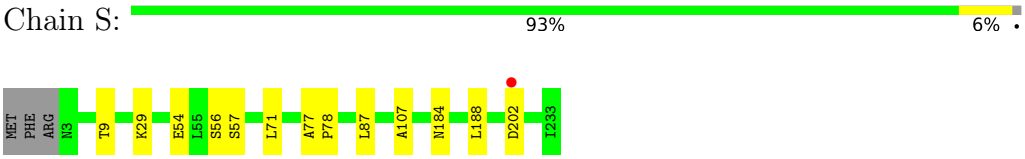
• Molecule 5: Proteasome subunit alpha type-6

Chain E:



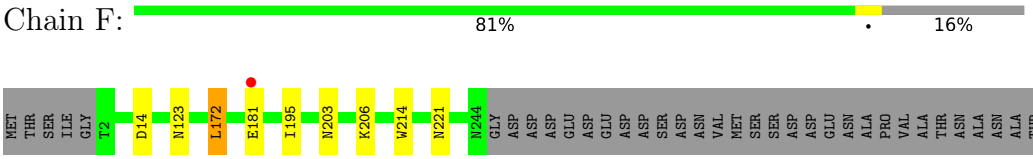
• Molecule 5: Proteasome subunit alpha type-6

Chain S:



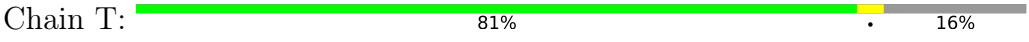
• Molecule 6: Probable proteasome subunit alpha type-7

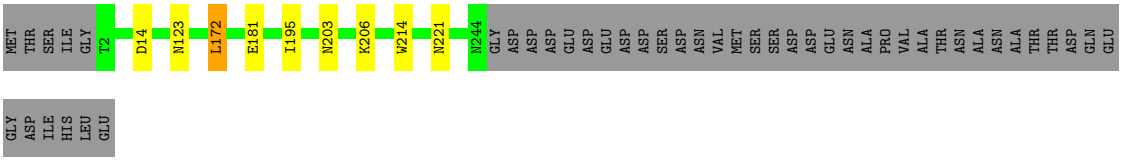
Chain F:



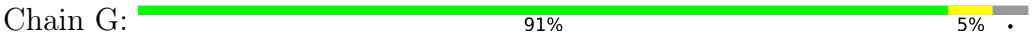
• Molecule 6: Probable proteasome subunit alpha type-7

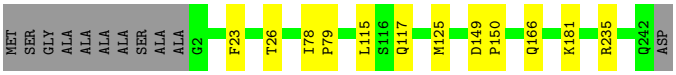
Chain T:



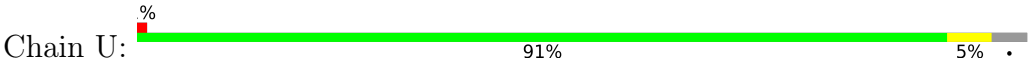


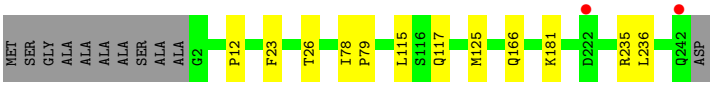
• Molecule 7: Proteasome subunit alpha type-1



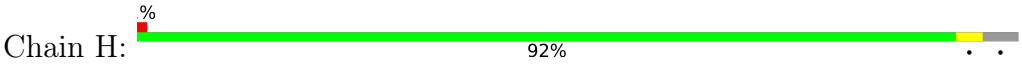


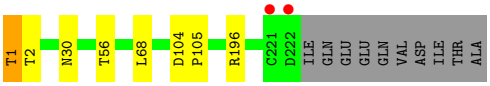
• Molecule 7: Proteasome subunit alpha type-1



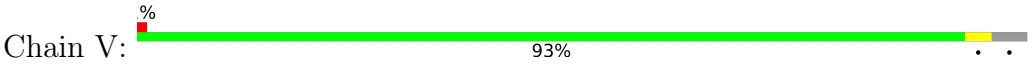


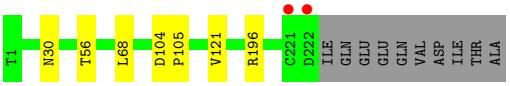
• Molecule 8: Proteasome subunit beta type-2





• Molecule 8: Proteasome subunit beta type-2



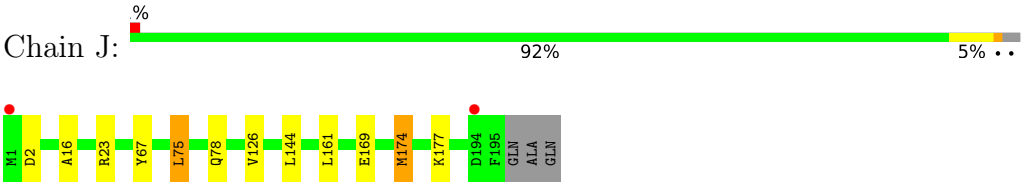


• Molecule 9: Proteasome subunit beta type-3

• Molecule 9: Proteasome subunit beta type-3

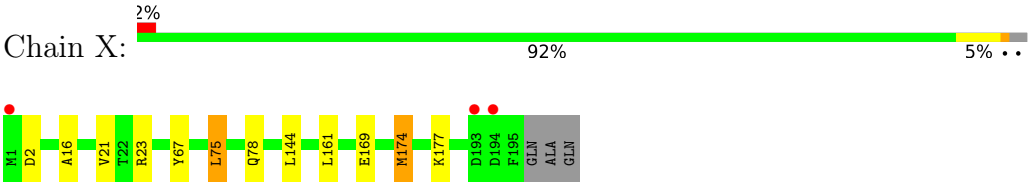
• Molecule 10: Proteasome subunit beta type-4

Chain J:



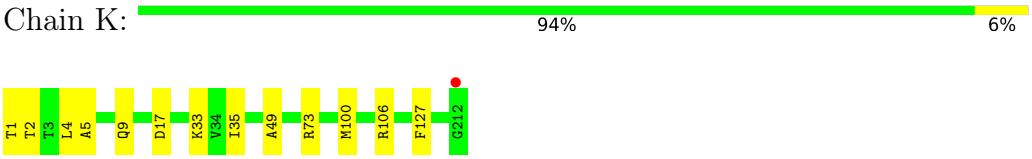
• Molecule 10: Proteasome subunit beta type-4

Chain X:



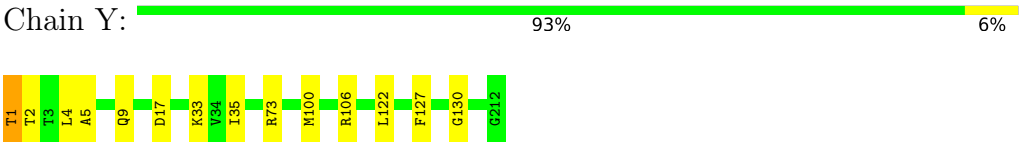
• Molecule 11: Proteasome subunit beta type-5

Chain K:



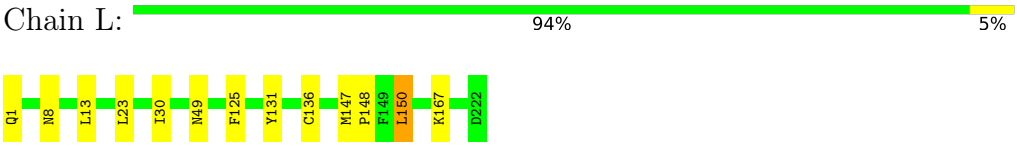
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



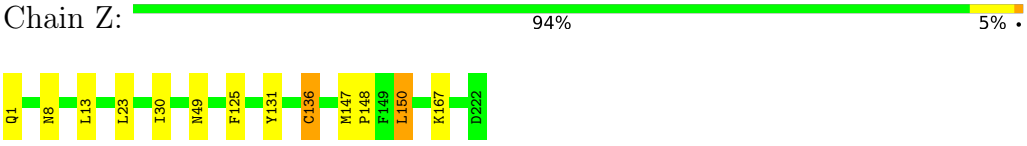
• Molecule 12: Proteasome subunit beta type-6

Chain L:



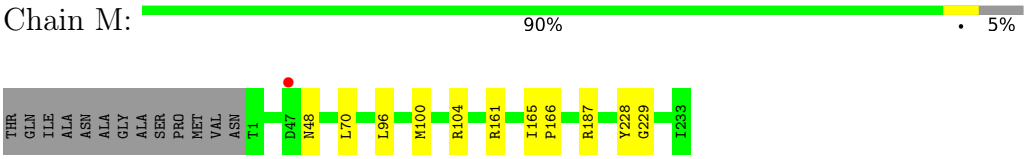
• Molecule 12: Proteasome subunit beta type-6

Chain Z:



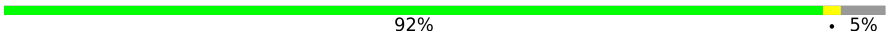
• Molecule 13: Proteasome subunit beta type-7

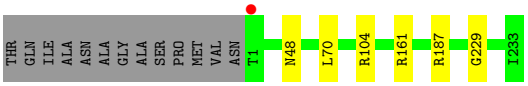
Chain M:



• Molecule 13: Proteasome subunit beta type-7

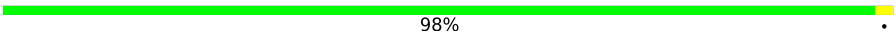
Chain a:





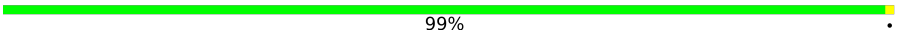
• Molecule 14: Proteasome subunit beta type-1

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	135.85Å 300.00Å 145.32Å 90.00° 113.17° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-3.00) 98.0 (15.00-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.170 , 0.203 0.176 , 0.204	Depositor DCC
R_{free} test set	10344 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	69.1	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 35.8	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	49501	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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, 6KG, MES, 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	0.27	0/1952	0.46	0/2642
1	O	0.27	0/1952	0.47	0/2642
2	B	0.27	0/1934	0.48	0/2618
2	P	0.27	0/1934	0.48	0/2618
3	C	0.28	0/1910	0.50	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.27	0/1837	0.47	0/2475
4	R	0.27	0/1837	0.47	0/2475
5	E	0.27	0/1800	0.46	0/2433
5	S	0.27	0/1800	0.46	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.44	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.27	0/1944	0.47	0/2632
8	H	0.25	0/1715	0.50	1/2326 (0.0%)
8	V	0.25	0/1715	0.48	0/2326
9	I	0.27	0/1611	0.50	0/2174
9	W	0.27	0/1611	0.50	0/2174
10	J	0.26	0/1589	0.48	0/2142
10	X	0.26	0/1589	0.48	0/2142
11	K	0.26	0/1681	0.51	0/2274
11	Y	0.28	0/1681	0.51	1/2274 (0.0%)
12	L	0.27	0/1795	0.47	0/2420
12	Z	0.27	0/1795	0.47	0/2420
13	M	0.26	0/1855	0.51	0/2514
13	a	0.26	0/1855	0.51	0/2514
14	N	0.25	0/1541	0.47	0/2087
14	b	0.25	0/1541	0.47	0/2087
All	All	0.27	0/50193	0.48	2/67866 (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})
11	Y	1	THR	CB-CA-C	-5.51	96.73	111.60
8	H	1	THR	N-CA-C	5.21	125.07	111.00

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	1	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	6	0
2	P	1904	0	1904	4	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	4	0
4	D	1813	0	1797	1	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	4	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	3	0
7	U	1906	0	1901	3	0
8	H	1684	0	1685	3	0
8	V	1684	0	1688	2	0
9	I	1581	0	1574	6	0
9	W	1581	0	1574	4	0
10	J	1561	0	1569	6	0
10	X	1561	0	1569	6	0
11	K	1644	0	1592	10	0
11	Y	1644	0	1592	17	0
12	L	1757	0	1711	5	0
12	Z	1757	0	1711	6	0
13	M	1824	0	1832	3	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	1	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	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	H	48	0	0	7	0
17	K	48	0	0	2	0
17	Y	48	0	0	2	0
18	H	12	0	13	0	0
18	K	12	0	13	0	0
18	V	12	0	13	0	0
18	Y	12	0	13	0	0
19	N	1	0	0	0	0
19	V	1	0	0	0	0
19	W	2	0	0	1	0
19	b	1	0	0	0	0
All	All	49501	0	49111	105	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 (105) 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:Y:1:THR:HG23	11:Y:33:LYS:HZ2	1.06	1.17
11:Y:1:THR:HG23	11:Y:33:LYS:NZ	1.61	1.16
11:Y:1:THR:CG2	11:Y:33:LYS:NZ	2.31	0.93
11:Y:1:THR:CG2	11:Y:17:ASP:OD1	2.22	0.88
17:H:301:6KG:C21	9:I:130:ASP:HB2	2.13	0.77
11:Y:1:THR:CG2	11:Y:33:LYS:HZ3	1.96	0.77
11:Y:1:THR:HG22	11:Y:2:THR:N	2.00	0.76
11:Y:1:THR:HG22	11:Y:17:ASP:OD1	1.86	0.75
11:Y:1:THR:HG21	11:Y:33:LYS:HD3	1.73	0.70
17:H:301:6KG:C30	17:H:301:6KG:C24	2.70	0.70
11:Y:1:THR:HG23	11:Y:17:ASP:OD1	1.91	0.69
17:H:301:6KG:C30	17:H:301:6KG:N26	2.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:1:THR:CG2	11:Y:33:LYS:HZ2	1.93	0.67
17:H:301:6KG:C12	17:H:301:6KG:C2	2.72	0.66
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.79	0.65
11:K:1:THR:HG23	11:K:33:LYS:NZ	2.14	0.61
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.82	0.61
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.83	0.61
17:H:301:6KG:C20	9:I:130:ASP:HB2	2.33	0.59
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.84	0.58
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.85	0.58
11:Y:1:THR:HG22	11:Y:2:THR:H	1.67	0.58
11:K:49:ALA:HA	17:K:301:6KG:C42	2.34	0.57
10:J:174:MET:HA	10:X:174:MET:HA	1.86	0.57
11:K:1:THR:HG22	11:K:2:THR:N	2.21	0.55
14:N:152:VAL:HA	14:N:175:MET:HE1	1.90	0.54
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.90	0.54
17:H:301:6KG:C2	17:H:301:6KG:O13	2.55	0.54
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.43	0.54
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.43	0.53
17:Y:301:6KG:N10	17:Y:301:6KG:C6	2.72	0.53
9:W:130:ASP:HB2	19:W:301:HOH:O	2.09	0.52
8:H:1:THR:HG22	8:H:2:THR:N	2.25	0.52
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.92	0.52
7:G:23:PHE:O	7:G:26:THR:HB	2.10	0.51
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.92	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.50
7:U:23:PHE:O	7:U:26:THR:HB	2.11	0.50
11:Y:1:THR:O	11:Y:130:GLY:HA3	2.11	0.50
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.95	0.48
17:H:301:6KG:O13	17:H:301:6KG:C1	2.60	0.48
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.96	0.48
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.96	0.48
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.44	0.47
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.97	0.47
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.97	0.47
11:K:1:THR:HG23	11:K:33:LYS:HZ2	1.77	0.47
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.97	0.46
17:Y:301:6KG:C6	17:Y:301:6KG:N11	2.79	0.46
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.46
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.46	0.46
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.51	0.45
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.51	0.45
11:K:100:MET:CE	11:K:127:PHE:HB2	2.46	0.45
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.98	0.45
10:J:177:LYS:NZ	10:X:169:GLU:O	2.50	0.45
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.52	0.45
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.98	0.45
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.52	0.45
13:M:228:TYR:HA	8:V:121:VAL:HG23	1.98	0.45
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.44	0.45
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.98	0.44
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.47	0.44
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.48	0.44
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.18	0.44
1:O:119:GLN:O	1:O:122:THR:HB	2.18	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.49	0.43
3:C:201:VAL:HG13	3:C:202:GLN:N	2.33	0.43
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.01	0.43
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.53	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.48	0.43
12:L:8:ASN:HA	12:L:30:ILE:O	2.19	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.34	0.42
11:K:5:ALA:HB3	11:K:100:MET:CE	2.49	0.42
12:Z:136:CYS:SG	12:Z:150:LEU:HB3	2.60	0.42
11:K:1:THR:HG23	11:K:17:ASP:OD1	2.20	0.42
12:L:147:MET:N	12:L:148:PRO:HD2	2.34	0.42
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.84	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.55	0.42
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.34	0.42
13:M:96:LEU:O	13:M:100:MET:HG2	2.20	0.42
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.41
1:A:119:GLN:O	1:A:122:THR:HB	2.20	0.41
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.02	0.41
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.85	0.41
4:R:158:ARG:HB3	5:S:57:SER:HB3	2.03	0.41
11:K:33:LYS:HE2	17:K:301:6KG:C41	2.50	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.03	0.41
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.03	0.41
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
2:B:86:LEU:HB3	2:B:114:LEU:HD21	2.03	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.41
8:H:1:THR:CG2	8:H:2:THR:N	2.85	0.40
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.03	0.40
2:B:161:ALA:HB3	3:C:52:LEU:HD23	2.04	0.40
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.86	0.40
10:J:169:GLU:O	10:X:177:LYS:NZ	2.54	0.40
9:I:123:PHE:HA	9:I:128:CYS:O	2.21	0.40
2:B:50:LYS:O	2:B:51:VAL:C	2.60	0.40
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.52	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	57
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	19	57
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	19	57
3	Q	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	19	57
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	234 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	T	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	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%)	189 (98%)	3 (2%)	1 (0%)	29	68
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	68
11	K	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
11	Y	210/212 (99%)	204 (97%)	6 (3%)	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%)	217 (94%)	13 (6%)	1 (0%)	34	72
13	a	231/246 (94%)	217 (94%)	13 (6%)	1 (0%)	34	72
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%)	6091 (97%)	173 (3%)	12 (0%)	47	82

All (12) 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
3	C	205	ALA
3	Q	205	ALA
2	B	221	ASP
10	J	2	ASP
2	P	221	ASP
10	X	2	ASP
13	M	229	GLY
13	a	229	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%)	206 (99%)	3 (1%)	67	88
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	88
2	B	203/216 (94%)	196 (97%)	7 (3%)	37	72
2	P	203/216 (94%)	197 (97%)	6 (3%)	41	75
3	C	212/226 (94%)	206 (97%)	6 (3%)	43	77
3	Q	212/226 (94%)	206 (97%)	6 (3%)	43	77
4	D	194/215 (90%)	188 (97%)	6 (3%)	40	75
4	R	194/215 (90%)	188 (97%)	6 (3%)	40	75
5	E	190/193 (98%)	183 (96%)	7 (4%)	34	70
5	S	190/193 (98%)	183 (96%)	7 (4%)	34	70
6	F	201/239 (84%)	193 (96%)	8 (4%)	31	68
6	T	201/239 (84%)	193 (96%)	8 (4%)	31	68
7	G	206/210 (98%)	200 (97%)	6 (3%)	42	76
7	U	206/210 (98%)	199 (97%)	7 (3%)	37	72
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%)	170 (99%)	2 (1%)	71	90
9	W	172/173 (99%)	170 (99%)	2 (1%)	71	90
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	76
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	76
11	K	169/169 (100%)	164 (97%)	5 (3%)	41	75
11	Y	169/169 (100%)	164 (97%)	5 (3%)	41	75
12	L	185/185 (100%)	179 (97%)	6 (3%)	39	74
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39	74
13	M	199/208 (96%)	194 (98%)	5 (2%)	47	79
13	a	199/208 (96%)	194 (98%)	5 (2%)	47	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	N	162/162 (100%)	161 (99%)	1 (1%)	86 95
14	b	162/162 (100%)	161 (99%)	1 (1%)	86 95
All	All	5312/5540 (96%)	5170 (97%)	142 (3%)	44 77

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	114	LEU
2	B	184	LYS
2	B	186	ASP
2	B	191	LEU
3	C	4	ARG
3	C	38	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	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN

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Mol	Chain	Res	Type
6	F	206	LYS
6	F	214	TRP
6	F	221	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
8	H	30	ASN
8	H	56	THR
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	182	TRP
10	J	23	ARG
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	73	ARG
11	K	106	ARG
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	136	CYS
12	L	150	LEU
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	39	ASP
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	55	LEU

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Mol	Chain	Res	Type
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	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	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	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	56	THR
8	V	68	LEU
8	V	196	ARG

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Mol	Chain	Res	Type
9	W	37	ASN
9	W	182	TRP
10	X	23	ARG
10	X	75	LEU
10	X	78	GLN
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	73	ARG
11	Y	106	ARG
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	136	CYS
12	Z	150	LEU
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	39	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
4	D	91	HIS
4	D	146	GLN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN

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Mol	Chain	Res	Type
5	E	184	ASN
6	F	86	ASN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	117	GLN
7	G	121	GLN
8	H	66	HIS
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	70	ASN
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	194	ASN
13	M	213	GLN
1	O	94	HIS
2	P	119	GLN
2	P	123	GLN
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	146	GLN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
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	117	GLN
7	U	121	GLN
10	X	55	GLN

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Mol	Chain	Res	Type
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	70	ASN
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	194	ASN
13	a	213	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 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
18	MES	Y	302	-	12,12,12	2.32	1 (8%)	14,16,16	1.25	2 (14%)
17	6KG	Y	301	11	49,50,50	2.22	5 (10%)	59,65,65	1.36	6 (10%)
17	6KG	H	301	8	49,50,50	1.38	4 (8%)	59,65,65	1.73	9 (15%)
18	MES	V	301	-	12,12,12	2.23	1 (8%)	14,16,16	1.22	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	6KG	K	301	11	49,50,50	1.36	4 (8%)	59,65,65	1.96	10 (16%)
18	MES	K	303	-	12,12,12	2.30	1 (8%)	14,16,16	1.41	1 (7%)
18	MES	H	302	-	12,12,12	2.13	1 (8%)	14,16,16	1.45	3 (21%)

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
18	MES	Y	302	-	-	0/6/14/14	0/1/1/1
17	6KG	Y	301	11	-	5/54/62/62	0/3/3/3
17	6KG	H	301	8	-	25/54/62/62	0/3/3/3
18	MES	V	301	-	-	0/6/14/14	0/1/1/1
17	6KG	K	301	11	-	9/54/62/62	0/3/3/3
18	MES	K	303	-	-	3/6/14/14	0/1/1/1
18	MES	H	302	-	-	5/6/14/14	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	301	6KG	N10-N9	-11.45	0.93	1.23
18	Y	302	MES	C8-S	-7.71	1.66	1.77
18	K	303	MES	C8-S	-7.71	1.66	1.77
18	V	301	MES	C8-S	-7.36	1.67	1.77
18	H	302	MES	C8-S	-6.99	1.67	1.77
17	Y	301	6KG	C28-C29	-6.00	1.36	1.51
17	H	301	6KG	C7-C1	-5.76	1.37	1.51
17	K	301	6KG	C7-C1	-5.54	1.38	1.51
17	Y	301	6KG	C7-C1	-5.24	1.38	1.51
17	H	301	6KG	C28-C29	-4.99	1.39	1.51
17	K	301	6KG	C28-C29	-4.68	1.40	1.51
17	K	301	6KG	C45-C43	3.42	1.59	1.53
17	H	301	6KG	N10-N9	-3.37	1.14	1.23
17	Y	301	6KG	O44-C43	-3.25	1.35	1.43
17	Y	301	6KG	C45-C43	-3.12	1.48	1.53
17	H	301	6KG	C45-C43	2.79	1.58	1.53
17	K	301	6KG	N10-N9	-2.07	1.17	1.23

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	H	301	6KG	C16-C17-C18	-7.81	102.28	115.17
17	K	301	6KG	C40-C39-C38	-7.43	101.06	115.84
17	K	301	6KG	C16-C17-C18	-6.51	104.43	115.17
17	Y	301	6KG	C39-C38-N37	-5.13	103.54	110.18
17	K	301	6KG	C41-C40-C42	-4.49	89.83	110.51
17	K	301	6KG	C8-N9-N10	4.32	119.78	115.24
17	H	301	6KG	C20-C19-C18	-4.21	104.19	112.15
17	K	301	6KG	C29-C28-C27	-3.87	102.70	113.39
17	Y	301	6KG	C8-N9-N10	3.69	119.12	115.24
17	H	301	6KG	O47-C46-C45	-3.66	103.85	111.33
17	Y	301	6KG	C16-C17-C18	-3.59	109.24	115.17
17	K	301	6KG	C39-C38-N37	-3.52	105.63	110.18
18	H	302	MES	O2S-S-C8	3.31	110.90	106.92
17	K	301	6KG	C7-C8-N9	3.27	114.69	109.30
18	K	303	MES	O2S-S-C8	3.24	110.82	106.92
17	H	301	6KG	C48-C45-C46	-2.94	106.01	109.88
17	H	301	6KG	C40-C39-C38	-2.92	110.02	115.84
18	Y	302	MES	O3S-S-C8	2.75	110.21	105.77
17	K	301	6KG	C46-C45-C43	-2.71	105.86	110.99
17	Y	301	6KG	C29-C28-C27	-2.60	106.20	113.39
18	H	302	MES	O1S-S-C8	2.50	109.93	106.92
17	K	301	6KG	C16-C15-C24	-2.49	104.39	110.20
17	K	301	6KG	C20-C19-C18	-2.41	107.59	112.15
18	V	301	MES	O3S-S-C8	2.35	109.57	105.77
18	H	302	MES	O3S-S-C8	2.35	109.57	105.77
17	Y	301	6KG	C16-C15-C24	-2.32	104.78	110.20
18	Y	302	MES	O2S-S-C8	2.27	109.65	106.92
17	Y	301	6KG	C16-C15-N14	-2.26	106.30	110.88
17	H	301	6KG	C22-C23-C18	-2.26	107.89	112.15
17	H	301	6KG	C29-C28-C27	-2.25	107.19	113.39
18	V	301	MES	O2S-S-C8	2.24	109.61	106.92
17	H	301	6KG	C21-C22-C23	-2.21	106.90	111.42
18	V	301	MES	O1S-S-C8	2.19	109.55	106.92
17	H	301	6KG	C24-C15-N14	-2.07	105.53	111.16

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	6KG	O13-C12-C8-N9
17	H	301	6KG	N14-C12-C8-N9
17	H	301	6KG	N11-N10-N9-C8
17	H	301	6KG	C38-C43-C45-C48

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Mol	Chain	Res	Type	Atoms
17	H	301	6KG	C38-C43-C45-C46
17	H	301	6KG	C43-C45-C46-O47
17	H	301	6KG	C48-C45-C46-O47
17	K	301	6KG	O44-C43-C45-C48
17	K	301	6KG	C48-C45-C46-O47
17	Y	301	6KG	C1-C7-C8-N9
18	H	302	MES	C7-C8-S-O1S
18	H	302	MES	C7-C8-S-O2S
18	H	302	MES	C7-C8-S-O3S
18	K	303	MES	C7-C8-S-O1S
18	K	303	MES	C7-C8-S-O3S
17	K	301	6KG	C38-C39-C40-C42
17	K	301	6KG	C38-C39-C40-C41
17	H	301	6KG	C38-C39-C40-C41
17	H	301	6KG	O44-C43-C45-C48
17	H	301	6KG	C38-C39-C40-C42
17	H	301	6KG	C24-C15-N14-C12
17	K	301	6KG	C38-C43-C45-C48
17	Y	301	6KG	C48-C45-C46-O47
17	H	301	6KG	C28-C27-C35-O36
17	H	301	6KG	C28-C27-C35-N37
17	H	301	6KG	O44-C43-C45-C46
17	H	301	6KG	C6-C1-C7-C8
17	H	301	6KG	C2-C1-C7-C8
17	H	301	6KG	C27-C28-C29-C34
17	H	301	6KG	C27-C28-C29-C30
17	K	301	6KG	N11-N10-N9-C8
17	H	301	6KG	N26-C27-C35-O36
17	H	301	6KG	C1-C7-C8-C12
17	H	301	6KG	C16-C15-N14-C12
18	K	303	MES	C7-C8-S-O2S
17	H	301	6KG	N26-C27-C35-N37
17	H	301	6KG	C1-C7-C8-N9
18	H	302	MES	C8-C7-N4-C5
17	K	301	6KG	N26-C27-C35-O36
17	Y	301	6KG	C1-C7-C8-C12
17	Y	301	6KG	N26-C27-C35-O36
17	Y	301	6KG	N26-C27-C35-N37
17	K	301	6KG	N26-C27-C35-N37
17	H	301	6KG	N37-C38-C43-O44
17	K	301	6KG	C38-C43-C45-C46
17	H	301	6KG	N37-C38-C43-C45

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Mol	Chain	Res	Type	Atoms
18	H	302	MES	C8-C7-N4-C3

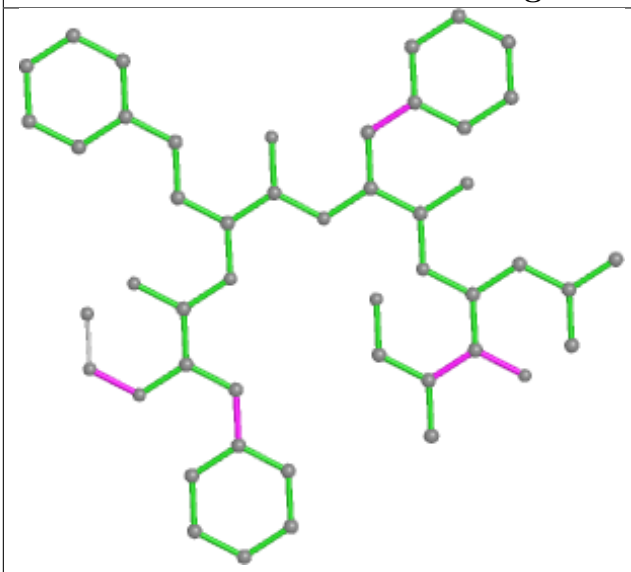
There are no ring outliers.

3 monomers are involved in 11 short contacts:

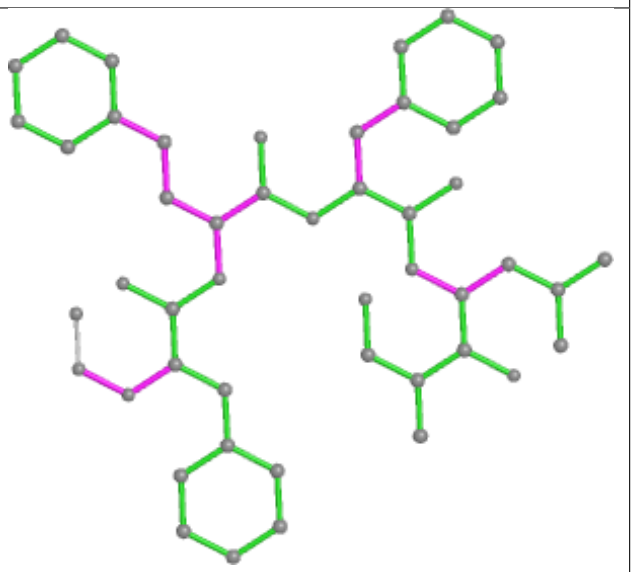
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	301	6KG	2	0
17	H	301	6KG	7	0
17	K	301	6KG	2	0

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

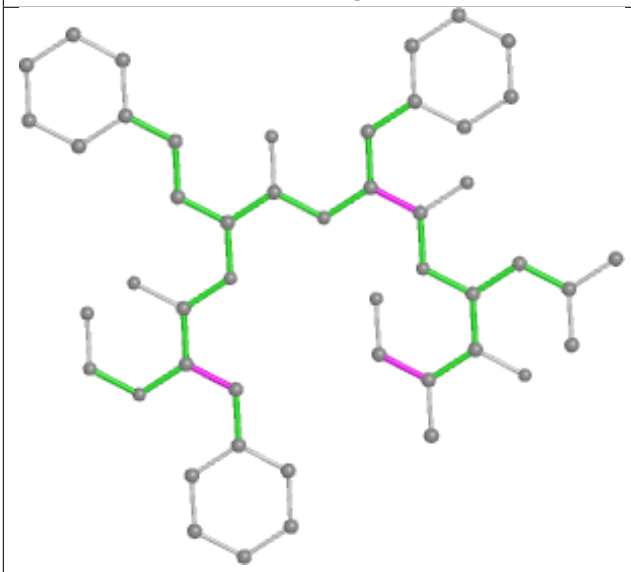
Ligand 6KG Y 301



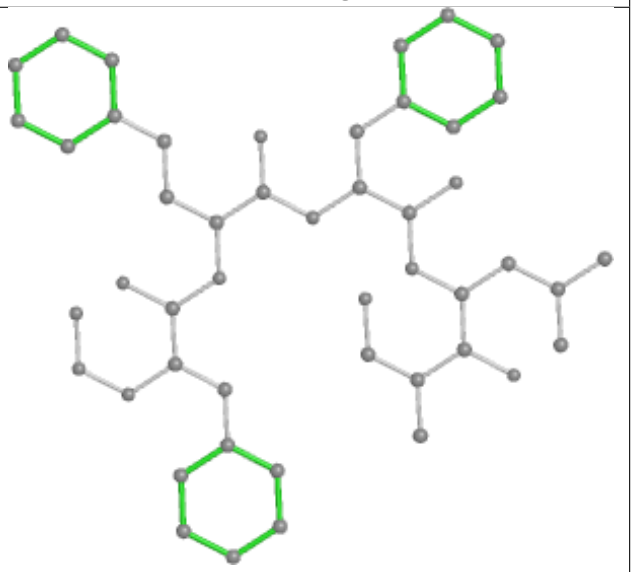
Bond lengths



Bond angles

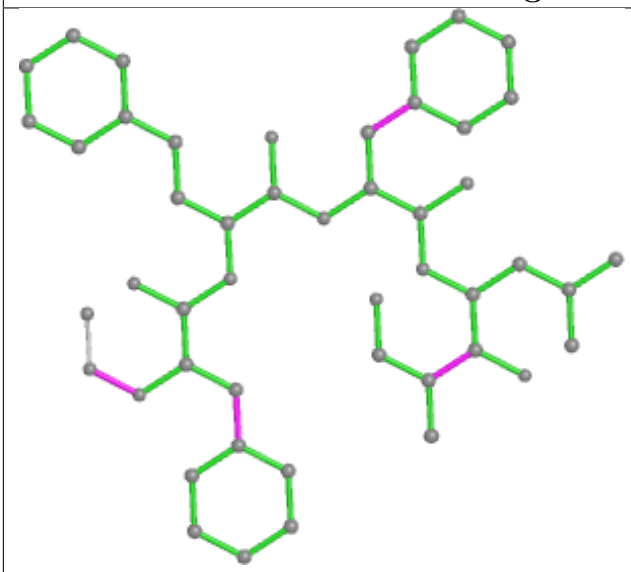


Torsions

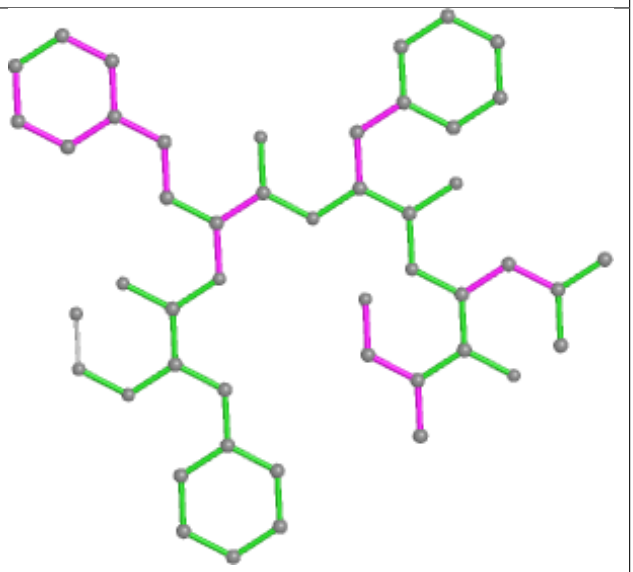


Rings

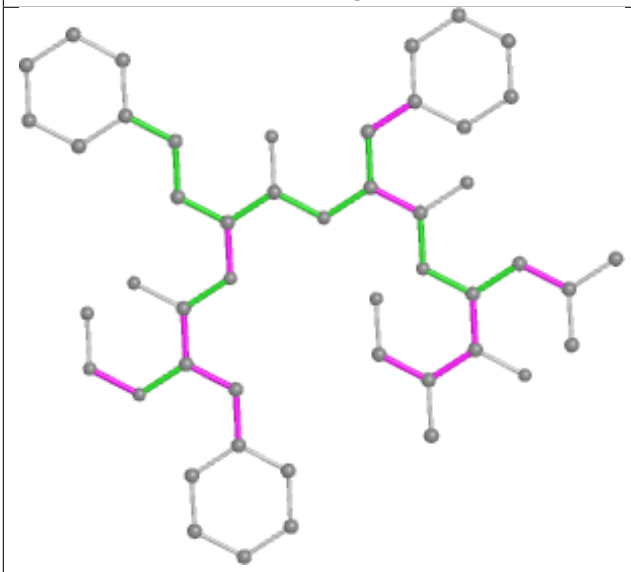
Ligand 6KG H 301



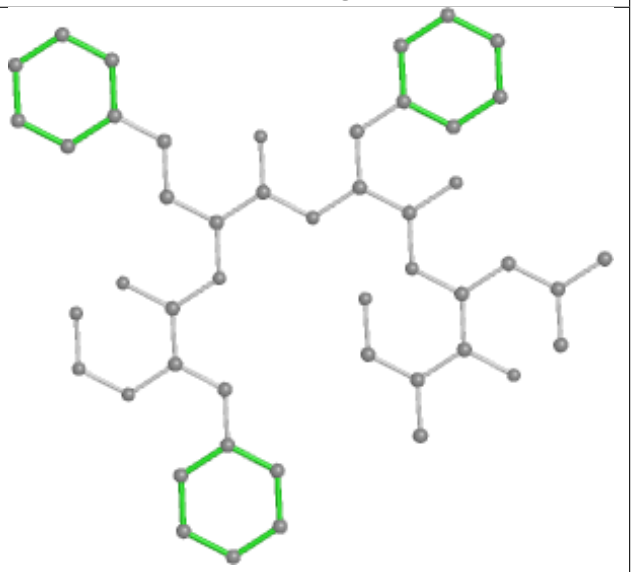
Bond lengths



Bond angles

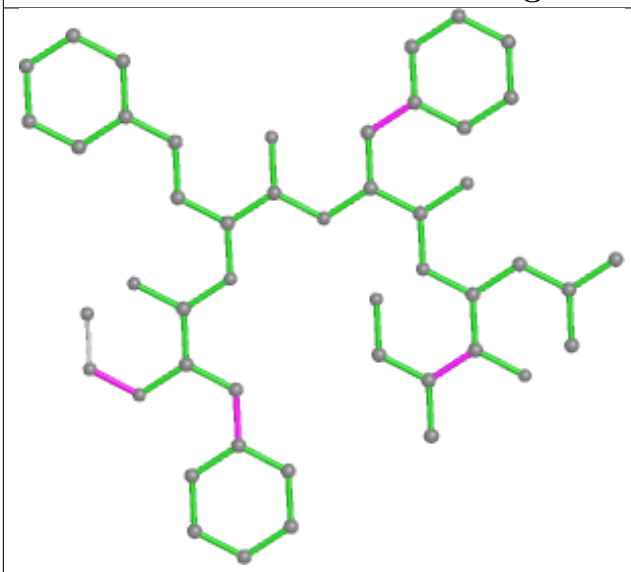


Torsions

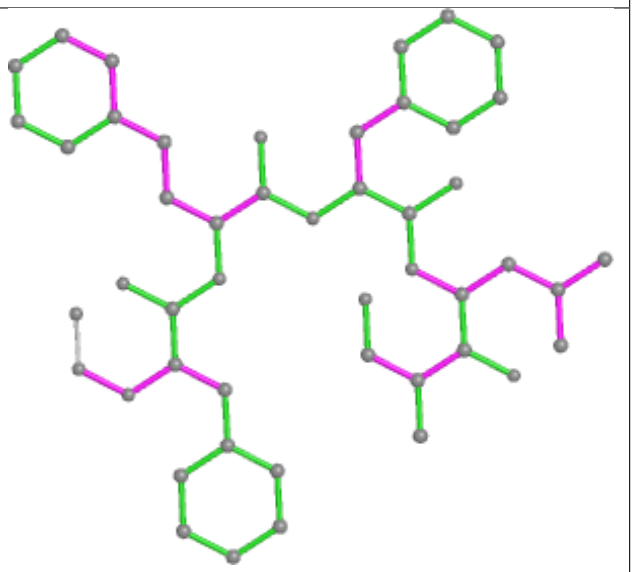


Rings

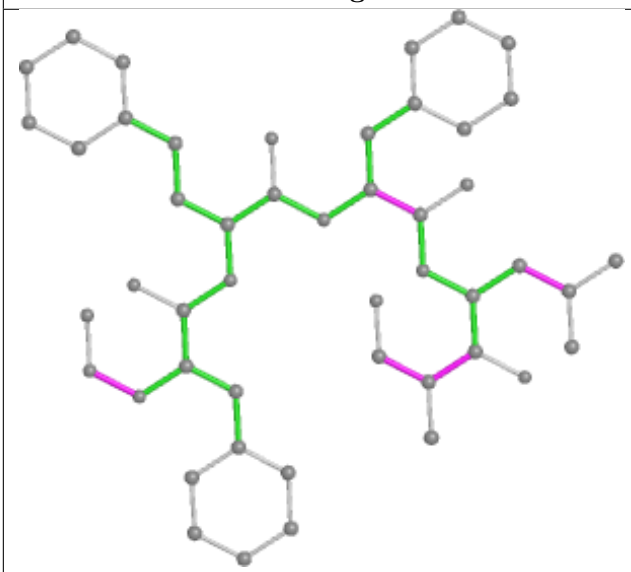
Ligand 6KG K 301



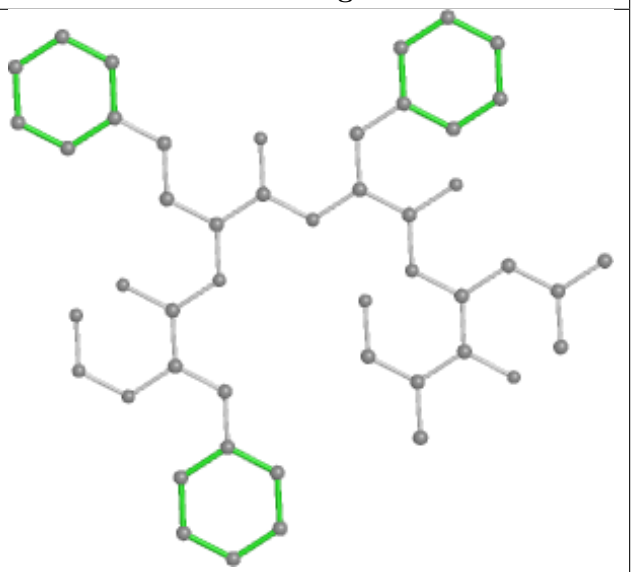
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.59	2 (0%)	86	65	48, 64, 102, 158	0
1	O	250/250 (100%)	-0.54	3 (1%)	79	54	53, 72, 114, 156	0
2	B	244/258 (94%)	-0.52	5 (2%)	65	36	49, 70, 118, 172	0
2	P	244/258 (94%)	-0.48	6 (2%)	57	29	53, 74, 119, 171	0
3	C	240/254 (94%)	-0.45	3 (1%)	77	51	50, 75, 138, 168	0
3	Q	240/254 (94%)	-0.31	9 (3%)	40	16	56, 87, 168, 197	0
4	D	235/260 (90%)	-0.57	1 (0%)	92	79	54, 79, 111, 154	0
4	R	235/260 (90%)	-0.54	1 (0%)	92	79	58, 79, 118, 159	0
5	E	231/234 (98%)	-0.49	1 (0%)	92	79	57, 82, 117, 158	0
5	S	231/234 (98%)	-0.49	1 (0%)	92	79	58, 85, 130, 163	0
6	F	243/288 (84%)	-0.62	1 (0%)	92	79	51, 74, 121, 163	0
6	T	243/288 (84%)	-0.57	0	100	100	47, 80, 135, 171	0
7	G	241/252 (95%)	-0.63	0	100	100	46, 67, 108, 156	0
7	U	241/252 (95%)	-0.65	2 (0%)	86	65	42, 68, 102, 145	0
8	H	222/232 (95%)	-0.63	2 (0%)	84	63	51, 65, 102, 132	0
8	V	222/232 (95%)	-0.60	2 (0%)	84	63	53, 69, 100, 142	0
9	I	204/205 (99%)	-0.80	1 (0%)	91	75	46, 63, 92, 115	0
9	W	204/205 (99%)	-0.73	0	100	100	48, 65, 94, 121	0
10	J	195/198 (98%)	-0.71	2 (1%)	82	59	44, 62, 93, 132	0
10	X	195/198 (98%)	-0.68	3 (1%)	73	46	48, 65, 92, 144	0
11	K	212/212 (100%)	-0.71	1 (0%)	91	75	46, 64, 94, 119	0
11	Y	212/212 (100%)	-0.75	0	100	100	48, 64, 95, 119	0
12	L	222/222 (100%)	-0.72	0	100	100	47, 66, 97, 118	0
12	Z	222/222 (100%)	-0.72	0	100	100	46, 65, 97, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.72	1 (0%) 92 79	46, 65, 92, 101	0
13	a	233/246 (94%)	-0.71	1 (0%) 92 79	46, 64, 87, 105	0
14	N	196/196 (100%)	-0.69	0 100 100	46, 62, 91, 116	0
14	b	196/196 (100%)	-0.69	0 100 100	49, 62, 93, 115	0
All	All	6336/6614 (95%)	-0.61	48 (0%) 86 65	42, 69, 115, 197	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	6.7
1	A	1	MET	5.5
3	C	206	LYS	5.3
2	B	220	ASN	5.2
8	V	222	ASP	4.3
1	O	1	MET	4.1
3	Q	206	LYS	4.1
2	B	218	GLY	4.0
2	P	220	ASN	3.9
2	B	221	ASP	3.7
2	B	219	ALA	3.7
2	P	219	ALA	3.6
8	H	221	CYS	3.5
4	R	241	ALA	3.4
5	E	202	ASP	3.4
1	O	249	ALA	3.4
2	P	221	ASP	3.4
10	X	1	MET	3.3
5	S	202	ASP	3.2
3	Q	50	LEU	3.2
3	C	49	THR	2.9
3	Q	239	GLN	2.9
3	Q	48	SER	2.8
13	a	1	THR	2.8
2	P	59	ASP	2.8
10	J	1	MET	2.7
3	Q	223	SER	2.7
8	V	221	CYS	2.7
3	Q	240	GLU	2.7
8	H	222	ASP	2.7
2	P	218	GLY	2.6
3	Q	238	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
9	I	1	SER	2.5
7	U	222	ASP	2.4
10	X	194	ASP	2.4
2	P	51	VAL	2.4
7	U	242	GLN	2.4
4	D	242	GLU	2.3
2	B	51	VAL	2.3
3	Q	236	GLN	2.2
6	F	181	GLU	2.2
1	A	249	ALA	2.1
3	C	238	LYS	2.1
1	O	231	LYS	2.1
13	M	47	ASP	2.1
10	J	194	ASP	2.1
11	K	212	GLY	2.0
10	X	193	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	6KG	H	301	48/48	0.66	0.46	43,53,60,63	48
18	MES	V	301	12/12	0.87	0.61	91,93,128,140	0
17	6KG	K	301	48/48	0.90	0.23	48,54,63,75	0
18	MES	H	302	12/12	0.91	0.47	87,91,117,120	12
17	6KG	Y	301	48/48	0.92	0.19	48,56,63,83	0
18	MES	Y	302	12/12	0.95	0.29	57,60,79,82	0
18	MES	K	303	12/12	0.96	0.28	54,59,74,77	0

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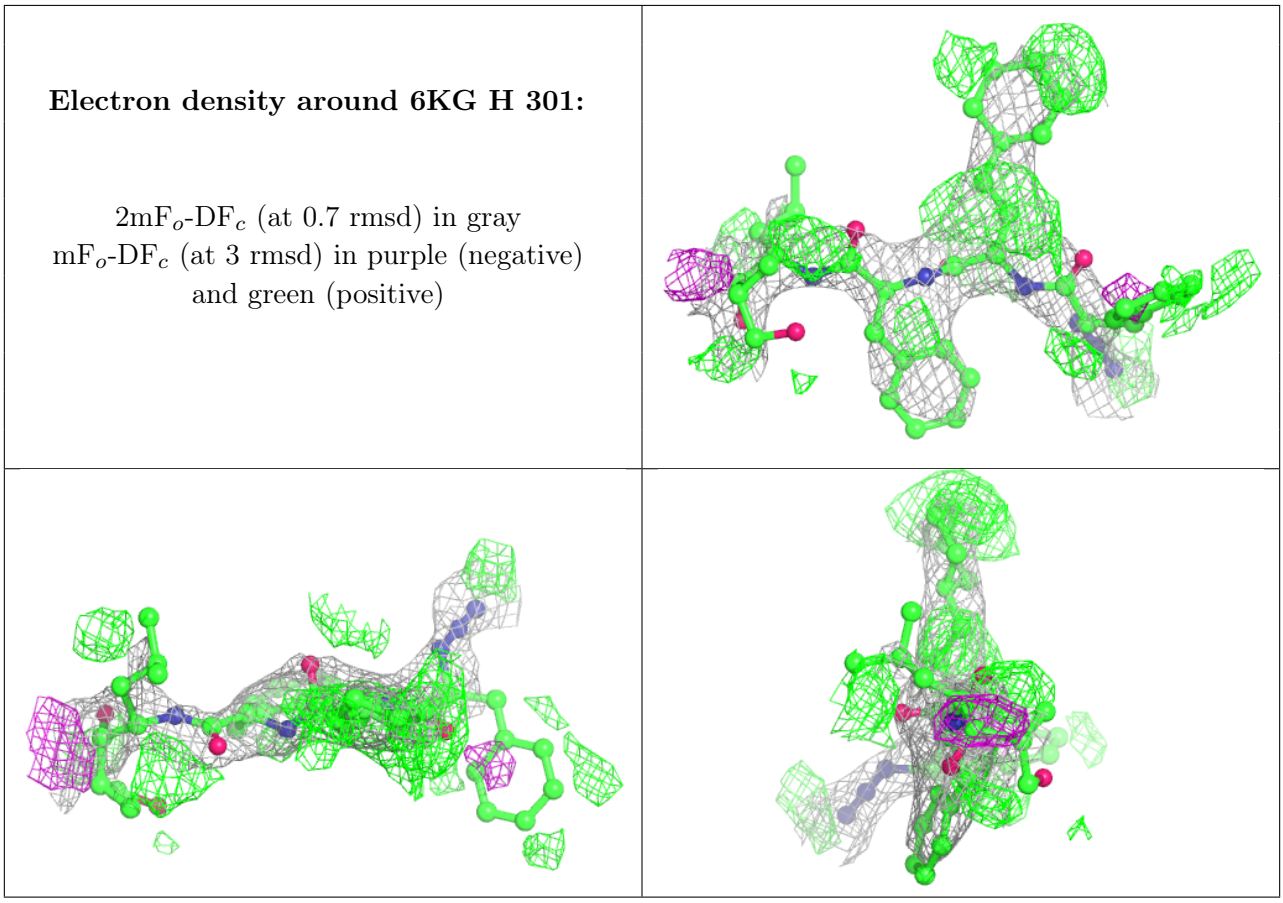
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	G	301	1/1	0.96	0.05	60,60,60,60	0
15	MG	N	201	1/1	0.96	0.18	50,50,50,50	0
15	MG	Z	301	1/1	0.97	0.23	77,77,77,77	0
15	MG	I	301	1/1	0.97	0.36	83,83,83,83	0
16	CL	U	301	1/1	0.98	0.22	64,64,64,64	0
15	MG	L	301	1/1	0.98	0.07	81,81,81,81	0
15	MG	I	302	1/1	0.98	0.06	65,65,65,65	0
15	MG	K	302	1/1	0.98	0.05	58,58,58,58	0
16	CL	G	302	1/1	0.99	0.22	51,51,51,51	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.

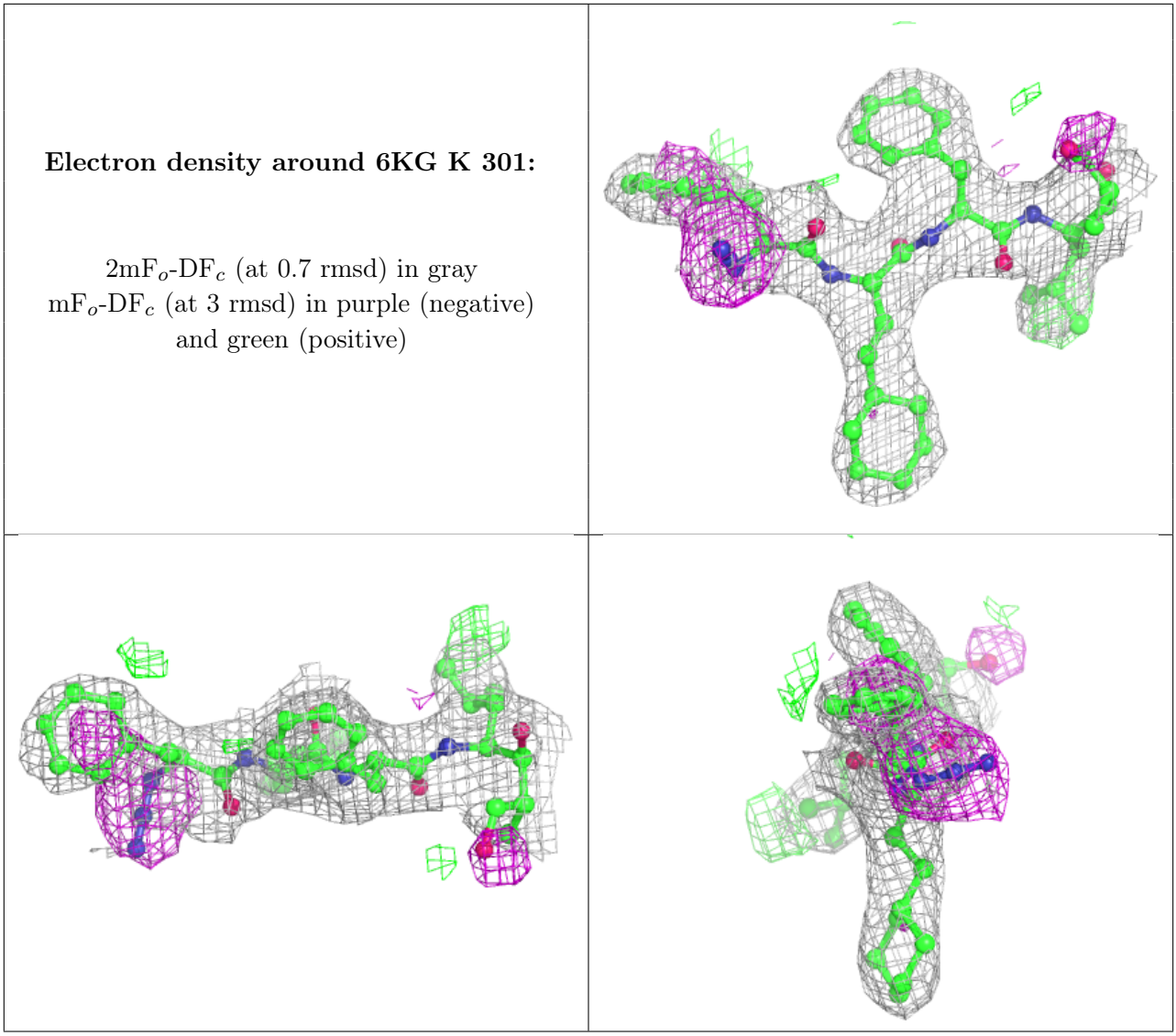
Electron density around 6KG H 301:

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



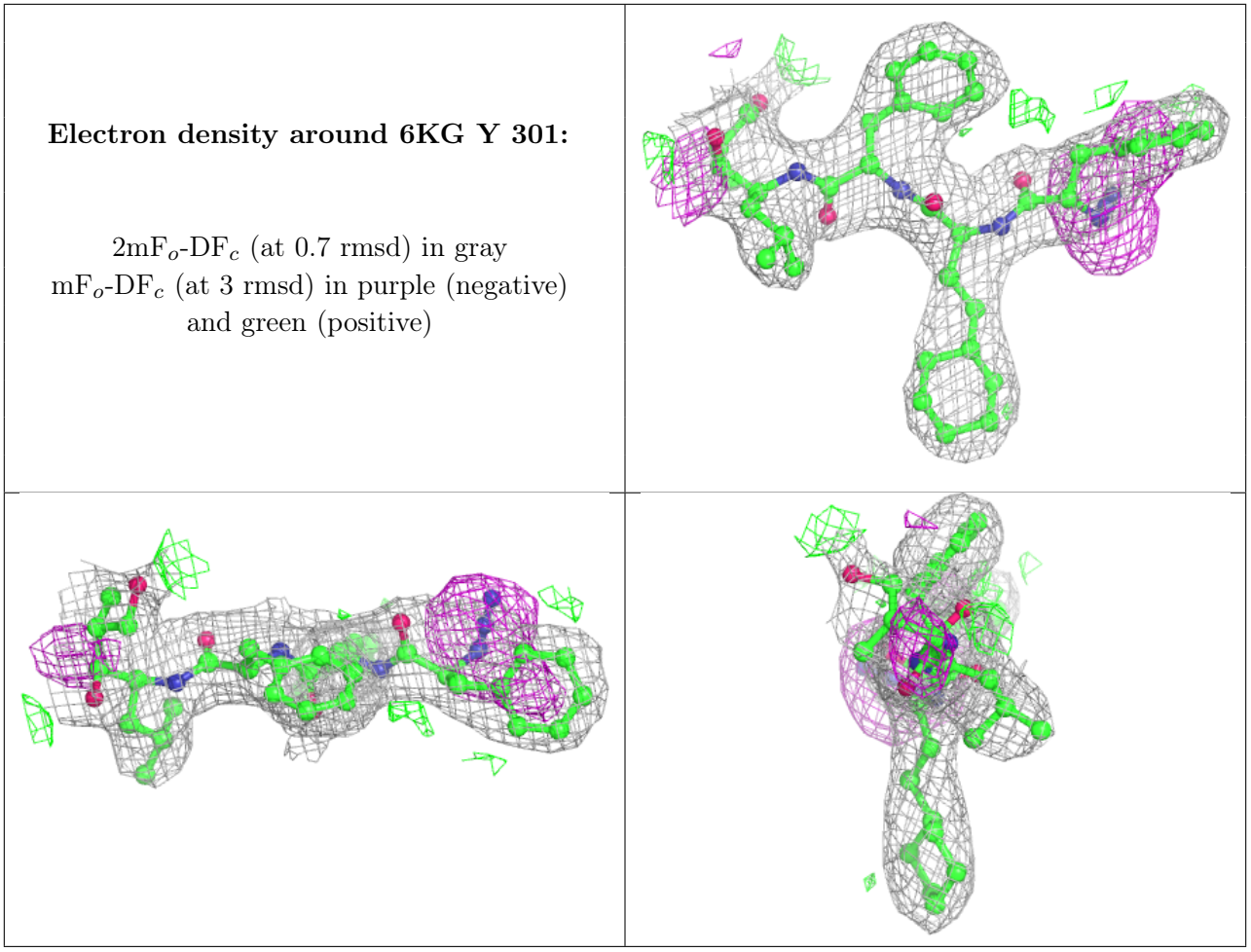
Electron density around 6KG K 301:

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



Electron density around 6KG 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.