Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2023 – 01:27 PM EDT

PDB ID	:	4LTC
Title	:	Crystal structure of yeast 20S proteasome in complex with enone carmaphycin analogue 6
Authors	:	Stein, M.; Trivella, D.B.B.; Groll, M.
Deposited on	:	2013-07-23
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

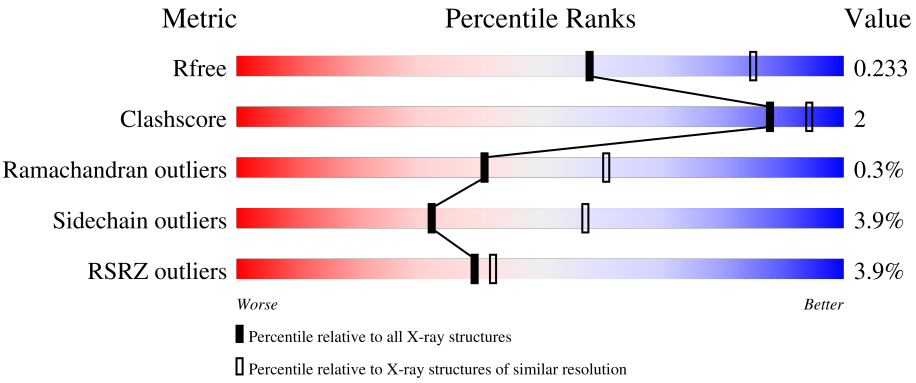
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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% 95% ·
1	O	250	4% 97% ·
2	B	258	6% 85% 8% · 5%
2	P	258	6% 85% 8% · 5%
3	C	254	7% 85% 8% · 5%

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Mol	Chain	Length	Quality of chain
3	Q	254	13% 86% 7% 5%
4	D	260	5% 85% 8% 7%
4	R	260	6% 86% 7% 7%
5	E	234	6% 88% 12%
5	S	234	7% 87% 13%
6	F	287	4% 77% 6% 15%
6	T	287	5% 80% 5% 15%
7	G	252	3% 89% 6%
7	U	252	2% 86% 10%
8	H	232	2% 91%
8	V	232	% 91%
9	I	205	% 95%
9	W	205	% 96%
10	J	198	4% 96%
10	X	198	3% 97%
11	K	212	90% 8%
11	Y	212	% 92% 7%
12	L	222	2% 91% 7%
12	Z	222	2% 91% 8%
13	M	233	% 92% 7%
13	a	233	% 97%
14	N	196	% 95%
14	b	196	2% 97%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 52219 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	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

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

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

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

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

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

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

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

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

- Molecule 8 is a protein called Proteasome 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	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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

- Molecule 11 is a protein called Proteasome 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			

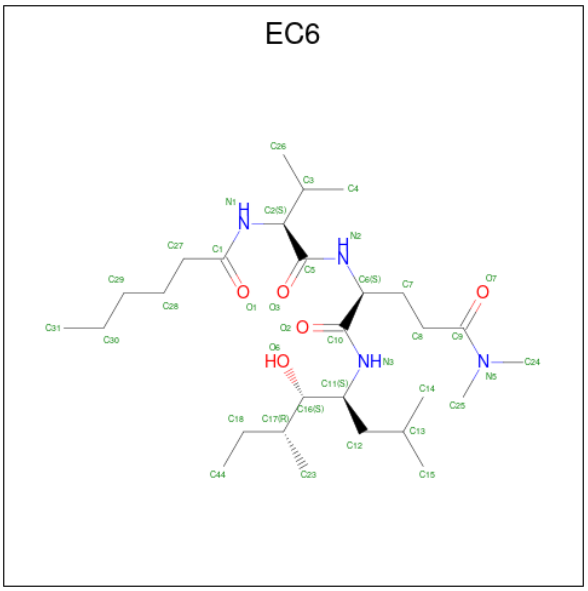
- Molecule 13 is a protein called Proteasome subunit beta type-7.

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 N-hexanoyl-L-valyl-N 1 -[(4S,5S,6R)-5-hydroxy-2,6-dimethyloctan-4-yl]-N 5 , N 5 -dimethyl-L-glutamamide (three-letter code: EC6) (formula: $C_{28}H_{54}N_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	1	Total C N O 37 28 4 5	0	0
15	Y	1	Total C N O 37 28 4 5	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	99	Total O 99 99	0	0
16	B	77	Total O 77 77	0	0
16	C	85	Total O 85 85	0	0
16	D	86	Total O 86 86	0	0
16	E	57	Total O 57 57	0	0
16	F	92	Total O 92 92	0	0
16	G	121	Total O 121 121	0	0
16	O	66	Total O 66 66	0	0
16	P	75	Total O 75 75	0	0
16	Q	73	Total O 73 73	0	0

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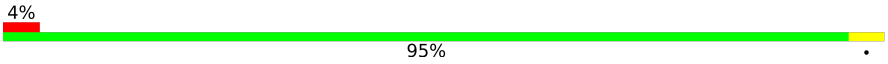
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	R	85	Total O 85 85	0	0
16	S	49	Total O 49 49	0	0
16	T	89	Total O 89 89	0	0
16	U	110	Total O 110 110	0	0
16	H	101	Total O 101 101	0	0
16	I	107	Total O 107 107	0	0
16	J	103	Total O 103 103	0	0
16	K	104	Total O 104 104	0	0
16	L	110	Total O 110 110	0	0
16	M	132	Total O 132 132	0	0
16	N	101	Total O 101 101	0	0
16	V	91	Total O 91 91	0	0
16	W	104	Total O 104 104	0	0
16	X	98	Total O 98 98	0	0
16	Y	73	Total O 73 73	0	0
16	Z	102	Total O 102 102	0	0
16	a	111	Total O 111 111	0	0
16	b	106	Total O 106 106	0	0

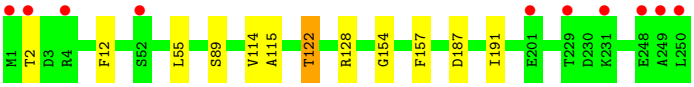
3 Residue-property plots (i)

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

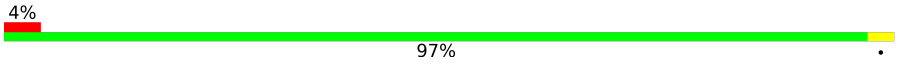
Chain A:

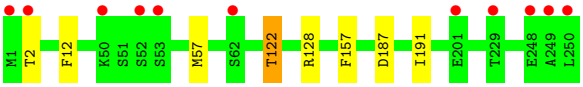




• Molecule 1: Proteasome subunit alpha type-2

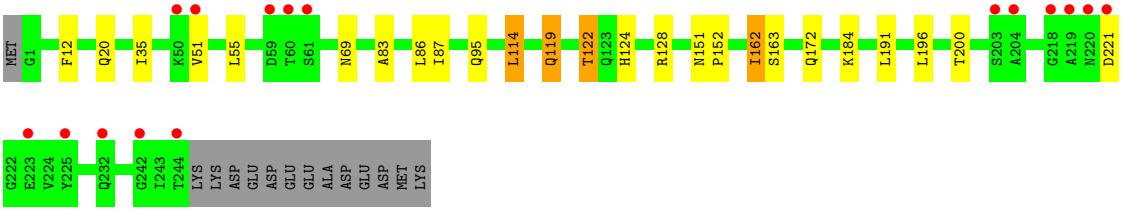
Chain O:





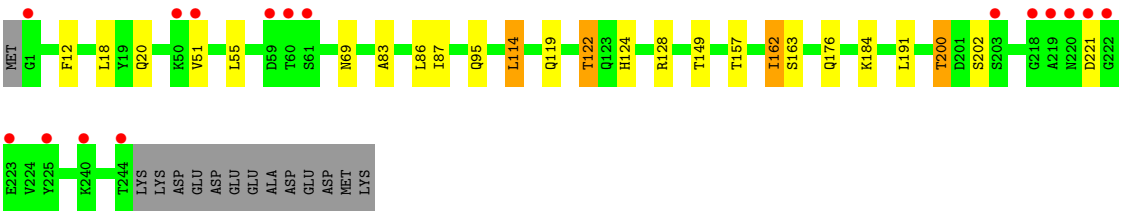
• Molecule 2: Proteasome subunit alpha type-3

Chain B:

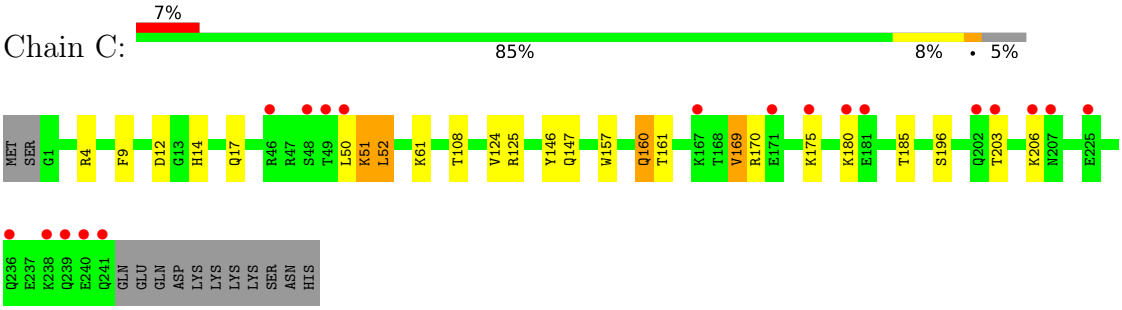


• Molecule 2: Proteasome subunit alpha type-3

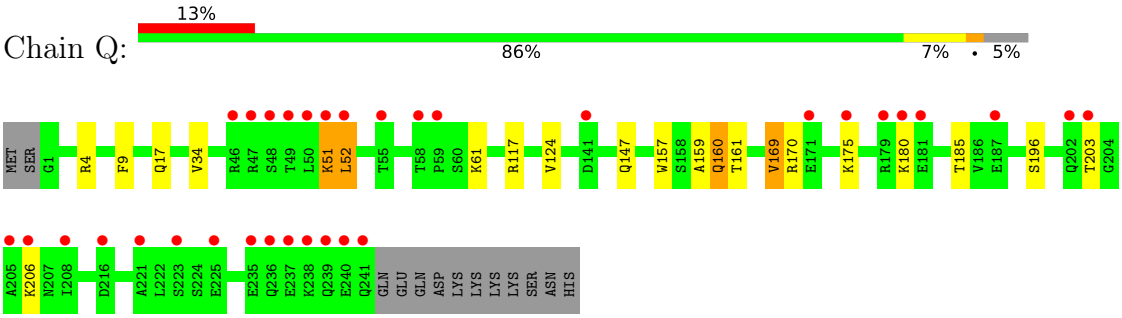
Chain P:



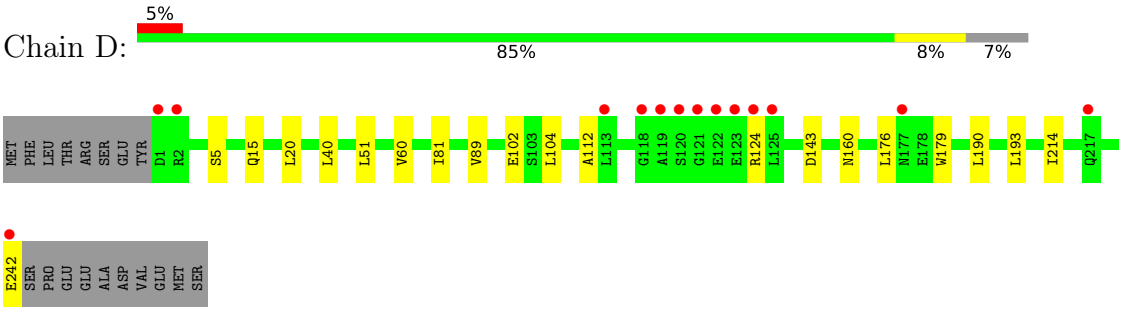
• Molecule 3: Proteasome subunit alpha type-4



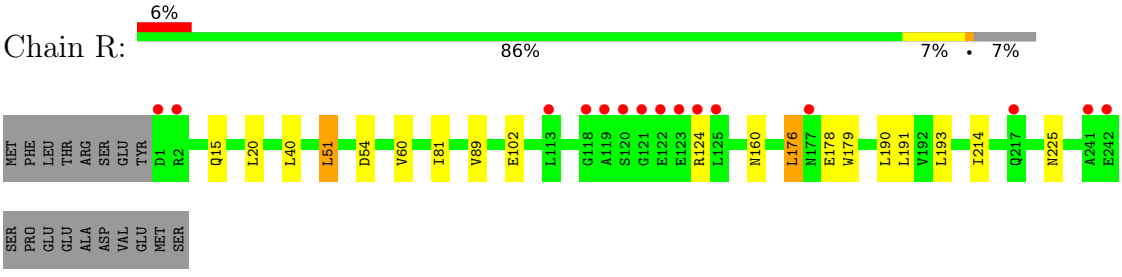
• Molecule 3: Proteasome subunit alpha type-4



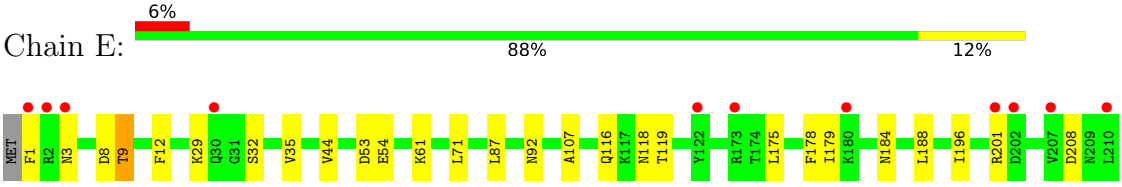
• Molecule 4: Proteasome subunit alpha type-5

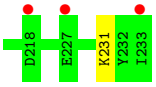


• Molecule 4: Proteasome subunit alpha type-5



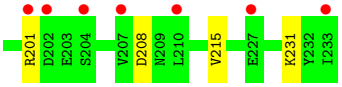
• Molecule 5: Proteasome subunit alpha type-6





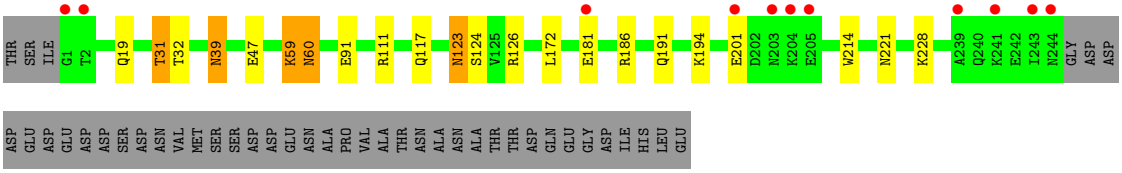
• Molecule 5: Proteasome subunit alpha type-6

Chain S:



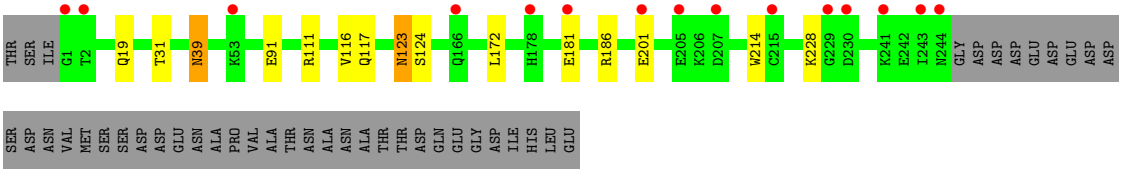
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



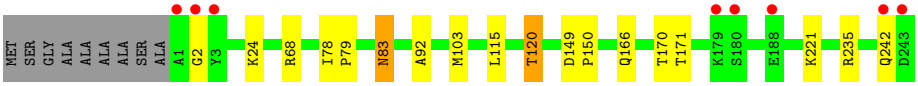
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



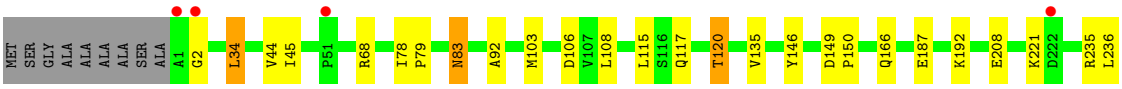
• Molecule 7: Proteasome subunit alpha type-1

Chain G:



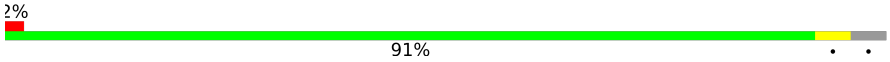
• Molecule 7: Proteasome subunit alpha type-1

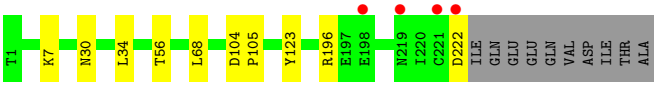
Chain U:



• Molecule 8: Proteasome subunit beta type-2

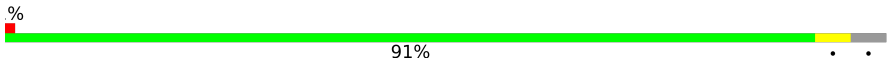
Chain H:





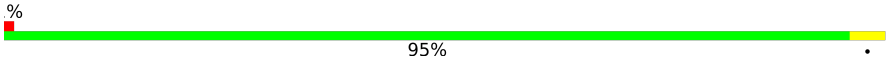
• Molecule 8: Proteasome subunit beta type-2

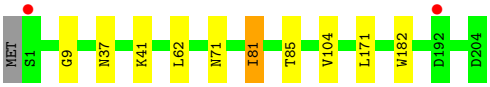
Chain V:



• Molecule 9: Proteasome subunit beta type-3

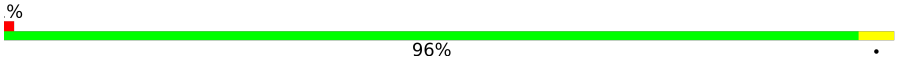
Chain I:

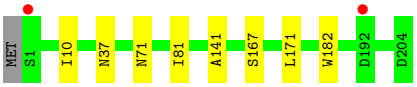




• Molecule 9: Proteasome subunit beta type-3

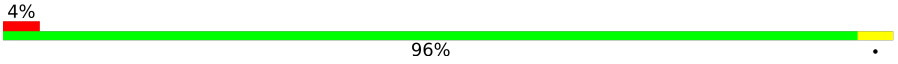
Chain W:

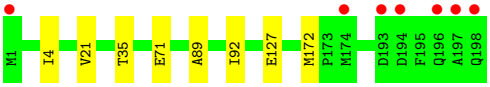




• Molecule 10: Proteasome subunit beta type-4

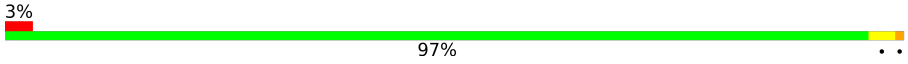
Chain J:





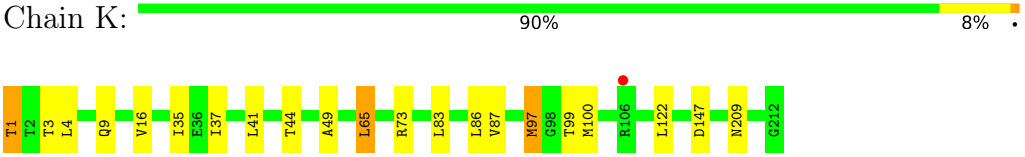
• Molecule 10: Proteasome subunit beta type-4

Chain X:



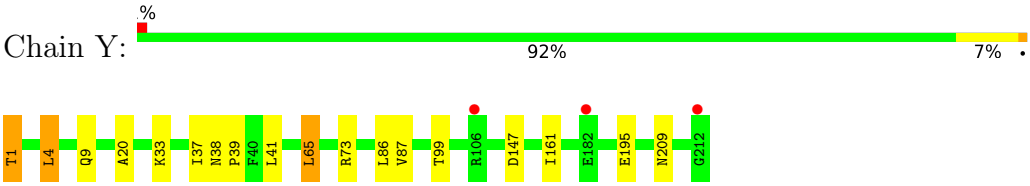
• Molecule 11: Proteasome subunit beta type-5

Chain K:



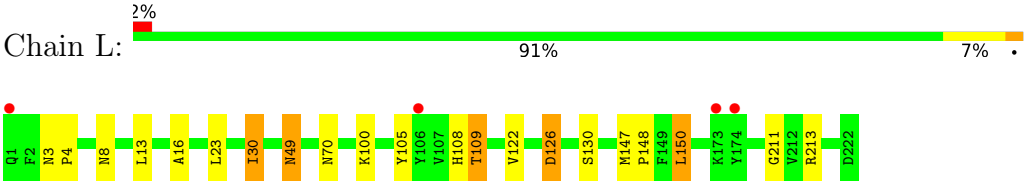
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



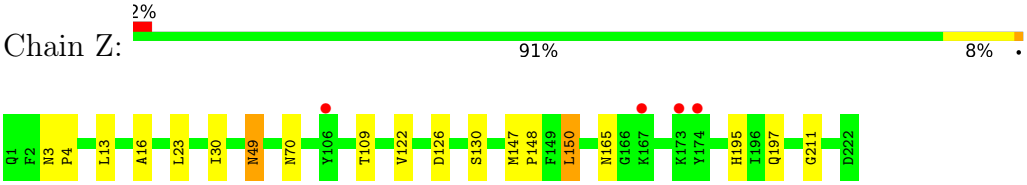
• Molecule 12: Proteasome subunit beta type-6

Chain L:



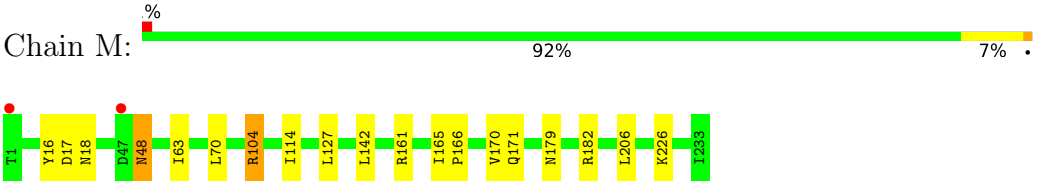
• Molecule 12: Proteasome subunit beta type-6

Chain Z:



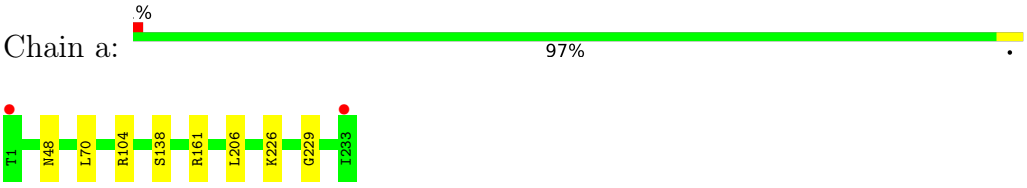
• Molecule 13: Proteasome subunit beta type-7

Chain M:



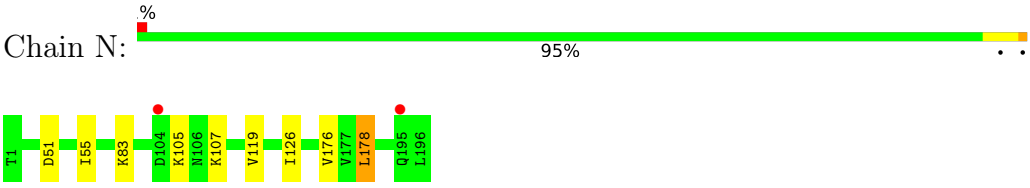
• Molecule 13: Proteasome subunit beta type-7

Chain a:



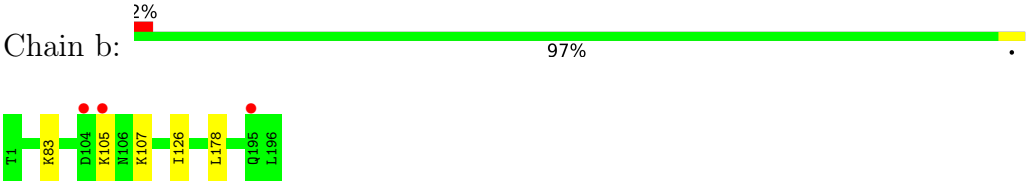
• Molecule 14: Proteasome subunit beta type-1

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	135.17Å 300.23Å 144.38Å 90.00° 112.79° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (15.00-2.50) 97.3 (15.00-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.204 , 0.233 0.206 , 0.233	Depositor DCC
R_{free} test set	17633 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	49.9	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.2	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	52219	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EC6

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	0.28	0/1952	0.48	0/2642
1	O	0.28	0/1952	0.47	0/2642
2	B	0.28	0/1934	0.50	0/2618
2	P	0.27	0/1934	0.49	0/2618
3	C	0.28	0/1919	0.51	0/2598
3	Q	0.27	0/1919	0.50	0/2598
4	D	0.27	0/1886	0.49	0/2541
4	R	0.28	0/1886	0.48	0/2541
5	E	0.28	0/1823	0.46	0/2463
5	S	0.27	0/1823	0.45	0/2463
6	F	0.28	0/1936	0.47	0/2614
6	T	0.27	0/1936	0.46	0/2614
7	G	0.28	0/1959	0.49	0/2652
7	U	0.28	0/1959	0.49	0/2652
8	H	0.26	0/1715	0.49	0/2326
8	V	0.26	0/1715	0.49	0/2326
9	I	0.29	0/1611	0.50	0/2174
9	W	0.28	0/1611	0.49	0/2174
10	J	0.27	0/1613	0.49	0/2173
10	X	0.27	0/1613	0.49	0/2173
11	K	0.32	1/1681 (0.1%)	0.51	0/2274
11	Y	0.32	1/1681 (0.1%)	0.52	0/2274
12	L	0.28	0/1795	0.51	0/2420
12	Z	0.29	0/1795	0.51	0/2420
13	M	0.29	0/1855	0.52	0/2514
13	a	0.28	0/1855	0.53	0/2514
14	N	0.27	0/1541	0.48	0/2087
14	b	0.26	0/1541	0.47	0/2087
All	All	0.28	2/50440 (0.0%)	0.49	0/68192

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	K	0	1
11	Y	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	1	THR	C-N	6.61	1.49	1.34
11	K	1	THR	C-N	6.59	1.49	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	1	THR	Peptide
11	Y	1	THR	Peptide

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	7	0
1	O	1915	0	1929	5	0
2	B	1904	0	1904	13	0
2	P	1904	0	1904	12	0
3	C	1890	0	1903	15	0
3	Q	1890	0	1903	12	0
4	D	1861	0	1839	7	0
4	R	1861	0	1839	7	0
5	E	1795	0	1800	12	0
5	S	1795	0	1800	12	0
6	F	1896	0	1889	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	1896	0	1889	8	0
7	G	1921	0	1913	8	0
7	U	1921	0	1913	14	0
8	H	1684	0	1688	4	0
8	V	1684	0	1688	4	0
9	I	1581	0	1574	4	0
9	W	1581	0	1574	4	0
10	J	1585	0	1590	4	0
10	X	1585	0	1590	3	0
11	K	1644	0	1592	9	0
11	Y	1644	0	1592	7	0
12	L	1757	0	1711	15	0
12	Z	1757	0	1711	12	0
13	M	1824	0	1832	8	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	2	0
14	b	1512	0	1481	0	0
15	K	37	0	52	1	0
15	Y	37	0	52	2	0
16	A	99	0	0	0	0
16	B	77	0	0	0	0
16	C	85	0	0	0	0
16	D	86	0	0	1	0
16	E	57	0	0	0	0
16	F	92	0	0	1	0
16	G	121	0	0	0	0
16	H	101	0	0	0	0
16	I	107	0	0	0	0
16	J	103	0	0	2	0
16	K	104	0	0	1	0
16	L	110	0	0	2	0
16	M	132	0	0	0	0
16	N	101	0	0	0	0
16	O	66	0	0	0	0
16	P	75	0	0	1	0
16	Q	73	0	0	1	0
16	R	85	0	0	0	0
16	S	49	0	0	0	0
16	T	89	0	0	2	0
16	U	110	0	0	2	0
16	V	91	0	0	1	0
16	W	104	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	X	98	0	0	2	0
16	Y	73	0	0	0	0
16	Z	102	0	0	1	0
16	a	111	0	0	0	0
16	b	106	0	0	0	0
All	All	52219	0	49394	184	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 2.

All (184) 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)
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.64	0.80
3:C:51:LYS:O	3:C:52:LEU:HB2	1.90	0.71
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.41	0.68
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.58	0.68
5:E:12:PHE:H	6:F:19:GLN:HE22	1.40	0.67
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.58	0.67
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.76	0.67
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.60	0.66
4:D:89:VAL:HG11	11:K:65:LEU:HD22	1.79	0.65
7:U:92:ALA:HA	7:U:103:MET:HE2	1.80	0.63
5:S:12:PHE:H	6:T:19:GLN:HE22	1.45	0.63
6:T:116:VAL:HA	16:T:377:HOH:O	1.99	0.62
10:X:13:VAL:HG22	16:X:291:HOH:O	2.00	0.62
2:B:12:PHE:H	3:C:17:GLN:HE22	1.48	0.62
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.82	0.62
5:E:35:VAL:HG23	5:E:196:ILE:HD12	1.83	0.60
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.48	0.60
6:F:31:THR:HG21	6:F:47:GLU:O	2.03	0.57
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.52	0.57
5:S:35:VAL:HG23	5:S:196:ILE:HD12	1.85	0.57
6:T:123:ASN:C	6:T:123:ASN:HD22	2.08	0.56
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.86	0.56
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.86	0.56
7:U:83:ASN:C	7:U:83:ASN:HD22	2.07	0.56
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.03	0.56
7:G:83:ASN:C	7:G:83:ASN:HD22	2.10	0.56
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.72	0.55
6:F:123:ASN:C	6:F:123:ASN:HD22	2.11	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.88	0.54
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.05	0.54
2:P:18:LEU:HD13	2:P:122:THR:HG23	1.90	0.53
7:G:92:ALA:HA	7:G:103:MET:HE2	1.90	0.53
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.09	0.53
3:C:161:THR:HG21	3:C:169:VAL:HG13	1.92	0.52
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.90	0.52
2:B:86:LEU:HB3	2:B:114:LEU:HD21	1.91	0.52
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.58	0.52
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.90	0.52
11:K:49:ALA:HA	15:K:301:EC6:H43	1.93	0.51
4:R:89:VAL:HG11	11:Y:65:LEU:HD22	1.93	0.51
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.93	0.51
6:F:123:ASN:HD22	6:F:124:SER:N	2.08	0.50
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.92	0.50
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.94	0.50
6:T:91:GLU:HG2	6:T:111:ARG:CB	2.39	0.50
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.10	0.50
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.93	0.50
6:F:19:GLN:NE2	16:F:311:HOH:O	2.45	0.49
7:U:45:ILE:HG21	16:U:399:HOH:O	2.12	0.49
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.77	0.49
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.48	0.49
6:F:39:ASN:C	6:F:39:ASN:HD22	2.15	0.49
12:L:109:THR:HG23	16:L:306:HOH:O	2.11	0.49
11:Y:33:LYS:HE2	15:Y:301:EC6:H43	1.95	0.49
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.96	0.48
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.94	0.48
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.78	0.47
2:P:86:LEU:HB3	2:P:114:LEU:HD21	1.95	0.47
3:C:9:PHE:H	4:D:15:GLN:HE22	1.62	0.47
12:L:4:PRO:O	13:M:104:ARG:NH1	2.44	0.47
2:P:176:GLN:NE2	16:P:330:HOH:O	2.46	0.47
11:K:37:ILE:HB	11:K:41:LEU:HB3	1.94	0.47
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.44	0.47
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.63	0.47
10:J:4:ILE:HG21	16:J:299:HOH:O	2.13	0.47
12:L:213:ARG:NH1	16:L:329:HOH:O	2.47	0.47
2:B:172:GLN:HG2	3:C:50:LEU:HD12	1.96	0.47
13:M:48:ASN:HD22	13:M:48:ASN:H	1.62	0.47
4:D:112:ALA:HB2	16:D:377:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.62	0.47
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.13	0.47
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.97	0.47
12:Z:49:ASN:ND2	16:Z:316:HOH:O	2.48	0.47
8:V:210:THR:HG21	9:W:167:SER:HB3	1.97	0.47
6:T:123:ASN:HD22	6:T:124:SER:N	2.13	0.47
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	1.97	0.46
3:Q:117:ARG:NH2	16:Q:309:HOH:O	2.47	0.46
14:N:51:ASP:O	14:N:55:ILE:HG12	2.15	0.46
7:U:83:ASN:C	7:U:83:ASN:ND2	2.67	0.46
1:A:12:PHE:H	2:B:20:GLN:HE22	1.62	0.46
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.45	0.46
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.98	0.46
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.50	0.46
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.63	0.46
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.27	0.46
6:F:59:LYS:O	6:F:60:ASN:C	2.54	0.46
7:G:78:ILE:N	7:G:79:PRO:CD	2.79	0.46
2:B:162:ILE:HD13	2:B:163:SER:O	2.16	0.45
3:C:157:TRP:CZ2	4:D:51:LEU:HD23	2.51	0.45
7:U:103:MET:HE1	7:U:108:LEU:HD13	1.99	0.45
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.81	0.45
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.98	0.45
7:G:83:ASN:C	7:G:83:ASN:ND2	2.70	0.45
11:K:83:LEU:HD11	11:K:97:MET:HE1	1.98	0.45
9:I:81:ILE:CD1	9:I:85:THR:HB	2.45	0.45
7:U:78:ILE:N	7:U:79:PRO:CD	2.79	0.45
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.65	0.45
11:K:35:ILE:HB	16:K:497:HOH:O	2.16	0.45
13:M:17:ASP:OD1	13:M:18:ASN:N	2.50	0.45
8:V:84:LYS:HE2	8:V:119:THR:HG23	1.99	0.45
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.37	0.45
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.32	0.45
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.47	0.44
4:R:176:LEU:HD22	5:S:55:LEU:HD13	1.98	0.44
7:U:34:LEU:C	7:U:34:LEU:HD12	2.38	0.44
11:Y:4:LEU:HD13	11:Y:161:ILE:HD11	2.00	0.44
3:Q:34:VAL:HG12	3:Q:159:ALA:HB1	2.00	0.44
6:T:19:GLN:NE2	16:T:308:HOH:O	2.48	0.44
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.00	0.44
6:T:39:ASN:HD22	6:T:39:ASN:C	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:172:MET:HE2	16:J:209:HOH:O	2.17	0.43
1:A:55:LEU:HD12	7:G:170:THR:HG23	2.00	0.43
5:S:44:VAL:HG21	5:S:188:LEU:HB3	1.99	0.43
7:U:44:VAL:CG1	7:U:135:VAL:HG11	2.47	0.43
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.82	0.43
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.84	0.43
3:Q:157:TRP:CZ2	4:R:51:LEU:HD23	2.54	0.43
1:A:187:ASP:O	1:A:191:ILE:HG12	2.19	0.43
13:M:63:ILE:HD13	13:M:114:ILE:HD11	1.99	0.43
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.01	0.42
4:R:178:GLU:HB3	4:R:191:LEU:HD21	2.01	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.49	0.42
10:X:174:MET:HB2	16:X:207:HOH:O	2.20	0.42
5:S:134:ILE:HD12	5:S:215:VAL:HG12	2.02	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.42
8:V:172:ASN:ND2	16:V:378:HOH:O	2.52	0.42
1:A:115:ALA:HB1	1:A:154:GLY:O	2.20	0.42
1:O:187:ASP:O	1:O:191:ILE:HG12	2.20	0.42
5:S:68:HIS:HE1	5:S:102:LEU:O	2.02	0.42
2:P:200:THR:HG22	2:P:202:SER:H	1.85	0.42
5:S:77:ALA:N	5:S:78:PRO:CD	2.83	0.42
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.54	0.42
9:I:62:LEU:HD12	9:I:104:VAL:HG11	2.02	0.42
11:K:3:THR:HG22	11:K:16:VAL:HG12	2.01	0.42
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.00	0.42
5:E:118:ASN:HD22	5:E:118:ASN:N	2.17	0.42
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.54	0.42
11:K:44:THR:HG21	11:K:100:MET:HE3	2.01	0.42
8:H:222:ASP:N	8:H:222:ASP:OD1	2.53	0.42
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.16	0.41
13:M:16:TYR:CE2	13:M:170:VAL:HG22	2.54	0.41
6:F:191:GLN:HE21	6:F:194:LYS:CE	2.33	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
2:B:83:ALA:O	2:B:87:ILE:HG12	2.20	0.41
6:F:91:GLU:HG3	6:F:111:ARG:HH11	1.85	0.41
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.67	0.41
7:U:103:MET:CE	7:U:108:LEU:HD13	2.50	0.41
12:L:147:MET:N	12:L:148:PRO:HD2	2.34	0.41
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.67	0.41
2:B:122:THR:CG2	3:C:125:ARG:HH21	2.33	0.41
2:P:83:ALA:O	2:P:87:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:60:VAL:HG21	4:R:81:ILE:HD13	2.02	0.41
12:L:126:ASP:HB3	12:L:130:SER:HB3	2.02	0.41
7:U:187:GLU:HG2	7:U:192:LYS:CB	2.50	0.41
2:B:35:ILE:HD12	2:B:196:LEU:HG	2.01	0.41
1:O:12:PHE:H	2:P:20:GLN:HE22	1.67	0.41
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.55	0.41
2:P:162:ILE:HD13	2:P:163:SER:O	2.20	0.41
5:E:9:THR:HG21	5:E:119:THR:HA	2.01	0.41
8:H:7:LYS:HG3	8:H:123:TYR:HA	2.02	0.41
3:C:51:LYS:O	3:C:52:LEU:CB	2.65	0.41
4:D:60:VAL:HG21	4:D:81:ILE:HD13	2.02	0.41
5:E:44:VAL:HG21	5:E:188:LEU:HB3	2.02	0.41
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.03	0.41
10:X:33:ASP:OD1	10:X:35:THR:HG22	2.20	0.41
11:Y:20:ALA:HB1	15:Y:301:EC6:H4	2.03	0.41
3:C:12:ASP:OD2	3:C:14:HIS:ND1	2.54	0.41
5:E:1:PHE:O	5:E:3:ASN:N	2.54	0.41
7:U:187:GLU:HG2	7:U:192:LYS:HB3	2.03	0.41
10:J:89:ALA:O	10:J:92:ILE:HG22	2.20	0.41
11:K:86:LEU:C	11:K:86:LEU:HD13	2.42	0.41
3:C:51:LYS:HD2	3:C:52:LEU:N	2.35	0.40
7:G:92:ALA:HA	7:G:103:MET:CE	2.51	0.40
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.40
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.40
4:D:104:LEU:C	4:D:104:LEU:HD13	2.42	0.40
1:O:57:MET:HE2	16:U:317:HOH:O	2.20	0.40
1:A:89:SER:OG	1:A:114:VAL:HG22	2.22	0.40
2:B:119:GLN:O	2:B:122:THR:HB	2.21	0.40
3:C:108:THR:HG21	3:C:146:TYR:HB3	2.03	0.40
5:E:32:SER:O	5:E:61:LYS:NZ	2.53	0.40
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.86	0.40
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.57	0.40
12:Z:126:ASP:CB	12:Z:130:SER:HB3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34	54
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34	54
2	B	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	19	35
2	P	242/258 (94%)	232 (96%)	8 (3%)	2 (1%)	19	35
3	C	239/254 (94%)	234 (98%)	3 (1%)	2 (1%)	19	35
3	Q	239/254 (94%)	232 (97%)	5 (2%)	2 (1%)	19	35
4	D	240/260 (92%)	234 (98%)	6 (2%)	0	100	100
4	R	240/260 (92%)	233 (97%)	7 (3%)	0	100	100
5	E	231/234 (99%)	224 (97%)	6 (3%)	1 (0%)	34	54
5	S	231/234 (99%)	222 (96%)	8 (4%)	1 (0%)	34	54
6	F	242/287 (84%)	234 (97%)	6 (2%)	2 (1%)	19	35
6	T	242/287 (84%)	233 (96%)	9 (4%)	0	100	100
7	G	241/252 (96%)	233 (97%)	6 (2%)	2 (1%)	19	35
7	U	241/252 (96%)	236 (98%)	3 (1%)	2 (1%)	19	35
8	H	220/232 (95%)	215 (98%)	5 (2%)	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%)	197 (98%)	5 (2%)	0	100	100
10	J	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
10	X	196/198 (99%)	190 (97%)	6 (3%)	0	100	100
11	K	210/212 (99%)	205 (98%)	4 (2%)	1 (0%)	29	48
11	Y	210/212 (99%)	203 (97%)	6 (3%)	1 (0%)	29	48
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
13	M	231/233 (99%)	223 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	a	231/233 (99%)	223 (96%)	7 (3%)	1 (0%)	34 54
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100 100
14	b	194/196 (99%)	186 (96%)	8 (4%)	0	100 100
All	All	6312/6586 (96%)	6111 (97%)	180 (3%)	21 (0%)	41 61

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	52	LEU
7	G	242	GLN
3	Q	52	LEU
5	E	201	ARG
7	G	2	GLY
5	S	201	ARG
7	U	2	GLY
7	U	242	GLN
6	F	60	ASN
11	K	209	ASN
2	B	221	ASP
3	C	203	THR
6	F	59	LYS
2	P	51	VAL
2	P	221	ASP
11	Y	209	ASN
2	B	51	VAL
1	O	2	THR
3	Q	203	THR
1	A	2	THR
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%)	207 (99%)	2 (1%)	76 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	209/209 (100%)	207 (99%)	2 (1%)	76 90
2	B	203/216 (94%)	194 (96%)	9 (4%)	28 52
2	P	203/216 (94%)	192 (95%)	11 (5%)	22 42
3	C	213/226 (94%)	203 (95%)	10 (5%)	26 49
3	Q	213/226 (94%)	203 (95%)	10 (5%)	26 49
4	D	198/215 (92%)	187 (94%)	11 (6%)	21 40
4	R	198/215 (92%)	187 (94%)	11 (6%)	21 40
5	E	192/193 (100%)	181 (94%)	11 (6%)	20 39
5	S	192/193 (100%)	180 (94%)	12 (6%)	18 34
6	F	201/238 (84%)	188 (94%)	13 (6%)	17 33
6	T	201/238 (84%)	191 (95%)	10 (5%)	24 46
7	G	207/210 (99%)	198 (96%)	9 (4%)	29 53
7	U	207/210 (99%)	196 (95%)	11 (5%)	22 43
8	H	181/190 (95%)	176 (97%)	5 (3%)	43 70
8	V	181/190 (95%)	177 (98%)	4 (2%)	52 77
9	I	172/173 (99%)	168 (98%)	4 (2%)	50 76
9	W	172/173 (99%)	168 (98%)	4 (2%)	50 76
10	J	175/175 (100%)	172 (98%)	3 (2%)	60 82
10	X	175/175 (100%)	172 (98%)	3 (2%)	60 82
11	K	169/169 (100%)	161 (95%)	8 (5%)	26 49
11	Y	169/169 (100%)	161 (95%)	8 (5%)	26 49
12	L	185/185 (100%)	178 (96%)	7 (4%)	33 58
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39 65
13	M	199/199 (100%)	192 (96%)	7 (4%)	36 62
13	a	199/199 (100%)	192 (96%)	7 (4%)	36 62
14	N	162/162 (100%)	156 (96%)	6 (4%)	34 60
14	b	162/162 (100%)	157 (97%)	5 (3%)	40 67
All	All	5332/5520 (97%)	5123 (96%)	209 (4%)	32 57

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR

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Mol	Chain	Res	Type
1	A	157	PHE
2	B	55	LEU
2	B	69	ASN
2	B	114	LEU
2	B	119	GLN
2	B	122	THR
2	B	162	ILE
2	B	184	LYS
2	B	191	LEU
2	B	200	THR
3	C	4	ARG
3	C	51	LYS
3	C	61	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	185	THR
3	C	206	LYS
4	D	5	SER
4	D	20	LEU
4	D	40	LEU
4	D	102	GLU
4	D	124	ARG
4	D	143	ASP
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	214	ILE
4	D	242	GLU
5	E	8	ASP
5	E	9	THR
5	E	29	LYS
5	E	53	ASP
5	E	54	GLU
5	E	71	LEU
5	E	116	GLN
5	E	179	ILE
5	E	184	ASN
5	E	208	ASP
5	E	231	LYS

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Mol	Chain	Res	Type
6	F	31	THR
6	F	32	THR
6	F	39	ASN
6	F	117	GLN
6	F	123	ASN
6	F	126	ARG
6	F	172	LEU
6	F	181	GLU
6	F	186	ARG
6	F	201	GLU
6	F	214	TRP
6	F	221	ASN
6	F	228	LYS
7	G	24	LYS
7	G	68	ARG
7	G	83	ASN
7	G	115	LEU
7	G	120	THR
7	G	166	GLN
7	G	171	THR
7	G	221	LYS
7	G	235	ARG
1	O	122	THR
1	O	157	PHE
2	P	55	LEU
2	P	69	ASN
2	P	114	LEU
2	P	119	GLN
2	P	122	THR
2	P	149	THR
2	P	157	THR
2	P	162	ILE
2	P	184	LYS
2	P	191	LEU
2	P	200	THR
3	Q	4	ARG
3	Q	51	LYS
3	Q	61	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	175	LYS

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Mol	Chain	Res	Type
3	Q	180	LYS
3	Q	185	THR
3	Q	206	LYS
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	54	ASP
4	R	102	GLU
4	R	124	ARG
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	214	ILE
4	R	225	ASN
5	S	8	ASP
5	S	9	THR
5	S	29	LYS
5	S	53	ASP
5	S	54	GLU
5	S	71	LEU
5	S	99	ASN
5	S	116	GLN
5	S	179	ILE
5	S	184	ASN
5	S	208	ASP
5	S	231	LYS
6	T	31	THR
6	T	39	ASN
6	T	117	GLN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	186	ARG
6	T	201	GLU
6	T	214	TRP
6	T	228	LYS
7	U	34	LEU
7	U	68	ARG
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	120	THR

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Mol	Chain	Res	Type
7	U	166	GLN
7	U	208	GLU
7	U	221	LYS
7	U	235	ARG
7	U	236	LEU
8	H	30	ASN
8	H	34	LEU
8	H	56	THR
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	81	ILE
9	I	171	LEU
9	I	182	TRP
10	J	35	THR
10	J	71	GLU
10	J	127	GLU
11	K	4	LEU
11	K	9	GLN
11	K	65	LEU
11	K	73	ARG
11	K	87	VAL
11	K	97	MET
11	K	99	THR
11	K	147	ASP
12	L	23	LEU
12	L	30	ILE
12	L	49	ASN
12	L	108	HIS
12	L	109	THR
12	L	126	ASP
12	L	150	LEU
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	171	GLN
13	M	206	LEU
13	M	226	LYS
14	N	83	LYS
14	N	105	LYS
14	N	107	LYS

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Mol	Chain	Res	Type
14	N	119	VAL
14	N	126	ILE
14	N	178	LEU
8	V	30	ASN
8	V	56	THR
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	81	ILE
9	W	171	LEU
9	W	182	TRP
10	X	35	THR
10	X	71	GLU
10	X	127	GLU
11	Y	4	LEU
11	Y	9	GLN
11	Y	65	LEU
11	Y	73	ARG
11	Y	87	VAL
11	Y	99	THR
11	Y	147	ASP
11	Y	195	GLU
12	Z	23	LEU
12	Z	30	ILE
12	Z	49	ASN
12	Z	109	THR
12	Z	150	LEU
12	Z	165	ASN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	138	SER
13	a	161	ARG
13	a	206	LEU
13	a	226	LYS
14	b	83	LYS
14	b	105	LYS
14	b	107	LYS
14	b	126	ILE
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (141) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	69	ASN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
2	B	220	ASN
3	C	17	GLN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	100	ASN
4	D	146	GLN
4	D	160	ASN
4	D	198	GLN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	39	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
7	G	186	ASN
1	O	94	HIS
2	P	20	GLN
2	P	95	GLN

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Mol	Chain	Res	Type
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
2	P	220	ASN
3	Q	17	GLN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	100	ASN
4	R	146	GLN
4	R	160	ASN
4	R	198	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	19	GLN
6	T	39	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	175	ASN
7	U	186	ASN
7	U	231	ASN
8	H	30	ASN
8	H	57	GLN
8	H	66	HIS
8	H	144	GLN
8	H	172	ASN
8	H	189	ASN

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Mol	Chain	Res	Type
9	I	88	GLN
10	J	55	GLN
10	J	146	HIS
10	J	191	GLN
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	80	ASN
12	L	95	HIS
12	L	152	ASN
12	L	153	GLN
12	L	158	ASN
12	L	165	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	171	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
8	V	30	ASN
8	V	57	GLN
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	88	GLN
10	X	55	GLN
10	X	118	GLN
10	X	191	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	49	ASN

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Mol	Chain	Res	Type
12	Z	70	ASN
12	Z	80	ASN
12	Z	165	ASN
12	Z	195	HIS
13	a	2	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	171	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS

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)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	EC6	K	301	11	36,36,36	1.39	3 (8%)	43,47,47	1.63	8 (18%)
15	EC6	Y	301	11	36,36,36	1.33	3 (8%)	43,47,47	1.49	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	EC6	K	301	11	-	17/52/52/52	-
15	EC6	Y	301	11	-	20/52/52/52	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	K	301	EC6	C17-C16	4.31	1.61	1.53
15	Y	301	EC6	C17-C16	3.80	1.60	1.53
15	K	301	EC6	C12-C11	3.67	1.58	1.52
15	Y	301	EC6	C12-C11	3.59	1.58	1.52
15	K	301	EC6	C16-C11	3.24	1.59	1.53
15	Y	301	EC6	C16-C11	2.38	1.57	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	Y	301	EC6	O3-C5-C2	-4.14	112.19	120.74
15	K	301	EC6	O3-C5-C2	-3.88	112.72	120.74
15	K	301	EC6	C12-C11-N3	-3.63	105.49	110.18
15	K	301	EC6	C18-C17-C16	3.28	116.49	111.46
15	K	301	EC6	O1-C1-C27	-3.15	116.25	122.02
15	Y	301	EC6	C11-N3-C10	-2.98	117.80	123.07
15	K	301	EC6	C23-C17-C18	-2.84	104.58	111.78
15	K	301	EC6	O7-C9-C8	-2.81	113.32	121.31
15	Y	301	EC6	O7-C9-C8	-2.73	113.55	121.31
15	Y	301	EC6	O2-C10-C6	-2.56	115.06	120.45
15	K	301	EC6	C11-N3-C10	-2.23	119.12	123.07
15	Y	301	EC6	C26-C3-C2	2.17	117.30	111.16
15	K	301	EC6	C13-C12-C11	2.08	119.99	115.84
15	Y	301	EC6	O1-C1-C27	-2.04	118.29	122.02

There are no chirality outliers.

All (37) torsion outliers are listed below:

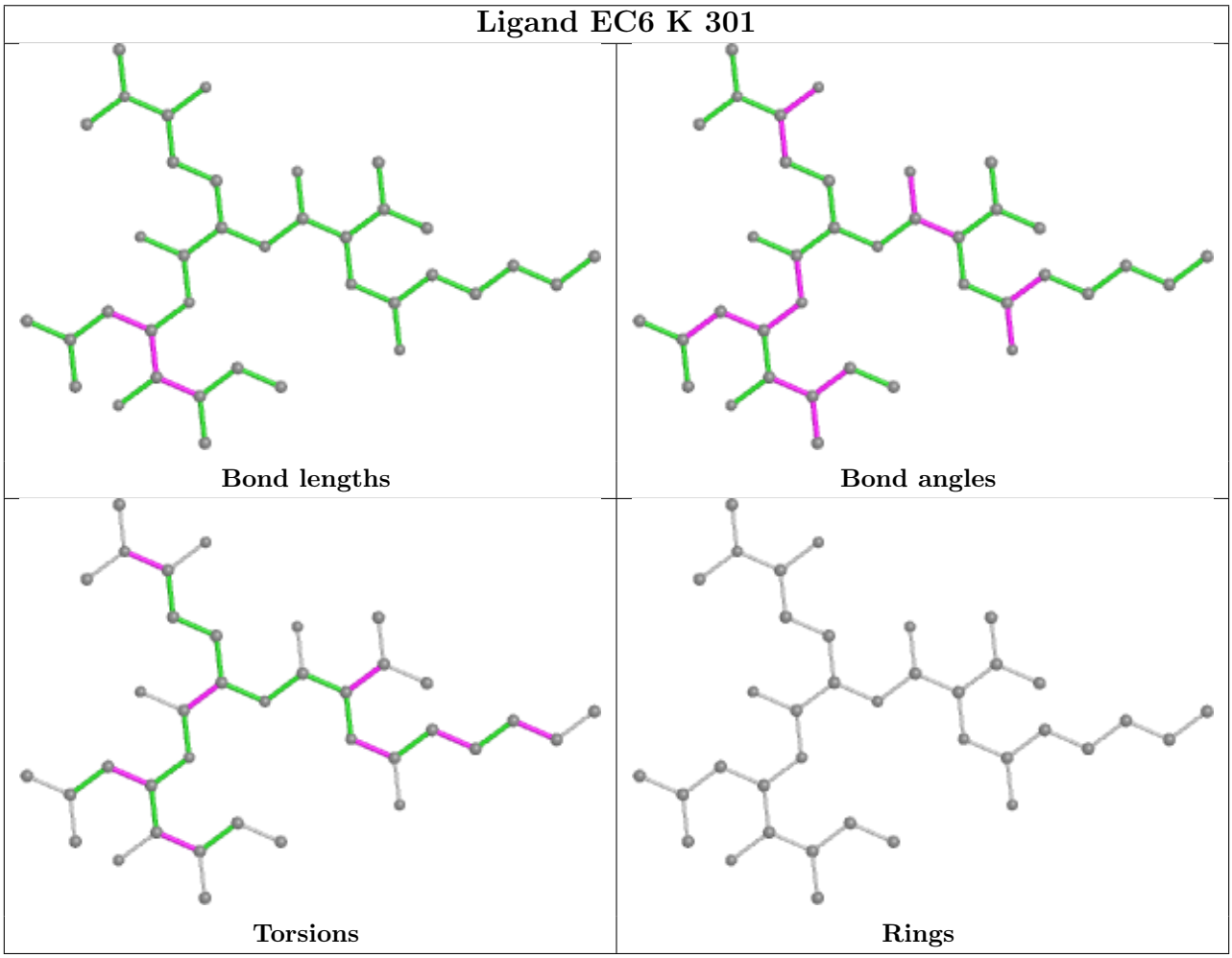
Mol	Chain	Res	Type	Atoms
15	K	301	EC6	C8-C9-N5-C24
15	K	301	EC6	C16-C11-C12-C13
15	K	301	EC6	C11-C16-C17-C23
15	K	301	EC6	C11-C16-C17-C18
15	Y	301	EC6	O1-C1-N1-C2
15	Y	301	EC6	C8-C9-N5-C24
15	Y	301	EC6	C8-C9-N5-C25
15	Y	301	EC6	O7-C9-N5-C24
15	Y	301	EC6	O7-C9-N5-C25
15	Y	301	EC6	C11-C16-C17-C23
15	Y	301	EC6	C11-C16-C17-C18
15	Y	301	EC6	C5-C2-C3-C26
15	Y	301	EC6	C23-C17-C18-C44
15	Y	301	EC6	N1-C2-C3-C26
15	Y	301	EC6	C5-C2-C3-C4
15	Y	301	EC6	N1-C2-C3-C4
15	K	301	EC6	O1-C1-N1-C2
15	K	301	EC6	C5-C2-C3-C4
15	K	301	EC6	O7-C9-N5-C25
15	Y	301	EC6	O2-C10-C6-C7
15	K	301	EC6	N1-C2-C3-C26
15	K	301	EC6	N1-C2-C3-C4
15	Y	301	EC6	C1-C27-C28-C29
15	K	301	EC6	O2-C10-C6-C7
15	Y	301	EC6	O2-C10-N3-C11
15	Y	301	EC6	O6-C16-C17-C23
15	Y	301	EC6	O6-C16-C17-C18
15	K	301	EC6	C1-C27-C28-C29
15	K	301	EC6	C28-C29-C30-C31
15	Y	301	EC6	C16-C17-C18-C44
15	K	301	EC6	O6-C16-C17-C23
15	K	301	EC6	O6-C16-C17-C18
15	K	301	EC6	N3-C11-C12-C13
15	K	301	EC6	C5-C2-C3-C26
15	Y	301	EC6	C27-C28-C29-C30
15	K	301	EC6	O2-C10-C6-N2
15	Y	301	EC6	O2-C10-C6-N2

There are no ring outliers.

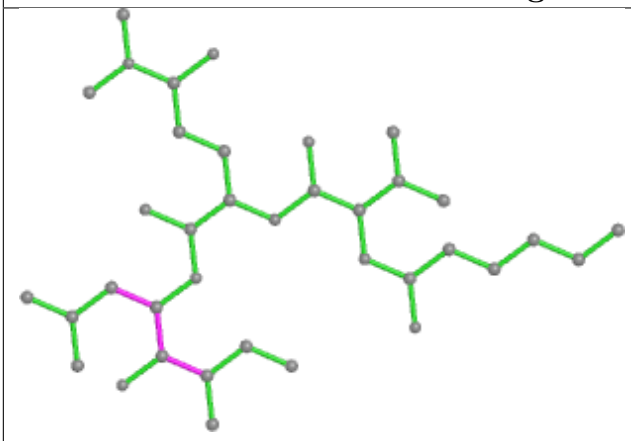
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	K	301	EC6	1	0
15	Y	301	EC6	2	0

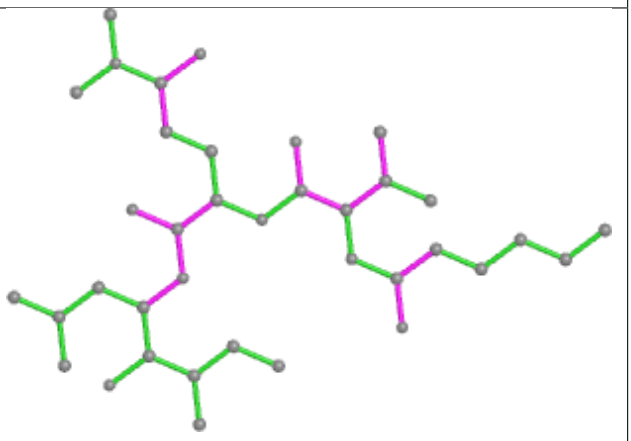
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



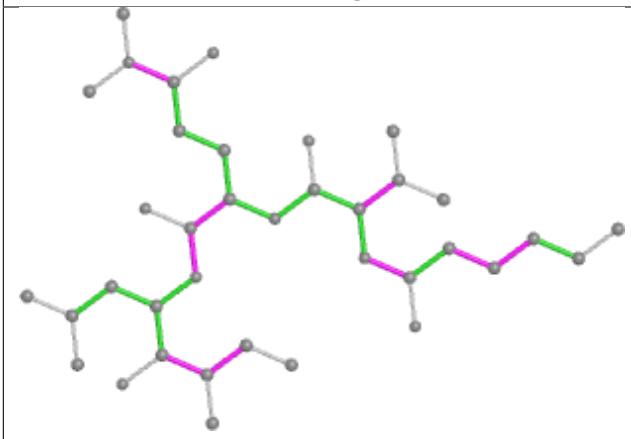
Ligand EC6 Y 301



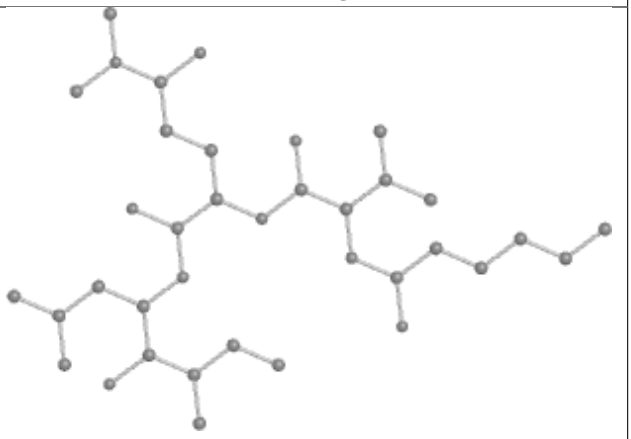
Bond lengths



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%)	-0.21	10 (4%) 38 41	38, 50, 81, 128	0
1	O	250/250 (100%)	-0.09	11 (4%) 34 37	43, 57, 94, 127	0
2	B	244/258 (94%)	0.02	16 (6%) 18 19	39, 55, 99, 138	0
2	P	244/258 (94%)	0.11	16 (6%) 18 19	45, 58, 100, 146	0
3	C	241/254 (94%)	0.17	19 (7%) 12 12	39, 58, 114, 137	0
3	Q	241/254 (94%)	0.46	33 (13%) 3 2	48, 69, 133, 150	0
4	D	242/260 (93%)	0.14	14 (5%) 23 24	41, 59, 107, 145	0
4	R	242/260 (93%)	0.14	15 (6%) 20 21	44, 62, 102, 149	0
5	E	233/234 (99%)	-0.06	14 (6%) 21 22	44, 58, 85, 123	0
5	S	233/234 (99%)	0.21	16 (6%) 16 17	48, 70, 100, 123	0
6	F	244/287 (85%)	-0.15	11 (4%) 33 36	38, 55, 92, 121	0
6	T	244/287 (85%)	0.01	15 (6%) 21 22	47, 63, 103, 130	0
7	G	243/252 (96%)	-0.20	8 (3%) 46 50	37, 51, 84, 135	0
7	U	243/252 (96%)	-0.16	6 (2%) 57 61	43, 55, 80, 121	0
8	H	222/232 (95%)	-0.28	4 (1%) 68 71	37, 48, 68, 113	0
8	V	222/232 (95%)	-0.24	2 (0%) 84 86	39, 50, 74, 125	0
9	I	204/205 (99%)	-0.49	2 (0%) 82 84	32, 46, 64, 90	0
9	W	204/205 (99%)	-0.44	2 (0%) 82 84	36, 48, 69, 87	0
10	J	198/198 (100%)	-0.21	7 (3%) 44 47	38, 49, 68, 143	0
10	X	198/198 (100%)	-0.16	6 (3%) 50 53	40, 52, 71, 148	0
11	K	212/212 (100%)	-0.39	1 (0%) 91 91	36, 49, 73, 85	0
11	Y	212/212 (100%)	-0.35	3 (1%) 75 77	38, 50, 76, 91	0
12	L	222/222 (100%)	-0.38	4 (1%) 68 71	36, 48, 73, 102	0
12	Z	222/222 (100%)	-0.35	4 (1%) 68 71	36, 49, 72, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/233 (100%)	-0.46	2 (0%) 84 86	34, 48, 63, 77	0
13	a	233/233 (100%)	-0.40	2 (0%) 84 86	36, 49, 65, 80	0
14	N	196/196 (100%)	-0.43	2 (1%) 82 84	37, 44, 65, 91	0
14	b	196/196 (100%)	-0.43	3 (1%) 73 75	37, 46, 65, 87	0
All	All	6368/6586 (96%)	-0.15	248 (3%) 39 42	32, 53, 93, 150	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	J	197	ALA	17.6
4	R	121	GLY	12.5
4	D	121	GLY	12.3
4	D	118	GLY	12.0
4	D	119	ALA	11.6
4	R	119	ALA	11.1
3	C	50	LEU	10.8
2	B	219	ALA	9.5
7	U	1	ALA	9.0
2	P	220	ASN	8.9
4	D	120	SER	8.7
10	X	197	ALA	8.6
3	Q	48	SER	8.5
2	B	220	ASN	8.4
4	R	118	GLY	8.2
10	X	198	GLN	8.0
7	G	1	ALA	8.0
4	D	125	LEU	8.0
8	V	222	ASP	7.7
9	W	1	SER	7.7
7	G	243	ASP	7.4
3	Q	49	THR	7.4
3	Q	203	THR	7.3
1	O	1	MET	7.3
3	Q	241	GLN	7.2
3	C	49	THR	7.2
2	P	219	ALA	7.2
3	Q	239	GLN	7.0
3	Q	50	LEU	7.0
10	J	198	GLN	6.9
2	P	51	VAL	6.9
5	S	1	PHE	6.4

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Mol	Chain	Res	Type	RSRZ
4	R	120	SER	6.4
12	L	174	TYR	6.3
4	D	124	ARG	6.3
2	B	51	VAL	6.2
8	V	221	CYS	6.2
5	E	1	PHE	6.1
3	C	241	GLN	6.1
4	R	125	LEU	6.1
10	X	196	GLN	6.0
1	A	1	MET	6.0
9	I	1	SER	5.9
6	F	1	GLY	5.8
5	S	2	ARG	5.8
4	D	122	GLU	5.6
8	H	221	CYS	5.6
1	A	250	LEU	5.5
4	R	124	ARG	5.5
5	S	173	ARG	5.4
5	S	202	ASP	5.3
7	U	243	ASP	5.3
4	R	122	GLU	5.3
1	A	2	THR	5.1
5	E	202	ASP	5.0
10	J	196	GLN	5.0
1	A	248	GLU	4.9
12	Z	174	TYR	4.9
3	Q	236	GLN	4.8
4	R	1	ASP	4.7
3	C	203	THR	4.7
3	C	206	LYS	4.6
2	B	221	ASP	4.6
3	C	238	LYS	4.6
2	P	221	ASP	4.6
2	P	222	GLY	4.5
1	O	2	THR	4.4
2	P	225	TYR	4.4
3	Q	240	GLU	4.4
6	F	244	ASN	4.3
6	F	205	GLU	4.3
5	E	2	ARG	4.2
6	T	244	ASN	4.2
2	B	218	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
4	D	1	ASP	4.0
6	T	1	GLY	4.0
3	Q	202	GLN	3.9
5	S	180	LYS	3.9
6	F	181	GLU	3.9
3	Q	52	LEU	3.9
6	T	243	ILE	3.8
1	O	248	GLU	3.8
2	P	203	SER	3.8
2	P	218	GLY	3.8
12	Z	173	LYS	3.8
5	E	3	ASN	3.8
8	H	222	ASP	3.7
3	Q	187	GLU	3.7
6	T	241	LYS	3.7
4	R	242	GLU	3.6
14	b	195	GLN	3.6
2	B	244	THR	3.6
7	G	242	GLN	3.6
6	T	2	THR	3.5
3	Q	225	GLU	3.5
4	D	242	GLU	3.5
4	D	2	ARG	3.4
2	P	59	ASP	3.4
2	B	50	LYS	3.4
3	Q	51	LYS	3.4
14	N	195	GLN	3.4
2	B	223	GLU	3.4
1	O	52	SER	3.3
2	P	61	SER	3.3
7	U	2	GLY	3.3
5	S	233	ILE	3.3
2	B	204	ALA	3.3
2	P	50	LYS	3.3
8	H	198	GLU	3.3
10	X	194	ASP	3.3
2	P	223	GLU	3.3
6	T	181	GLU	3.2
12	L	173	LYS	3.2
1	A	249	ALA	3.2
5	S	204	SER	3.2
4	R	2	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
5	S	201	ARG	3.2
1	O	201	GLU	3.2
3	C	225	GLU	3.2
14	N	104	ASP	3.2
2	B	203	SER	3.1
9	W	192	ASP	3.1
3	C	180	LYS	3.1
5	E	201	ARG	3.1
6	F	203	ASN	3.1
1	O	50	LYS	3.0
3	C	175	LYS	3.0
6	F	2	THR	3.0
4	R	177	ASN	3.0
5	S	163	ARG	3.0
10	X	193	ASP	3.0
1	O	62	SER	3.0
3	Q	55	THR	3.0
4	D	113	LEU	3.0
6	F	204	LYS	3.0
4	R	123	GLU	3.0
10	X	1	MET	2.9
3	C	239	GLN	2.9
3	C	202	GLN	2.9
14	b	105	LYS	2.9
4	D	123	GLU	2.9
10	J	1	MET	2.9
8	H	219	ASN	2.9
11	Y	106	ARG	2.9
11	Y	212	GLY	2.8
6	F	243	ILE	2.8
2	B	232	GLN	2.8
2	B	61	SER	2.8
6	T	166	GLN	2.7
1	A	231	LYS	2.7
5	E	173	ARG	2.7
7	G	2	GLY	2.7
6	F	241	LYS	2.7
4	R	113	LEU	2.7
12	Z	106	TYR	2.7
13	M	47	ASP	2.7
3	Q	181	GLU	2.7
11	K	106	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	59	ASP	2.7
14	b	104	ASP	2.7
5	E	227	GLU	2.6
3	Q	180	LYS	2.6
12	Z	167	LYS	2.6
3	Q	58	THR	2.6
13	a	233	ILE	2.6
3	Q	206	LYS	2.6
13	a	1	THR	2.6
3	C	240	GLU	2.6
7	U	242	GLN	2.6
2	B	225	TYR	2.6
3	C	48	SER	2.5
6	T	53	LYS	2.5
4	R	241	ALA	2.5
9	I	192	ASP	2.5
3	Q	47	ARG	2.5
11	Y	182	GLU	2.5
7	G	3	TYR	2.5
5	S	3	ASN	2.5
5	S	165	GLN	2.5
10	J	194	ASP	2.5
1	O	250	LEU	2.4
7	G	179	LYS	2.4
5	E	218	ASP	2.4
4	R	217	GLN	2.4
6	T	207	ASP	2.4
6	T	230	ASP	2.4
2	P	1	GLY	2.4
5	E	233	ILE	2.4
3	Q	59	PRO	2.4
1	A	52	SER	2.4
5	E	210	LEU	2.4
10	J	193	ASP	2.4
3	Q	46	ARG	2.4
3	C	236	GLN	2.4
7	G	188	GLU	2.4
3	C	46	ARG	2.4
6	F	201	GLU	2.4
3	Q	237	GLU	2.3
13	M	1	THR	2.3
3	Q	238	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
12	L	1	GLN	2.3
2	B	60	THR	2.3
2	P	240	LYS	2.3
5	S	51	ASN	2.3
4	D	217	GLN	2.3
3	Q	171	GLU	2.3
5	E	30	GLN	2.2
5	S	52	ALA	2.2
1	A	201	GLU	2.2
3	Q	235	GLU	2.2
2	B	242	GLY	2.2
3	Q	223	SER	2.2
3	Q	205	ALA	2.2
2	P	60	THR	2.2
5	E	122	TYR	2.2
12	L	106	TYR	2.2
10	J	174	MET	2.2
2	P	244	THR	2.2
1	A	229	THR	2.2
6	T	229	GLY	2.2
1	O	229	THR	2.2
4	D	177	ASN	2.2
1	O	249	ALA	2.2
3	Q	216	ASP	2.1
3	C	171	GLU	2.1
5	S	227	GLU	2.1
1	O	53	SER	2.1
6	T	178	HIS	2.1
3	Q	179	ARG	2.1
5	S	207	VAL	2.1
6	T	201	GLU	2.1
5	E	180	LYS	2.1
3	C	207	ASN	2.1
6	F	239	ALA	2.1
7	U	222	ASP	2.1
3	C	181	GLU	2.1
7	U	51	PRO	2.1
7	G	180	SER	2.1
3	C	167	LYS	2.1
3	Q	221	ALA	2.0
5	E	207	VAL	2.0
6	T	215	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	Q	208	ILE	2.0
6	T	205	GLU	2.0
3	Q	175	LYS	2.0
1	A	4	ARG	2.0
5	S	210	LEU	2.0
3	Q	141	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)

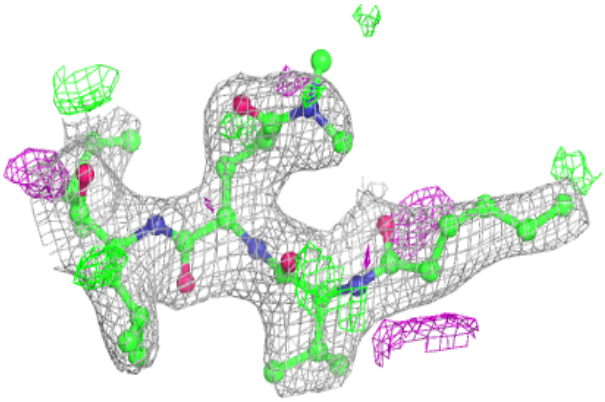
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

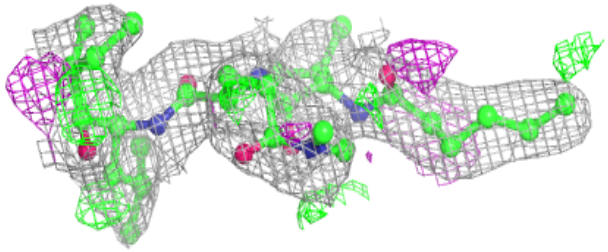
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	EC6	Y	301	37/37	0.88	0.20	52,59,75,76	0
15	EC6	K	301	37/37	0.89	0.18	47,54,69,69	0

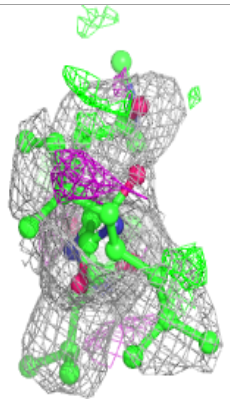
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EC6 Y 301:

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

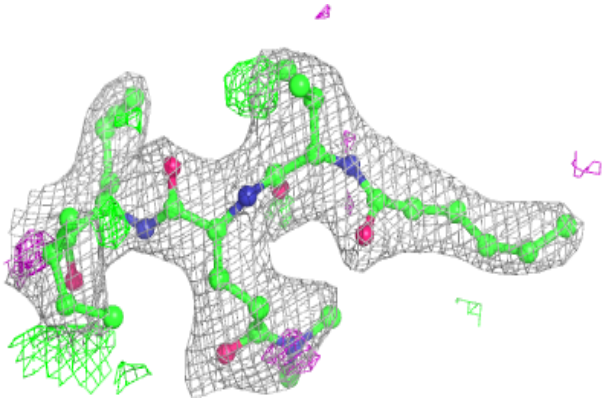


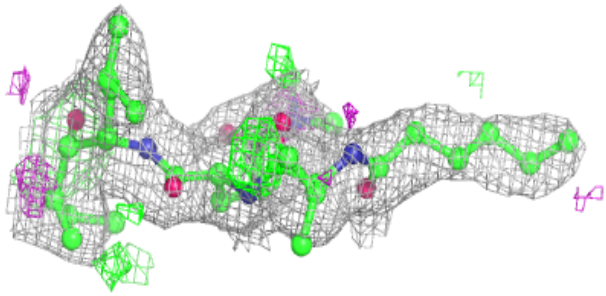


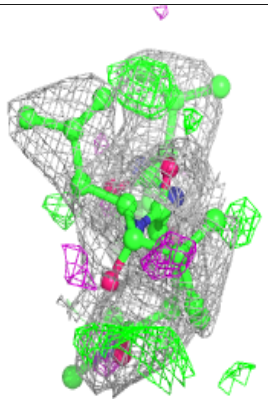


Electron density around EC6 K 301:

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







6.5 Other polymers (i)

There are no such residues in this entry.