Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 06:24 PM EDT

PDB ID	:	4QLV
Title	:	yCP in complex with tripeptidic epoxyketone inhibitor 17
Authors	:	de Bruin, G.; Huber, E.; Xin, B.; van Rooden, E.; Al-Ayed, K.; Kim, K.; Kisselev, A.; Driessen, C.; van der Marel, G.; Groll, M.; Overkleeft, H.
Deposited on	:	2014-06-13
Resolution	:	2.90 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:

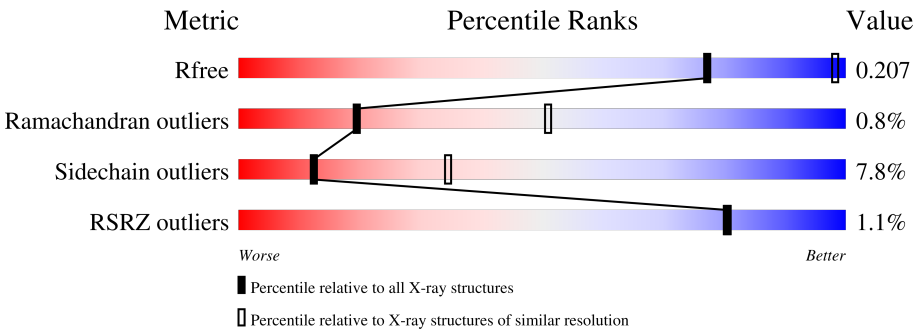
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	250	2%, 92%, 7%
1	O	250	.%, 92%, 7%
2	B	258	2%, 85%, 9%, 5%
2	P	258	3%, 86%, 9%, 5%
3	C	254	2%, 84%, 10%, 6%
3	Q	254	4%, 84%, 10%, 6%

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Mol	Chain	Length	Quality of chain
4	D	260	81% 10% 10%
4	R	260	.% 81% 10% 10%
5	E	234	.% 90% 9% •
5	S	234	.% 90% 9% •
6	F	288	.% 78% 6% 16%
6	T	288	.% 78% 6% 16%
7	G	252	2% 87% 9% •
7	U	252	.% 87% 9% •
8	H	232	.% 92% • •
8	V	232	.% 92% • •
9	I	205	95% •
9	W	205	95% •
10	J	198	.% 91% 7% • •
10	X	198	.% 91% 7% • •
11	K	212	95% •
11	Y	212	96% •
12	L	222	94% 6%
12	Z	222	94% 6%
13	M	246	.% 88% 6% 5%
13	a	246	.% 88% 7% 5%
14	N	196	2% 97% •
14	b	196	.% 97% •

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 49622 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	222	1684	1061	293	323	7	0	0	0
8	V	222	1683	1061	293	322	7	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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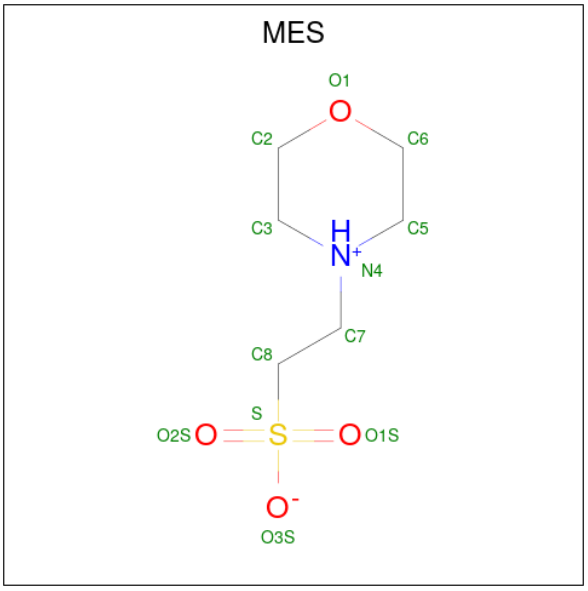
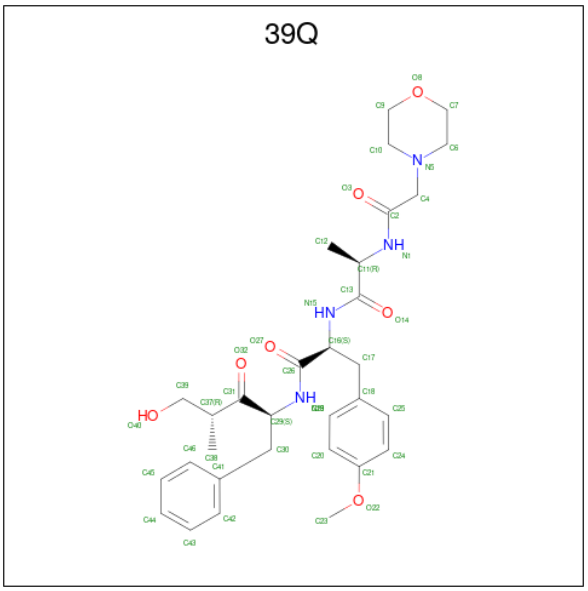
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	1	Total Mg 1 1	0	0
15	N	2	Total Mg 2 2	0	0
15	V	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

- Molecule 16 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 17 is N-(morpholin-4-ylacetyl)-D-alanyl-N-[(2S,4R)-5-hydroxy-4-methyl-3-oxo-1-phenylpentan-2-yl]-O-methyl-L-tyrosinamide (three-letter code: 39Q) (formula: $C_{31}H_{42}N_4O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
17	K	1	42	31	4	7	0	0
17	Y	1	42	31	4	7	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	A	5	5	5	0	0
18	B	10	10	10	0	0
18	C	9	9	9	0	0
18	D	4	4	4	0	0
18	E	5	5	5	0	0
18	F	6	6	6	0	0
18	G	6	6	6	0	0
18	H	9	9	9	0	0
18	I	6	6	6	0	0
18	J	7	7	7	0	0

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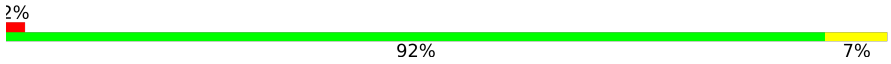
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	K	13	13	13	0	0
			Total	O		
18	L	8	8	8	0	0
			Total	O		
18	M	15	15	15	0	0
			Total	O		
18	N	7	7	7	0	0
			Total	O		
18	O	2	2	2	0	0
			Total	O		
18	P	6	6	6	0	0
			Total	O		
18	Q	9	9	9	0	0
			Total	O		
18	R	3	3	3	0	0
			Total	O		
18	S	5	5	5	0	0
			Total	O		
18	T	5	5	5	0	0
			Total	O		
18	U	9	9	9	0	0
			Total	O		
18	V	11	11	11	0	0
			Total	O		
18	W	4	4	4	0	0
			Total	O		
18	X	8	8	8	0	0
			Total	O		
18	Y	10	10	10	0	0
			Total	O		
18	Z	7	7	7	0	0
			Total	O		
18	a	13	13	13	0	0
			Total	O		
18	b	9	9	9	0	0

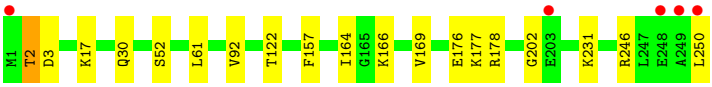
3 Residue-property plots (i)

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

• Molecule 1: Proteasome subunit alpha type-2

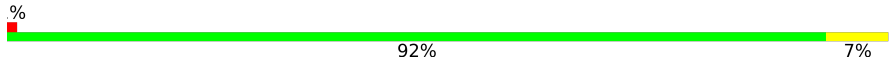
Chain A:





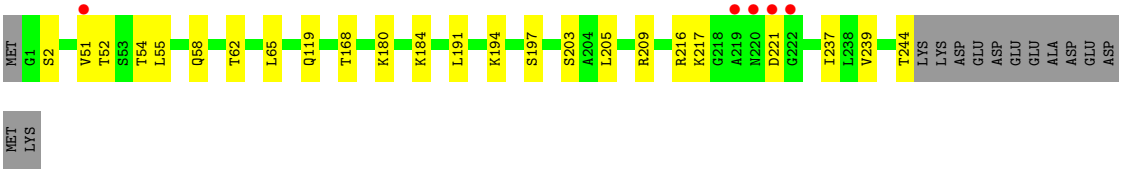
• Molecule 1: Proteasome subunit alpha type-2

Chain O:



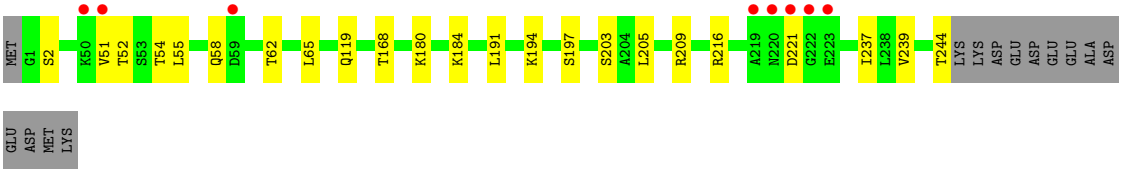
• Molecule 2: Proteasome subunit alpha type-3

Chain B:



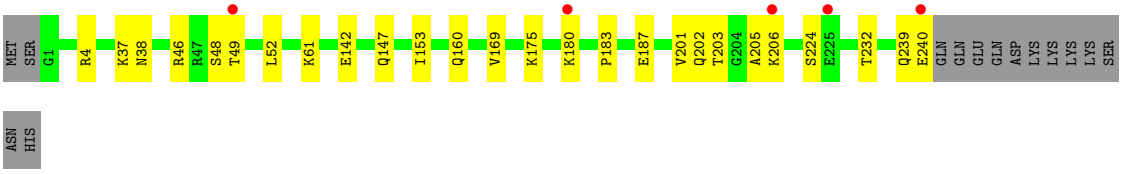
• Molecule 2: Proteasome subunit alpha type-3

Chain P:



• Molecule 3: Proteasome subunit alpha type-4

Chain C:

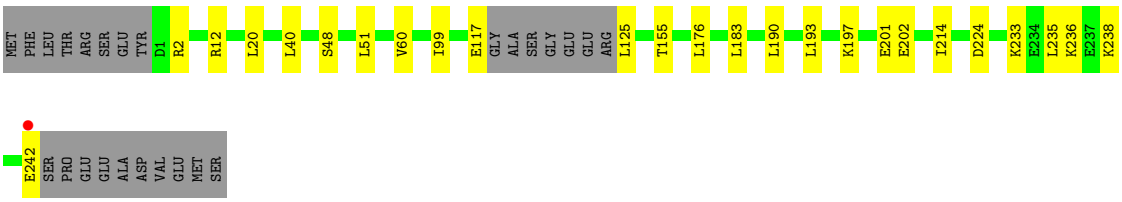


• Molecule 3: Proteasome subunit alpha type-4

Chain Q:

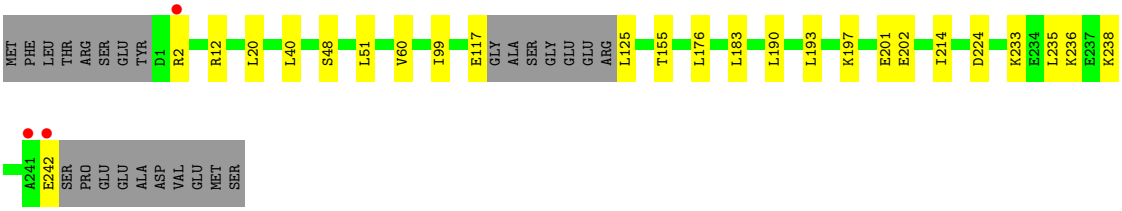
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



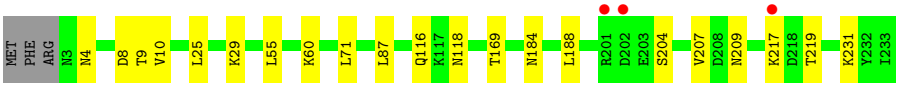
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



• Molecule 5: Proteasome subunit alpha type-6

Chain E:

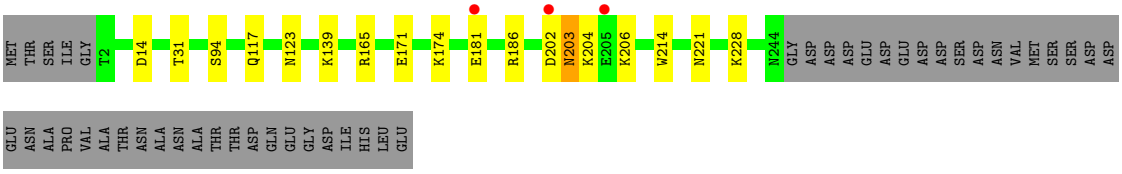


• Molecule 5: Proteasome subunit alpha type-6

Chain S:

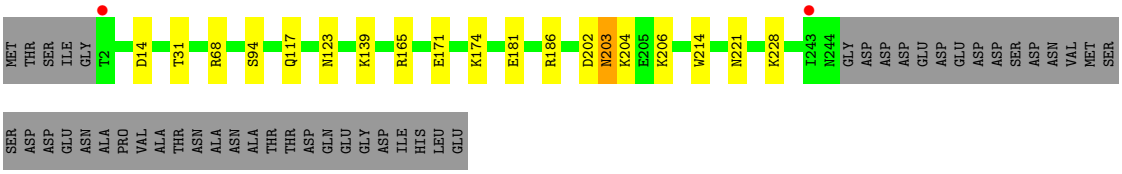
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



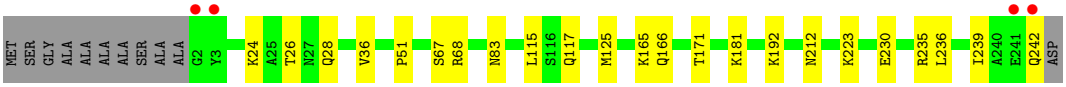
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



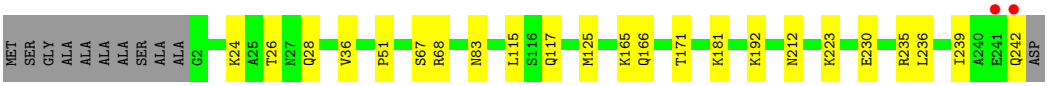
• Molecule 7: Proteasome subunit alpha type-1

Chain G:



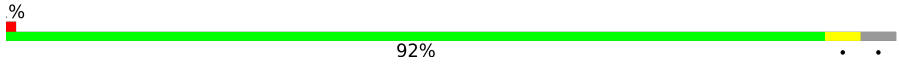
• Molecule 7: Proteasome subunit alpha type-1

Chain U:



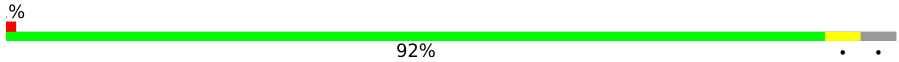
• Molecule 8: Proteasome subunit beta type-2

Chain H:



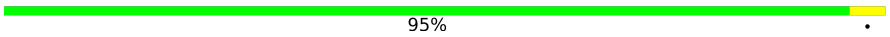
• Molecule 8: Proteasome subunit beta type-2

Chain V:



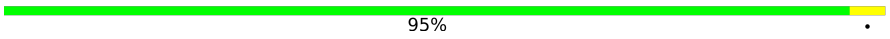
• Molecule 9: Proteasome subunit beta type-3

Chain I:



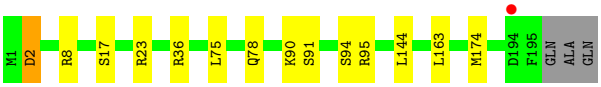
• Molecule 9: Proteasome subunit beta type-3

Chain W:



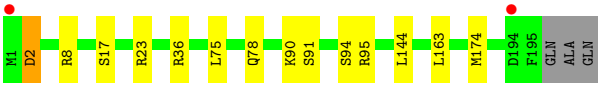
• Molecule 10: Proteasome subunit beta type-4

Chain J:



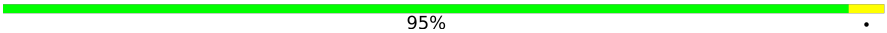
• Molecule 10: Proteasome subunit beta type-4

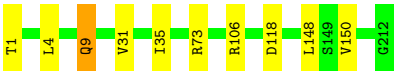
Chain X:



• Molecule 11: Proteasome subunit beta type-5

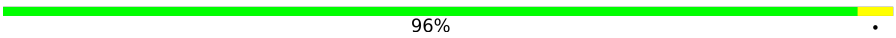
Chain K:

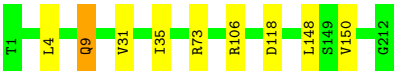




• Molecule 11: Proteasome subunit beta type-5

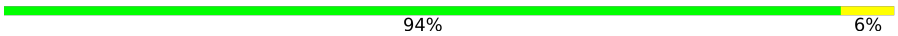
Chain Y:

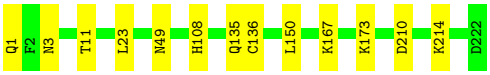




• Molecule 12: Proteasome subunit beta type-6

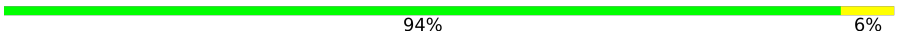
Chain L:

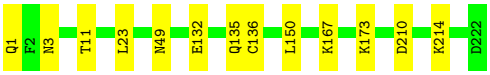




• Molecule 12: Proteasome subunit beta type-6

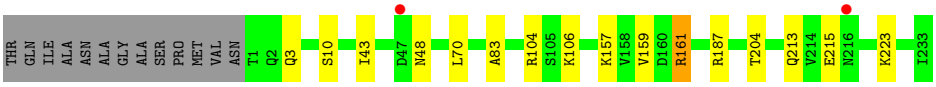
Chain Z:





• Molecule 13: Proteasome subunit beta type-7

Chain M:

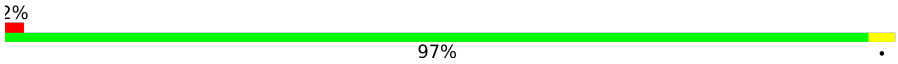


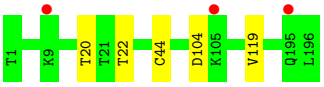
• Molecule 13: Proteasome subunit beta type-7

Chain a:

• Molecule 14: Proteasome subunit beta type-1

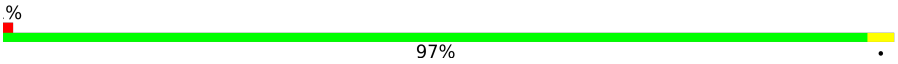
Chain N:

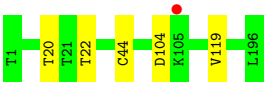




• Molecule 14: Proteasome subunit beta type-1

Chain b:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.04Å 300.38Å 146.52Å 90.00° 112.97° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.5 (15.00-2.90) 95.6 (15.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.184 , 0.209 0.185 , 0.207	Depositor DCC
R_{free} test set	11308 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	71.8	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 56.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	49622	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, MG, 39Q

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	0.29	0/1952	0.56	0/2642
1	O	0.29	0/1952	0.56	0/2642
2	B	0.30	0/1934	0.62	0/2618
2	P	0.30	0/1934	0.62	0/2618
3	C	0.30	0/1910	0.61	0/2586
3	Q	0.30	0/1910	0.61	0/2586
4	D	0.30	0/1837	0.59	0/2475
4	R	0.31	0/1837	0.59	0/2475
5	E	0.30	0/1800	0.58	0/2433
5	S	0.30	0/1800	0.58	0/2433
6	F	0.30	0/1932	0.57	0/2609
6	T	0.30	0/1932	0.57	0/2609
7	G	0.31	0/1945	0.58	0/2634
7	U	0.30	0/1945	0.58	0/2634
8	H	0.27	0/1715	0.55	0/2326
8	V	0.27	0/1714	0.55	0/2325
9	I	0.30	0/1611	0.57	0/2174
9	W	0.30	0/1611	0.57	0/2174
10	J	0.29	0/1589	0.57	0/2142
10	X	0.29	0/1589	0.57	0/2142
11	K	0.30	0/1681	0.58	0/2274
11	Y	0.31	0/1681	0.58	0/2274
12	L	0.30	0/1795	0.56	0/2420
12	Z	0.30	0/1795	0.56	0/2420
13	M	0.30	0/1855	0.60	1/2514 (0.0%)
13	a	0.30	0/1855	0.60	1/2514 (0.0%)
14	N	0.27	0/1541	0.54	0/2087
14	b	0.27	0/1541	0.54	0/2087
All	All	0.30	0/50193	0.58	2/67867 (0.0%)

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
6	F	0	1
6	T	0	1
11	K	0	1
12	L	0	1
12	Z	0	1
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	161	ARG	NE-CZ-NH1	5.21	122.91	120.30
13	M	161	ARG	NE-CZ-NH1	5.20	122.90	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	203	ASN	Peptide
11	K	1	THR	Peptide
12	L	135	GLN	Peptide
6	T	203	ASN	Peptide
12	Z	135	GLN	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	235 (95%)	9 (4%)	4 (2%)	9	32
1	O	248/250 (99%)	235 (95%)	9 (4%)	4 (2%)	9	32
2	B	242/258 (94%)	227 (94%)	11 (4%)	4 (2%)	9	31
2	P	242/258 (94%)	227 (94%)	12 (5%)	3 (1%)	13	40
3	C	238/254 (94%)	223 (94%)	8 (3%)	7 (3%)	4	18
3	Q	238/254 (94%)	223 (94%)	8 (3%)	7 (3%)	4	18
4	D	231/260 (89%)	223 (96%)	6 (3%)	2 (1%)	17	48
4	R	231/260 (89%)	223 (96%)	6 (3%)	2 (1%)	17	48
5	E	229/234 (98%)	214 (93%)	12 (5%)	3 (1%)	12	37
5	S	229/234 (98%)	213 (93%)	13 (6%)	3 (1%)	12	37
6	F	241/288 (84%)	231 (96%)	10 (4%)	0	100	100
6	T	241/288 (84%)	231 (96%)	10 (4%)	0	100	100
7	G	239/252 (95%)	228 (95%)	10 (4%)	1 (0%)	34	66
7	U	239/252 (95%)	228 (95%)	10 (4%)	1 (0%)	34	66
8	H	220/232 (95%)	211 (96%)	8 (4%)	1 (0%)	29	61
8	V	220/232 (95%)	211 (96%)	8 (4%)	1 (0%)	29	61
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	186 (96%)	6 (3%)	1 (0%)	29	61
10	X	193/198 (98%)	186 (96%)	6 (3%)	1 (0%)	29	61
11	K	210/212 (99%)	202 (96%)	6 (3%)	2 (1%)	15	45
11	Y	210/212 (99%)	201 (96%)	7 (3%)	2 (1%)	15	45
12	L	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
12	Z	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
13	M	231/246 (94%)	221 (96%)	9 (4%)	1 (0%)	34	66
13	a	231/246 (94%)	221 (96%)	8 (4%)	2 (1%)	17	48
14	N	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
14	b	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
All	All	6276/6614 (95%)	5982 (95%)	242 (4%)	52 (1%)	19	51

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	52	THR
3	C	202	GLN
3	C	206	LYS
5	E	231	LYS
1	O	2	THR
2	P	52	THR
3	Q	202	GLN
3	Q	206	LYS
5	S	231	LYS
1	A	3	ASP
1	A	166	LYS
2	B	51	VAL
3	C	201	VAL
3	C	205	ALA
4	D	2	ARG
5	E	217	LYS
8	H	9	ASN
10	J	2	ASP
1	O	3	ASP
1	O	166	LYS
2	P	51	VAL
3	Q	201	VAL
3	Q	205	ALA
4	R	2	ARG
5	S	217	LYS
8	V	9	ASN
10	X	2	ASP
5	E	209	ASN
7	G	51	PRO
5	S	209	ASN
7	U	51	PRO
3	C	183	PRO
3	Q	183	PRO
3	C	52	LEU
3	C	224	SER
4	D	201	GLU
13	M	83	ALA
3	Q	52	LEU
3	Q	224	SER
4	R	201	GLU
13	a	83	ALA
2	B	217	LYS

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Mol	Chain	Res	Type
2	B	221	ASP
11	K	9	GLN
2	P	221	ASP
11	Y	9	GLN
1	A	202	GLY
1	O	202	GLY
11	K	150	VAL
11	Y	150	VAL
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%)	193 (92%)	16 (8%)	13	35
1	O	209/209 (100%)	193 (92%)	16 (8%)	13	35
2	B	203/216 (94%)	183 (90%)	20 (10%)	8	24
2	P	203/216 (94%)	183 (90%)	20 (10%)	8	24
3	C	212/226 (94%)	193 (91%)	19 (9%)	9	29
3	Q	212/226 (94%)	193 (91%)	19 (9%)	9	29
4	D	194/215 (90%)	171 (88%)	23 (12%)	5	15
4	R	194/215 (90%)	171 (88%)	23 (12%)	5	15
5	E	190/193 (98%)	172 (90%)	18 (10%)	8	26
5	S	190/193 (98%)	172 (90%)	18 (10%)	8	26
6	F	201/239 (84%)	183 (91%)	18 (9%)	9	29
6	T	201/239 (84%)	182 (90%)	19 (10%)	8	26
7	G	206/210 (98%)	184 (89%)	22 (11%)	6	20
7	U	206/210 (98%)	184 (89%)	22 (11%)	6	20
8	H	181/190 (95%)	173 (96%)	8 (4%)	28	61
8	V	181/190 (95%)	173 (96%)	8 (4%)	28	61
9	I	172/173 (99%)	163 (95%)	9 (5%)	23	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	172/173 (99%)	163 (95%)	9 (5%)	23	55
10	J	173/175 (99%)	159 (92%)	14 (8%)	11	33
10	X	173/175 (99%)	159 (92%)	14 (8%)	11	33
11	K	169/169 (100%)	161 (95%)	8 (5%)	26	59
11	Y	169/169 (100%)	161 (95%)	8 (5%)	26	59
12	L	185/185 (100%)	173 (94%)	12 (6%)	17	45
12	Z	185/185 (100%)	173 (94%)	12 (6%)	17	45
13	M	199/208 (96%)	184 (92%)	15 (8%)	13	37
13	a	199/208 (96%)	184 (92%)	15 (8%)	13	37
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	74
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	74
All	All	5312/5540 (96%)	4897 (92%)	415 (8%)	12	34

All (415) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	17	LYS
1	A	30	GLN
1	A	52	SER
1	A	61	LEU
1	A	92	VAL
1	A	122	THR
1	A	157	PHE
1	A	164	ILE
1	A	169	VAL
1	A	176	GLU
1	A	177	LYS
1	A	178	ARG
1	A	231	LYS
1	A	246	ARG
1	A	250	LEU
2	B	2	SER
2	B	54	THR
2	B	55	LEU
2	B	58	GLN
2	B	62	THR
2	B	65	LEU

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Mol	Chain	Res	Type
2	B	119	GLN
2	B	168	THR
2	B	180	LYS
2	B	184	LYS
2	B	191	LEU
2	B	194	LYS
2	B	197	SER
2	B	203	SER
2	B	205	LEU
2	B	209	ARG
2	B	216	ARG
2	B	237	ILE
2	B	239	VAL
2	B	244	THR
3	C	4	ARG
3	C	37	LYS
3	C	38	ASN
3	C	46	ARG
3	C	48	SER
3	C	49	THR
3	C	61	LYS
3	C	142	GLU
3	C	147	GLN
3	C	153	ILE
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	187	GLU
3	C	203	THR
3	C	232	THR
3	C	239	GLN
3	C	240	GLU
4	D	12	ARG
4	D	20	LEU
4	D	40	LEU
4	D	48	SER
4	D	51	LEU
4	D	60	VAL
4	D	99	ILE
4	D	117	GLU
4	D	125	LEU

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Mol	Chain	Res	Type
4	D	155	THR
4	D	176	LEU
4	D	183	LEU
4	D	190	LEU
4	D	193	LEU
4	D	197	LYS
4	D	202	GLU
4	D	214	ILE
4	D	224	ASP
4	D	233	LYS
4	D	235	LEU
4	D	236	LYS
4	D	238	LYS
4	D	242	GLU
5	E	4	ASN
5	E	8	ASP
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	55	LEU
5	E	60	LYS
5	E	71	LEU
5	E	87	LEU
5	E	116	GLN
5	E	118	ASN
5	E	169	THR
5	E	184	ASN
5	E	188	LEU
5	E	204	SER
5	E	207	VAL
5	E	219	THR
6	F	14	ASP
6	F	31	THR
6	F	94	SER
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	165	ARG
6	F	171	GLU
6	F	174	LYS
6	F	181	GLU

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Mol	Chain	Res	Type
6	F	186	ARG
6	F	202	ASP
6	F	203	ASN
6	F	204	LYS
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
6	F	228	LYS
7	G	24	LYS
7	G	26	THR
7	G	28	GLN
7	G	36	VAL
7	G	67	SER
7	G	68	ARG
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	125	MET
7	G	165	LYS
7	G	166	GLN
7	G	171	THR
7	G	181	LYS
7	G	192	LYS
7	G	212	ASN
7	G	223	LYS
7	G	230	GLU
7	G	235	ARG
7	G	236	LEU
7	G	239	ILE
7	G	242	GLN
8	H	30	ASN
8	H	34	LEU
8	H	56	THR
8	H	68	LEU
8	H	153	LYS
8	H	156	SER
8	H	191	LEU
8	H	198	GLU
9	I	31	GLN
9	I	37	ASN
9	I	114	LYS
9	I	126	ILE

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Mol	Chain	Res	Type
9	I	133	LYS
9	I	151	SER
9	I	171	LEU
9	I	182	TRP
9	I	192	ASP
10	J	2	ASP
10	J	8	ARG
10	J	17	SER
10	J	23	ARG
10	J	36	ARG
10	J	75	LEU
10	J	78	GLN
10	J	90	LYS
10	J	91	SER
10	J	94	SER
10	J	95	ARG
10	J	144	LEU
10	J	163	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	31	VAL
11	K	35	ILE
11	K	73	ARG
11	K	106	ARG
11	K	118	ASP
11	K	148	LEU
12	L	1	GLN
12	L	3	ASN
12	L	11	THR
12	L	23	LEU
12	L	49	ASN
12	L	108	HIS
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
12	L	173	LYS
12	L	210	ASP
12	L	214	LYS
13	M	3	GLN
13	M	10	SER
13	M	43	ILE

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Mol	Chain	Res	Type
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	106	LYS
13	M	157	LYS
13	M	159	VAL
13	M	161	ARG
13	M	187	ARG
13	M	204	THR
13	M	213	GLN
13	M	215	GLU
13	M	223	LYS
14	N	20	THR
14	N	22	THR
14	N	44	CYS
14	N	104	ASP
14	N	119	VAL
1	O	2	THR
1	O	17	LYS
1	O	30	GLN
1	O	52	SER
1	O	61	LEU
1	O	92	VAL
1	O	122	THR
1	O	157	PHE
1	O	164	ILE
1	O	169	VAL
1	O	176	GLU
1	O	177	LYS
1	O	178	ARG
1	O	231	LYS
1	O	246	ARG
1	O	250	LEU
2	P	2	SER
2	P	54	THR
2	P	55	LEU
2	P	58	GLN
2	P	62	THR
2	P	65	LEU
2	P	119	GLN
2	P	168	THR
2	P	180	LYS

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Mol	Chain	Res	Type
2	P	184	LYS
2	P	191	LEU
2	P	194	LYS
2	P	197	SER
2	P	203	SER
2	P	205	LEU
2	P	209	ARG
2	P	216	ARG
2	P	237	ILE
2	P	239	VAL
2	P	244	THR
3	Q	4	ARG
3	Q	37	LYS
3	Q	38	ASN
3	Q	46	ARG
3	Q	48	SER
3	Q	49	THR
3	Q	61	LYS
3	Q	142	GLU
3	Q	147	GLN
3	Q	153	ILE
3	Q	160	GLN
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	187	GLU
3	Q	203	THR
3	Q	232	THR
3	Q	239	GLN
3	Q	240	GLU
4	R	12	ARG
4	R	20	LEU
4	R	40	LEU
4	R	48	SER
4	R	51	LEU
4	R	60	VAL
4	R	99	ILE
4	R	117	GLU
4	R	125	LEU
4	R	155	THR
4	R	176	LEU
4	R	183	LEU

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Mol	Chain	Res	Type
4	R	190	LEU
4	R	193	LEU
4	R	197	LYS
4	R	202	GLU
4	R	214	ILE
4	R	224	ASP
4	R	233	LYS
4	R	235	LEU
4	R	236	LYS
4	R	238	LYS
4	R	242	GLU
5	S	4	ASN
5	S	8	ASP
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	55	LEU
5	S	60	LYS
5	S	71	LEU
5	S	87	LEU
5	S	116	GLN
5	S	118	ASN
5	S	169	THR
5	S	184	ASN
5	S	188	LEU
5	S	204	SER
5	S	207	VAL
5	S	219	THR
6	T	14	ASP
6	T	31	THR
6	T	68	ARG
6	T	94	SER
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	165	ARG
6	T	171	GLU
6	T	174	LYS
6	T	181	GLU
6	T	186	ARG
6	T	202	ASP

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Mol	Chain	Res	Type
6	T	203	ASN
6	T	204	LYS
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
6	T	228	LYS
7	U	24	LYS
7	U	26	THR
7	U	28	GLN
7	U	36	VAL
7	U	67	SER
7	U	68	ARG
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	125	MET
7	U	165	LYS
7	U	166	GLN
7	U	171	THR
7	U	181	LYS
7	U	192	LYS
7	U	212	ASN
7	U	223	LYS
7	U	230	GLU
7	U	235	ARG
7	U	236	LEU
7	U	239	ILE
7	U	242	GLN
8	V	30	ASN
8	V	34	LEU
8	V	56	THR
8	V	68	LEU
8	V	153	LYS
8	V	156	SER
8	V	191	LEU
8	V	198	GLU
9	W	31	GLN
9	W	37	ASN
9	W	114	LYS
9	W	126	ILE
9	W	133	LYS
9	W	151	SER

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Mol	Chain	Res	Type
9	W	171	LEU
9	W	182	TRP
9	W	192	ASP
10	X	2	ASP
10	X	8	ARG
10	X	17	SER
10	X	23	ARG
10	X	36	ARG
10	X	75	LEU
10	X	78	GLN
10	X	90	LYS
10	X	91	SER
10	X	94	SER
10	X	95	ARG
10	X	144	LEU
10	X	163	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	31	VAL
11	Y	35	ILE
11	Y	73	ARG
11	Y	106	ARG
11	Y	118	ASP
11	Y	148	LEU
12	Z	1	GLN
12	Z	3	ASN
12	Z	11	THR
12	Z	23	LEU
12	Z	49	ASN
12	Z	132	GLU
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
12	Z	173	LYS
12	Z	210	ASP
12	Z	214	LYS
13	a	3	GLN
13	a	10	SER
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU

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Mol	Chain	Res	Type
13	a	104	ARG
13	a	106	LYS
13	a	157	LYS
13	a	159	VAL
13	a	161	ARG
13	a	187	ARG
13	a	204	THR
13	a	213	GLN
13	a	215	GLU
13	a	223	LYS
14	b	20	THR
14	b	22	THR
14	b	44	CYS
14	b	104	ASP
14	b	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (150) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	102	ASN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	233	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	139	HIS
4	D	146	GLN
4	D	225	ASN
5	E	30	GLN
5	E	59	GLN
5	E	68	HIS

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Mol	Chain	Res	Type
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	147	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	167	GLN
7	G	175	ASN
7	G	184	HIS
7	G	186	ASN
8	H	30	ASN
8	H	66	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
9	I	63	ASN
10	J	55	GLN
10	J	78	GLN
10	J	86	GLN
10	J	118	GLN
10	J	191	GLN
11	K	66	HIS
11	K	85	ASN
11	K	176	ASN
12	L	1	GLN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN

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Mol	Chain	Res	Type
12	L	80	ASN
12	L	195	HIS
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	69	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	233	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	139	HIS
4	R	146	GLN
4	R	225	ASN
5	S	30	GLN
5	S	59	GLN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	147	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN

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Mol	Chain	Res	Type
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
7	U	175	ASN
7	U	184	HIS
7	U	186	ASN
8	V	30	ASN
8	V	66	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	37	ASN
9	W	63	ASN
10	X	55	GLN
10	X	78	GLN
10	X	86	GLN
10	X	118	GLN
10	X	191	GLN
11	Y	66	HIS
11	Y	85	ASN
11	Y	176	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	108	HIS
12	Z	195	HIS
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	69	GLN

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Mol	Chain	Res	Type
14	b	161	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	MES	K	302	-	12,12,12	2.27	1 (8%)	14,16,16	1.21	2 (14%)
16	MES	Y	302	-	12,12,12	2.24	1 (8%)	14,16,16	1.23	1 (7%)
17	39Q	Y	303	-	43,44,44	1.76	3 (6%)	51,58,58	1.80	6 (11%)
17	39Q	K	303	-	43,44,44	1.92	3 (6%)	51,58,58	1.55	9 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	MES	K	302	-	-	0/6/14/14	0/1/1/1
16	MES	Y	302	-	-	0/6/14/14	0/1/1/1
17	39Q	Y	303	-	-	11/44/52/52	0/3/3/3
17	39Q	K	303	-	-	9/44/52/52	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	303	39Q	O32-C31	9.04	1.36	1.21
17	Y	303	39Q	O32-C31	7.71	1.34	1.21
16	K	302	MES	C8-S	-7.61	1.66	1.77
16	Y	302	MES	C8-S	-7.46	1.66	1.77
17	K	303	39Q	C17-C18	-5.54	1.38	1.51
17	Y	303	39Q	C30-C41	-5.50	1.38	1.51
17	Y	303	39Q	C17-C18	-5.42	1.38	1.51
17	K	303	39Q	C30-C41	-4.99	1.39	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Y	303	39Q	O32-C31-C37	-7.90	106.60	121.26
17	K	303	39Q	O32-C31-C37	-6.08	109.99	121.26
17	Y	303	39Q	C13-C11-N1	-4.15	101.33	111.60
17	Y	303	39Q	C11-N1-C2	3.78	127.01	121.34
17	K	303	39Q	C4-N5-C6	-3.73	105.31	111.09
17	Y	303	39Q	C30-C29-N28	-3.72	102.96	110.79
17	Y	303	39Q	C6-N5-C10	3.67	117.09	108.83
17	K	303	39Q	C12-C11-N1	-2.98	104.78	110.38
16	Y	302	MES	O3S-S-C8	2.97	110.58	105.77
17	K	303	39Q	C6-N5-C10	2.85	115.24	108.83
17	Y	303	39Q	O8-C7-C6	-2.70	105.85	111.80
16	K	302	MES	O2S-S-C8	2.67	110.13	106.92
17	K	303	39Q	O8-C9-C10	-2.65	105.96	111.80
17	K	303	39Q	C13-C11-N1	-2.53	105.33	111.60
17	K	303	39Q	O8-C7-C6	-2.50	106.28	111.80
17	K	303	39Q	C30-C29-N28	-2.37	105.80	110.79
17	K	303	39Q	C17-C16-N15	-2.27	106.00	110.79
16	K	302	MES	O3S-S-C8	2.12	109.19	105.77

There are no chirality outliers.

All (20) torsion outliers are listed below:

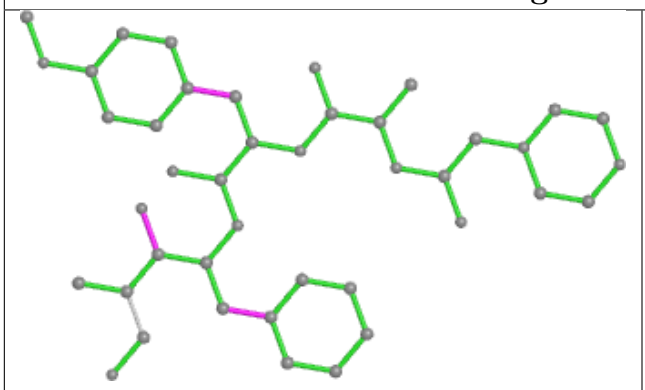
Mol	Chain	Res	Type	Atoms
17	K	303	39Q	O32-C31-C37-C38
17	Y	303	39Q	O32-C31-C37-C38
17	K	303	39Q	C20-C21-O22-C23
17	K	303	39Q	C24-C21-O22-C23
17	K	303	39Q	C29-C30-C41-C42
17	K	303	39Q	C29-C30-C41-C46
17	Y	303	39Q	C29-C30-C41-C42
17	Y	303	39Q	C29-C30-C41-C46
17	Y	303	39Q	C31-C37-C39-O40
17	Y	303	39Q	N15-C16-C26-O27
17	Y	303	39Q	N15-C16-C26-N28
17	Y	303	39Q	C38-C37-C39-O40
17	Y	303	39Q	N28-C29-C30-C41
17	K	303	39Q	N15-C16-C26-O27
17	K	303	39Q	N15-C16-C26-N28
17	Y	303	39Q	C17-C16-C26-O27
17	Y	303	39Q	N1-C11-C13-N15
17	K	303	39Q	C30-C29-C31-O32
17	K	303	39Q	N28-C29-C31-C37
17	Y	303	39Q	N28-C29-C31-C37

There are no ring outliers.

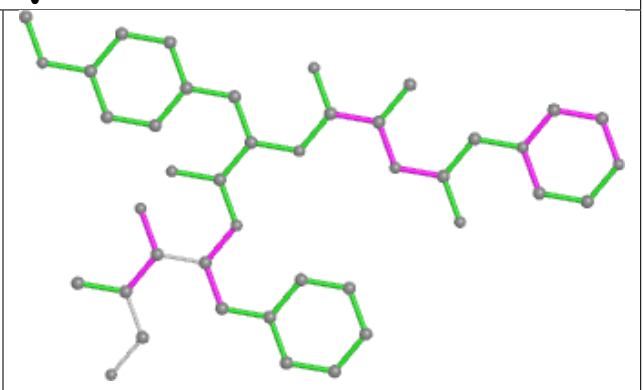
No monomer is involved in short contacts.

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.

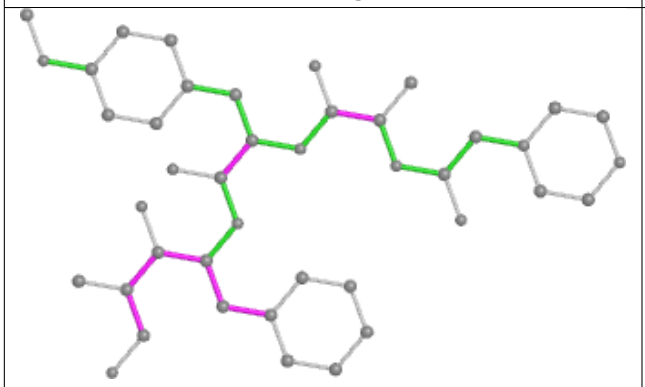
Ligand 39Q Y 303



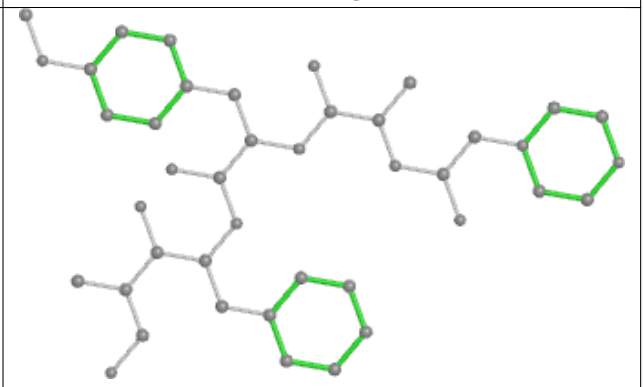
Bond lengths



Bond angles

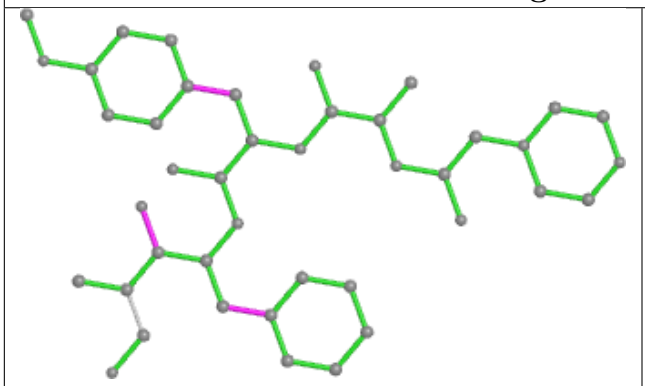


Torsions

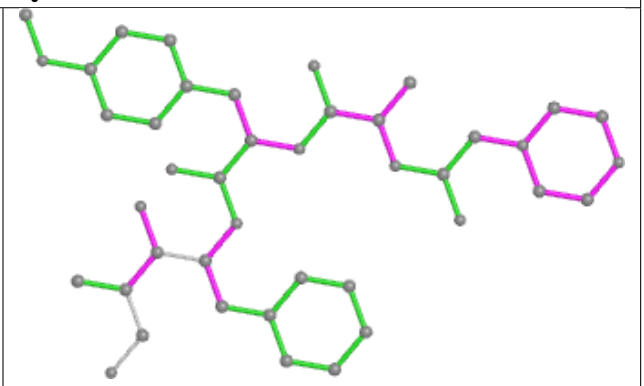


Rings

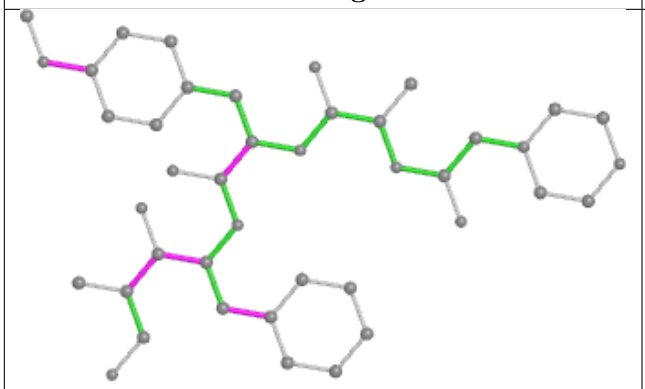
Ligand 39Q K 303



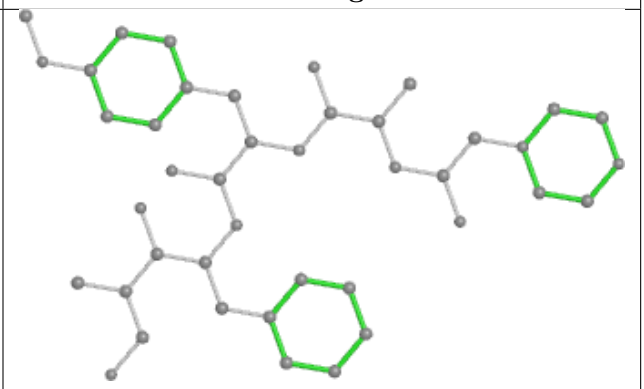
Bond lengths



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.57	5 (2%)	65	63	47, 67, 100, 134	0
1	O	250/250 (100%)	-0.53	2 (0%)	86	86	48, 72, 114, 143	0
2	B	244/258 (94%)	-0.46	5 (2%)	65	63	49, 73, 114, 161	0
2	P	244/258 (94%)	-0.43	8 (3%)	46	41	54, 75, 123, 162	0
3	C	240/254 (94%)	-0.36	5 (2%)	63	61	49, 77, 127, 148	0
3	Q	240/254 (94%)	-0.26	9 (3%)	40	36	54, 82, 142, 156	0
4	D	235/260 (90%)	-0.49	1 (0%)	92	93	54, 80, 110, 149	0
4	R	235/260 (90%)	-0.47	3 (1%)	77	77	55, 78, 109, 145	0
5	E	231/234 (98%)	-0.42	3 (1%)	77	77	53, 84, 112, 149	0
5	S	231/234 (98%)	-0.38	3 (1%)	77	77	51, 83, 119, 150	0
6	F	243/288 (84%)	-0.48	3 (1%)	79	79	52, 74, 115, 153	0
6	T	243/288 (84%)	-0.51	2 (0%)	86	86	51, 74, 117, 136	0
7	G	241/252 (95%)	-0.59	4 (1%)	70	69	43, 68, 105, 139	0
7	U	241/252 (95%)	-0.57	2 (0%)	86	86	47, 68, 98, 124	0
8	H	222/232 (95%)	-0.53	2 (0%)	84	84	46, 66, 90, 135	0
8	V	222/232 (95%)	-0.54	2 (0%)	84	84	51, 70, 95, 139	0
9	I	204/205 (99%)	-0.77	0	100	100	47, 62, 88, 117	0
9	W	204/205 (99%)	-0.71	1 (0%)	91	91	46, 66, 89, 127	0
10	J	195/198 (98%)	-0.67	1 (0%)	91	91	46, 64, 93, 144	0
10	X	195/198 (98%)	-0.57	2 (1%)	82	82	45, 67, 93, 156	0
11	K	212/212 (100%)	-0.68	0	100	100	47, 67, 90, 116	0
11	Y	212/212 (100%)	-0.69	0	100	100	43, 65, 88, 116	0
12	L	222/222 (100%)	-0.64	0	100	100	48, 69, 96, 114	0
12	Z	222/222 (100%)	-0.65	0	100	100	44, 66, 89, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.62	2 (0%)	84	84	45, 66, 91, 119	0
13	a	233/246 (94%)	-0.64	2 (0%)	84	84	47, 65, 93, 109	0
14	N	196/196 (100%)	-0.66	3 (1%)	73	73	47, 64, 91, 110	0
14	b	196/196 (100%)	-0.68	1 (0%)	91	91	47, 63, 88, 118	0
All	All	6336/6614 (95%)	-0.55	71 (1%)	80	80	43, 70, 109, 162	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	222	ASP	5.4
3	Q	49	THR	5.1
2	B	220	ASN	5.0
1	A	1	MET	4.5
10	X	194	ASP	4.3
5	S	202	ASP	4.3
2	P	219	ALA	4.3
2	B	221	ASP	4.2
2	B	219	ALA	4.1
2	P	220	ASN	4.0
3	C	206	LYS	4.0
8	H	222	ASP	3.9
2	P	222	GLY	3.8
3	Q	50	LEU	3.8
3	C	49	THR	3.6
2	B	222	GLY	3.5
1	O	1	MET	3.5
3	Q	238	LYS	3.4
6	F	181	GLU	3.4
8	V	221	CYS	3.4
4	D	242	GLU	3.2
3	Q	206	LYS	3.2
3	C	240	GLU	3.1
2	P	59	ASP	3.1
3	Q	236	GLN	3.0
2	B	51	VAL	3.0
4	R	241	ALA	2.9
3	Q	240	GLU	2.9
7	G	2	GLY	2.9
2	P	221	ASP	2.9
1	A	249	ALA	2.9
3	Q	239	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
2	P	50	LYS	2.8
3	Q	48	SER	2.7
9	W	1	SER	2.6
3	Q	203	THR	2.6
8	H	22	GLN	2.6
5	E	202	ASP	2.6
1	O	249	ALA	2.6
7	G	241	GLU	2.6
3	C	225	GLU	2.5
6	F	202	ASP	2.4
7	G	3	TYR	2.4
7	U	241	GLU	2.4
14	b	105	LYS	2.3
6	F	205	GLU	2.3
4	R	2	ARG	2.3
14	N	195	GLN	2.3
2	P	223	GLU	2.3
5	S	52	ALA	2.3
5	E	201	ARG	2.3
10	X	1	MET	2.2
10	J	194	ASP	2.2
7	U	242	GLN	2.2
13	M	47	ASP	2.2
2	P	51	VAL	2.2
1	A	250	LEU	2.1
14	N	105	LYS	2.1
4	R	242	GLU	2.1
6	T	2	THR	2.1
1	A	248	GLU	2.1
14	N	9	LYS	2.1
6	T	243	ILE	2.1
13	a	233	ILE	2.1
1	A	203	GLU	2.1
13	a	1	THR	2.1
5	S	173	ARG	2.1
13	M	216	ASN	2.0
7	G	242	GLN	2.0
3	C	180	LYS	2.0
5	E	217	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

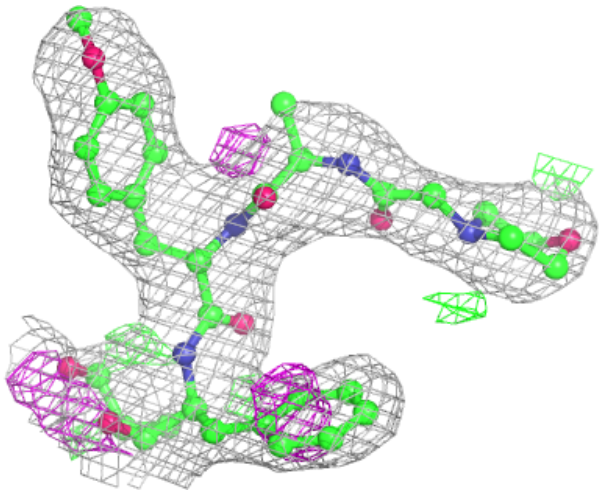
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

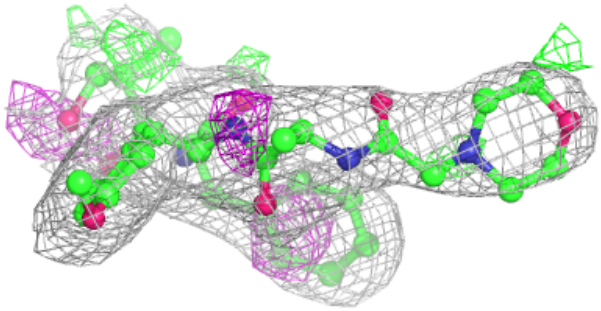
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	N	202	1/1	0.64	0.25	78,78,78,78	0
15	MG	N	201	1/1	0.88	0.17	68,68,68,68	0
17	39Q	K	303	42/42	0.91	0.20	36,65,95,101	0
17	39Q	Y	303	42/42	0.92	0.18	47,63,90,97	0
15	MG	Z	301	1/1	0.96	0.26	69,69,69,69	0
16	MES	K	302	12/12	0.97	0.17	69,75,87,93	0
16	MES	Y	302	12/12	0.97	0.21	64,76,80,80	0
15	MG	K	301	1/1	0.97	0.10	78,78,78,78	0
15	MG	G	301	1/1	0.97	0.04	63,63,63,63	0
15	MG	Y	301	1/1	0.98	0.06	57,57,57,57	0
15	MG	V	301	1/1	0.98	0.19	68,68,68,68	0
15	MG	I	301	1/1	0.99	0.14	51,51,51,51	0

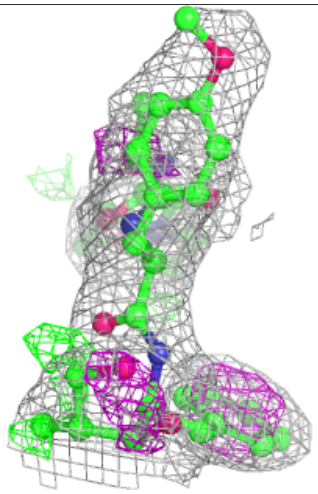
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 39Q K 303:

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

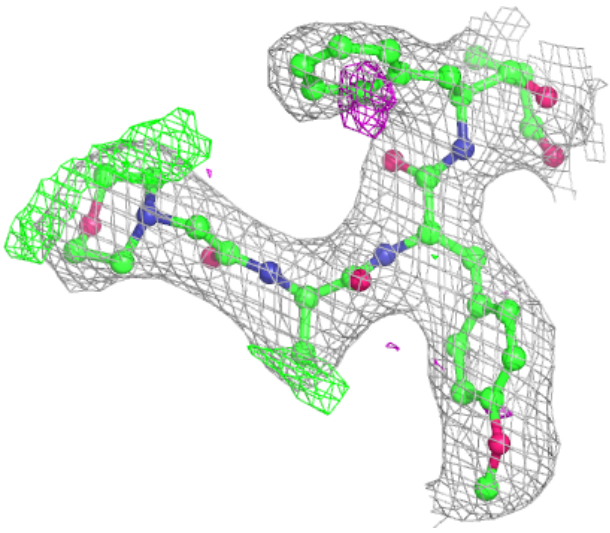


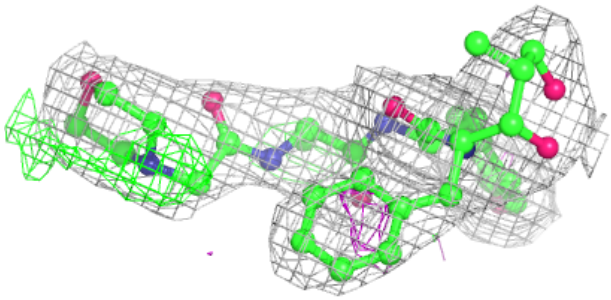


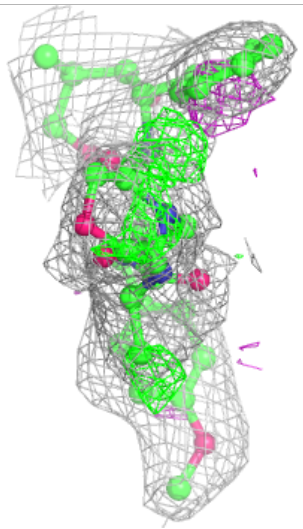


Electron density around 39Q Y 303:

$2mF_o$-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.