Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 08:19 AM EDT

PDB ID	:	4QWK
Title	:	yCP beta5-A49T-A50V-double mutant in complex with carfilzomib
Authors	:	Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on	:	2014-07-16
Resolution	:	2.80 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:

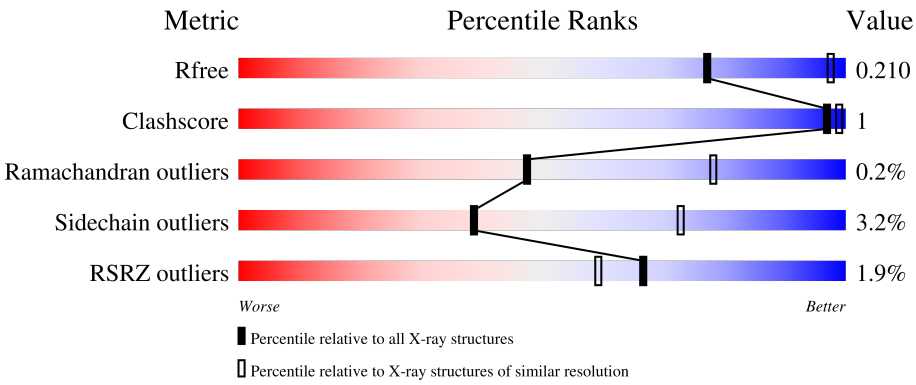
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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%, 98%, •
1	O	250	2%, 98%, •
2	B	258	5%, 90%, 5%, 5%
2	P	258	4%, 90%, • • 5%
3	C	254	5%, 89%, • • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	6% 89% 6%
4	D	260	.% 87% 10%
4	R	260	2% 87% 10%
5	E	234	.% 92% 6%
5	S	234	2% 92% 6%
6	F	288	2% 81% 16%
6	T	288	2% 81% 16%
7	G	252	2% 90% 5%
7	U	252	.% 91% 5%
8	H	232	.% 93%
8	V	232	.% 93%
9	I	205	.% 95%
9	W	205	.% 95% 5%
10	J	198	.% 92% 5%
10	X	198	2% 93%
11	K	212	93% 7%
11	Y	212	.% 92% 8%
12	L	222	96%
12	Z	222	95%
13	M	246	.% 89% 5% 7%
13	a	246	.% 91% 7%
14	N	196	97%
14	b	196	.% 98%

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 49853 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	212	1648	1048	280	313	7	0	0	0
			Total	C	N	O	S			
11	Y	212	1648	1048	280	313	7	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	49	THR	ALA	engineered mutation	UNP P30656
K	50	VAL	ALA	engineered mutation	UNP P30656
Y	49	THR	ALA	engineered mutation	UNP P30656
Y	50	VAL	ALA	engineered mutation	UNP P30656

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	230	1797	1137	307	346	7	0	0	0
			Total	C	N	O	S			
13	a	230	1797	1137	307	346	7	0	0	0

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

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

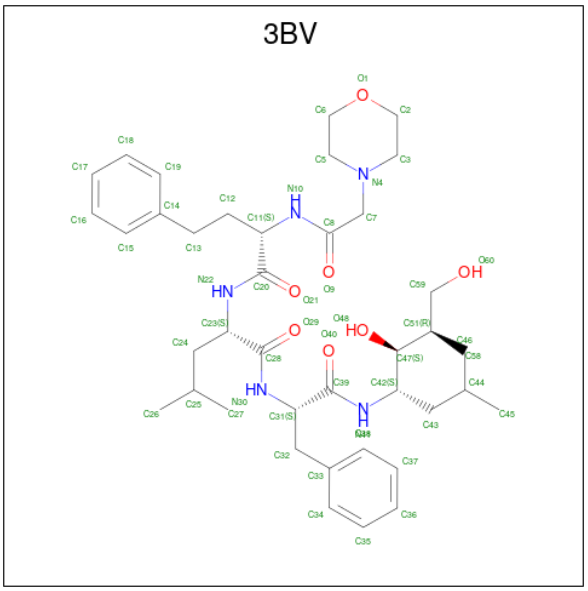
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	I	1	Total Mg 1 1	0	0
15	K	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

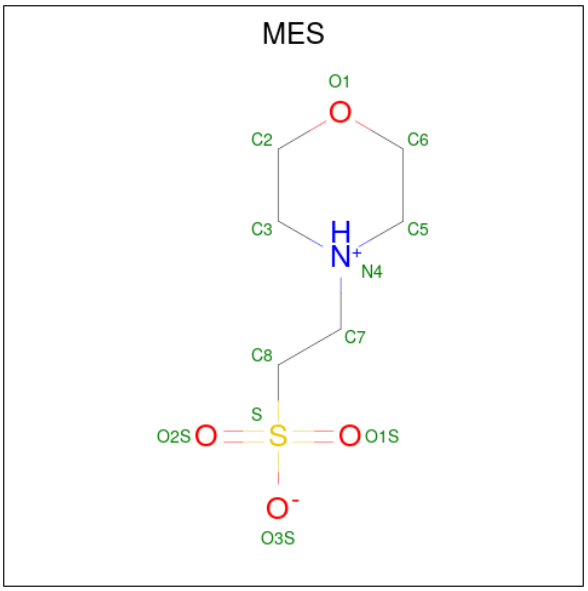
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	N	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0
16	b	1	Total Cl 1 1	0	0

- Molecule 17 is N-{(2S)-2-[(morpholin-4-ylacetyl)amino]-4-phenylbutanoyl}-L-leucyl-N-[(2R,3S,4S)-1,3-dihydroxy-2,6-dimethylheptan-4-yl]-L-phenylalaninamide (three-letter code: 3BV) (formula: $C_{40}H_{61}N_5O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
17	H	1	52	40	5	7	0	0
			Total	C	N	O		
17	K	1	52	40	5	7	0	0
			Total	C	N	O		
17	N	1	52	40	5	7	0	0
			Total	C	N	O		
17	V	1	52	40	5	7	0	0
			Total	C	N	O		
17	Y	1	52	40	5	7	0	0
			Total	C	N	O		
17	b	1	52	40	5	7	0	0

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



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
19	A	5	5	5	0	0
			Total	O		
19	B	14	14	14	0	0
			Total	O		
19	C	7	7	7	0	0
			Total	O		
19	D	6	6	6	0	0
			Total	O		
19	E	2	2	2	0	0
			Total	O		
19	F	11	11	11	0	0
			Total	O		
19	G	10	10	10	0	0
			Total	O		
19	H	11	11	11	0	0
			Total	O		
19	I	8	8	8	0	0
			Total	O		
19	J	13	13	13	0	0

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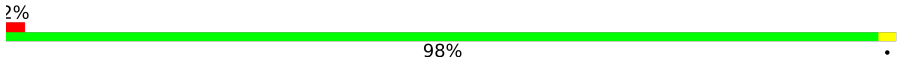
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
19	K	16	16	16	0	0
			Total	O		
19	L	15	15	15	0	0
			Total	O		
19	M	14	14	14	0	0
			Total	O		
19	N	5	5	5	0	0
			Total	O		
19	O	4	4	4	0	0
			Total	O		
19	P	6	6	6	0	0
			Total	O		
19	Q	3	3	3	0	0
			Total	O		
19	R	6	6	6	0	0
			Total	O		
19	S	3	3	3	0	0
			Total	O		
19	T	9	9	9	0	0
			Total	O		
19	U	13	13	13	0	0
			Total	O		
19	V	7	7	7	0	0
			Total	O		
19	W	2	2	2	0	0
			Total	O		
19	X	19	19	19	0	0
			Total	O		
19	Y	12	12	12	0	0
			Total	O		
19	Z	14	14	14	0	0
			Total	O		
19	a	13	13	13	0	0
			Total	O		
19	b	8	8	8	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.

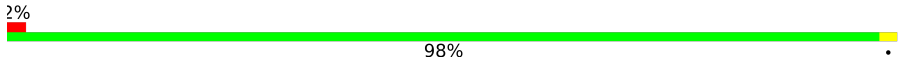
• Molecule 1: Proteasome subunit alpha type-2

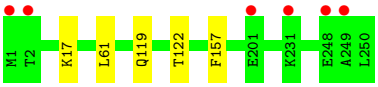
Chain A:



• Molecule 1: Proteasome subunit alpha type-2

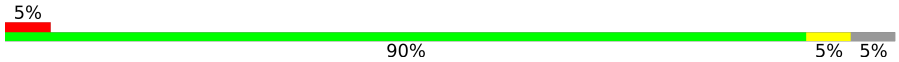
Chain O:

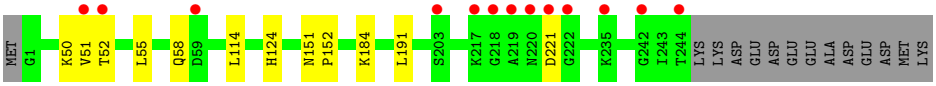




• Molecule 2: Proteasome subunit alpha type-3

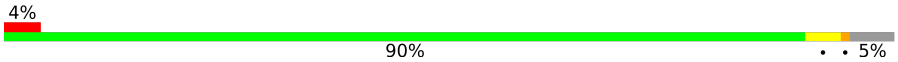
Chain B:





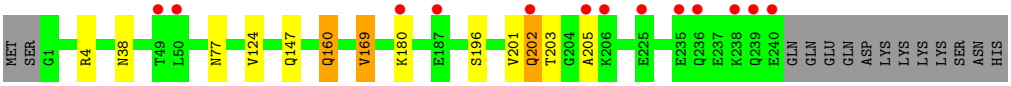
• Molecule 2: Proteasome subunit alpha type-3

Chain P:



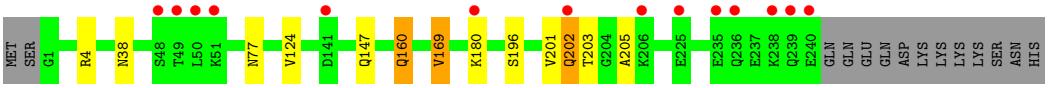
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



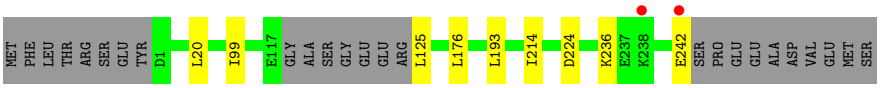
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



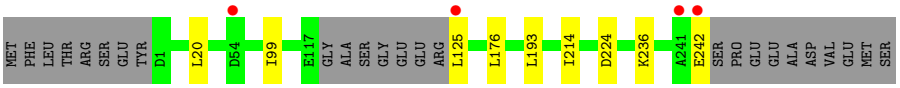
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



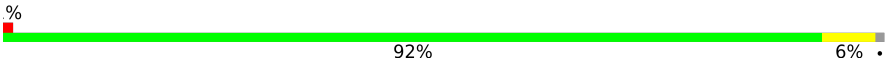
• Molecule 4: Proteasome subunit alpha type-5

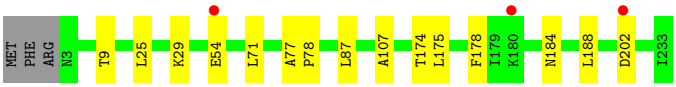
Chain R:



• Molecule 5: Proteasome subunit alpha type-6

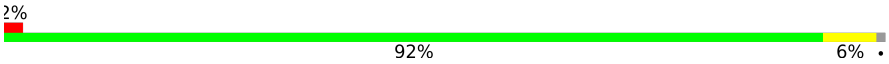
Chain E:

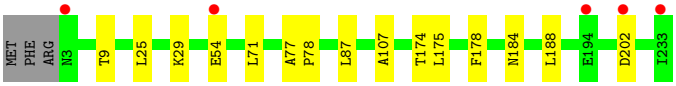




• Molecule 5: Proteasome subunit alpha type-6

Chain S:



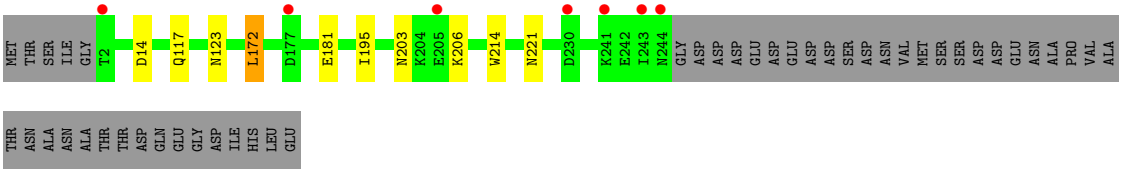


• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:

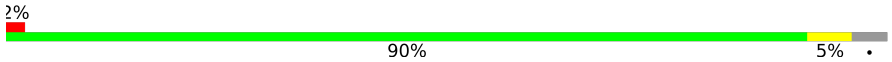
• Molecule 6: Probable proteasome subunit alpha type-7

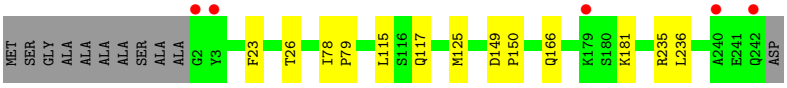
Chain T:



• Molecule 7: Proteasome subunit alpha type-1

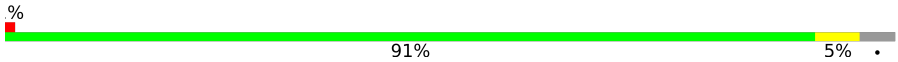
Chain G:

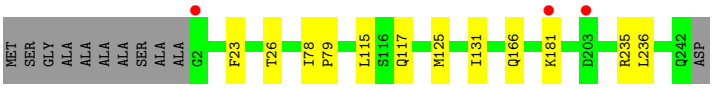




• Molecule 7: Proteasome subunit alpha type-1

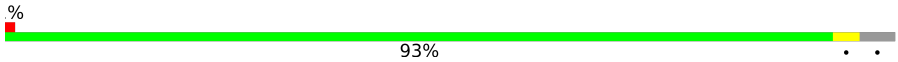
Chain U:

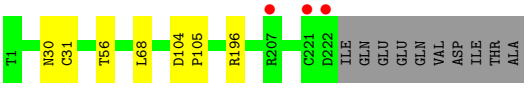




• Molecule 8: Proteasome subunit beta type-2

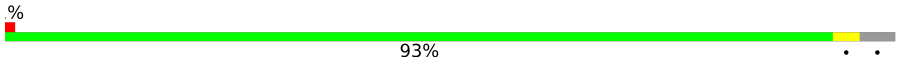
Chain H:

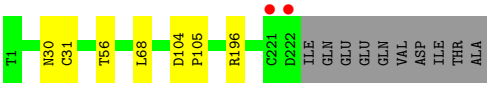




• Molecule 8: Proteasome subunit beta type-2

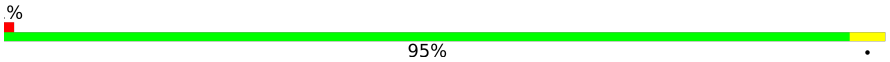
Chain V:





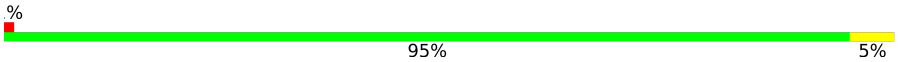
• Molecule 9: Proteasome subunit beta type-3

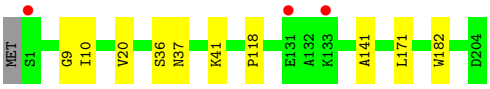
Chain I:



• Molecule 9: Proteasome subunit beta type-3

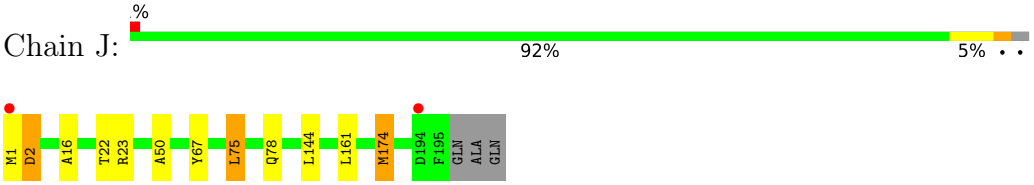
Chain W:





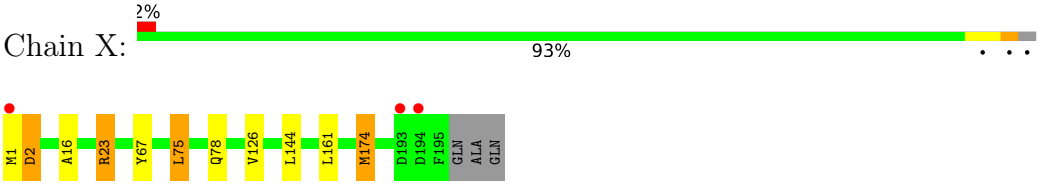
• Molecule 10: Proteasome subunit beta type-4

Chain J:



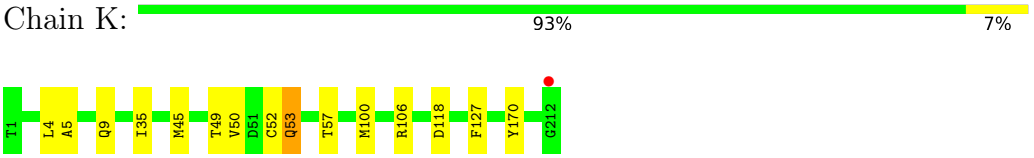
• Molecule 10: Proteasome subunit beta type-4

Chain X:



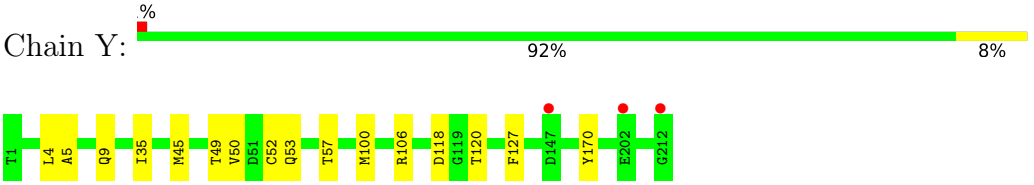
• Molecule 11: Proteasome subunit beta type-5

Chain K:



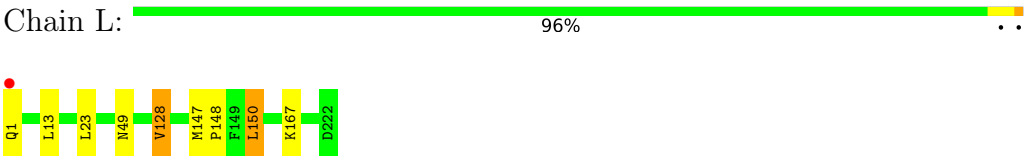
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



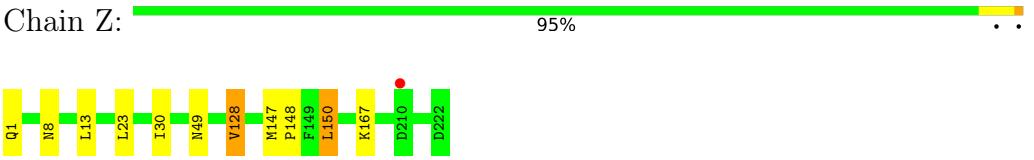
• Molecule 12: Proteasome subunit beta type-6

Chain L:



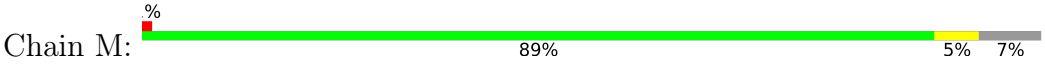
• Molecule 12: Proteasome subunit beta type-6

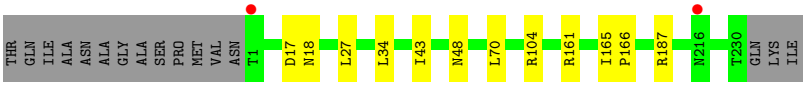
Chain Z:



• Molecule 13: Proteasome subunit beta type-7

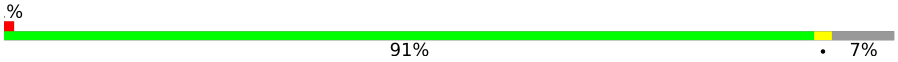
Chain M:

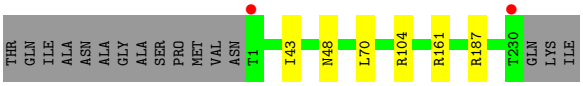




• Molecule 13: Proteasome subunit beta type-7

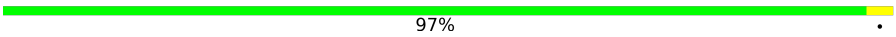
Chain a:

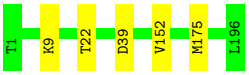




• Molecule 14: Proteasome subunit beta type-1

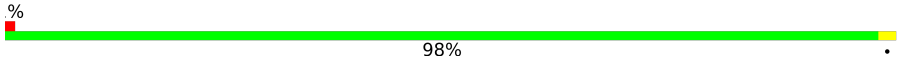
Chain N:

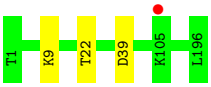




• Molecule 14: Proteasome subunit beta type-1

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	136.69Å 300.21Å 145.62Å 90.00° 112.79° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (15.00-2.80) 99.0 (15.00-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.182 , 0.209 0.185 , 0.210	Depositor DCC
R_{free} test set	13004 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	60.7	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 40.7	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	49853	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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, CL, 3BV

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.27	0/1952	0.47	0/2642
1	O	0.27	0/1952	0.47	0/2642
2	B	0.27	0/1934	0.49	0/2618
2	P	0.27	0/1934	0.49	0/2618
3	C	0.28	0/1910	0.50	0/2586
3	Q	0.28	0/1910	0.50	0/2586
4	D	0.27	0/1837	0.47	0/2475
4	R	0.27	0/1837	0.47	0/2475
5	E	0.27	0/1800	0.46	0/2433
5	S	0.27	0/1800	0.46	0/2433
6	F	0.28	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.28	0/1945	0.47	0/2634
7	U	0.28	0/1945	0.46	0/2634
8	H	0.26	0/1715	0.46	0/2326
8	V	0.26	0/1715	0.46	0/2326
9	I	0.27	0/1611	0.48	0/2174
9	W	0.27	0/1611	0.47	0/2174
10	J	0.28	0/1589	0.48	0/2142
10	X	0.28	0/1589	0.48	0/2142
11	K	0.28	0/1685	0.49	0/2280
11	Y	0.29	0/1685	0.49	0/2280
12	L	0.27	0/1795	0.47	0/2420
12	Z	0.27	0/1795	0.47	0/2420
13	M	0.28	0/1828	0.50	0/2480
13	a	0.28	0/1828	0.51	0/2480
14	N	0.26	0/1541	0.47	0/2087
14	b	0.26	0/1541	0.47	0/2087
All	All	0.27	0/50148	0.48	0/67812

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	1	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	2	0
2	P	1904	0	1904	5	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	0	0
4	R	1813	0	1797	0	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	3	0
8	H	1684	0	1685	1	0
8	V	1684	0	1685	1	0
9	I	1581	0	1574	3	0
9	W	1581	0	1574	4	0
10	J	1561	0	1569	8	0
10	X	1561	0	1569	6	0
11	K	1648	0	1599	8	0
11	Y	1648	0	1599	11	0
12	L	1757	0	1711	3	0
12	Z	1757	0	1711	5	0
13	M	1797	0	1800	3	0
13	a	1797	0	1800	0	0
14	N	1512	0	1478	1	0
14	b	1512	0	1478	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	H	52	0	59	1	0
17	K	52	0	59	4	0
17	N	52	0	59	1	0
17	V	52	0	59	1	0
17	Y	52	0	59	2	0
17	b	52	0	59	0	0
18	K	12	0	13	0	0
18	Y	12	0	13	0	0
19	A	5	0	0	0	0
19	B	14	0	0	0	0
19	C	7	0	0	0	0
19	D	6	0	0	0	0
19	E	2	0	0	0	0
19	F	11	0	0	0	0
19	G	10	0	0	0	0
19	H	11	0	0	0	0
19	I	8	0	0	0	0
19	J	13	0	0	0	0
19	K	16	0	0	0	0
19	L	15	0	0	0	0
19	M	14	0	0	0	0
19	N	5	0	0	0	0
19	O	4	0	0	0	0
19	P	6	0	0	0	0
19	Q	3	0	0	0	0
19	R	6	0	0	0	0
19	S	3	0	0	0	0
19	T	9	0	0	0	0
19	U	13	0	0	0	0
19	V	7	0	0	0	0
19	W	2	0	0	0	0
19	X	19	0	0	0	0
19	Y	12	0	0	0	0
19	Z	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	a	13	0	0	0	0
19	b	8	0	0	0	0
All	All	49853	0	49380	86	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (86) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:53:GLN:O	11:K:57:THR:OG1	2.11	0.67
11:Y:53:GLN:O	11:Y:57:THR:OG1	2.10	0.65
17:N:201:3BV:O60	17:N:201:3BV:O48	2.16	0.58
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.85	0.58
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.85	0.57
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.88	0.55
17:H:301:3BV:O60	17:H:301:3BV:O48	2.25	0.55
7:G:23:PHE:O	7:G:26:THR:HB	2.08	0.54
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.90	0.53
7:U:23:PHE:O	7:U:26:THR:HB	2.09	0.53
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.45	0.52
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.91	0.52
17:V:301:3BV:O60	17:V:301:3BV:O48	2.26	0.51
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.45	0.51
10:J:174:MET:HA	10:X:174:MET:HA	1.93	0.50
10:J:22:THR:O	10:J:23:ARG:HD2	2.12	0.50
11:K:170:TYR:O	17:K:301:3BV:H57	2.12	0.49
10:J:22:THR:O	10:J:23:ARG:CD	2.61	0.49
3:C:201:VAL:O	3:C:202:GLN:CB	2.60	0.49
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.77	0.49
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.78	0.49
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.60	0.49
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.94	0.49
11:Y:170:TYR:O	17:Y:301:3BV:H57	2.12	0.49
11:Y:49:THR:OG1	17:Y:301:3BV:H52	2.13	0.48
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.97	0.47
11:K:49:THR:OG1	17:K:301:3BV:H52	2.14	0.47
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.97	0.47
10:J:23:ARG:NH2	10:J:50:ALA:CB	2.78	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.46
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.98	0.46
10:X:1:MET:O	10:X:2:ASP:HB2	2.16	0.46
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.31	0.46
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.97	0.46
3:C:201:VAL:HG13	3:C:202:GLN:N	2.31	0.45
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.98	0.45
10:J:1:MET:O	10:J:2:ASP:HB2	2.16	0.45
1:O:119:GLN:O	1:O:122:THR:HB	2.17	0.45
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.97	0.45
10:J:23:ARG:NH2	10:J:50:ALA:HB1	2.31	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.00	0.44
11:Y:50:VAL:HG11	12:Z:128:VAL:CG2	2.48	0.44
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.99	0.44
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.00	0.44
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.00	0.43
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.99	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.99	0.43
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.49	0.43
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.49	0.43
17:K:301:3BV:O48	17:K:301:3BV:O60	2.35	0.42
10:X:23:ARG:NH2	11:Y:120:THR:OG1	2.52	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
1:A:119:GLN:O	1:A:122:THR:HB	2.19	0.42
14:N:152:VAL:HA	14:N:175:MET:HE1	2.01	0.42
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.19	0.42
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.02	0.42
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.51	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.02	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.41
17:K:301:3BV:H62	17:K:301:3BV:H55	1.64	0.41
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.02	0.41
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.03	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
13:M:17:ASP:OD1	13:M:18:ASN:N	2.54	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
11:Y:45:MET:HE1	11:Y:53:GLN:HG3	2.02	0.41
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.36	0.41
3:C:201:VAL:O	3:C:202:GLN:HB2	2.19	0.41
11:K:45:MET:HG2	11:K:52:CYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:100:MET:CE	11:K:127:PHE:HB2	2.51	0.41
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.86	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.56	0.41
11:Y:50:VAL:HG11	12:Z:128:VAL:HG23	2.03	0.41
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.04	0.40
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.52	0.40
12:L:147:MET:N	12:L:148:PRO:HD2	2.35	0.40
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.56	0.40
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	2.03	0.40
11:K:50:VAL:HG11	12:L:128:VAL:CG2	2.52	0.40
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.04	0.40
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.04	0.40
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
2	B	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	19	49
2	P	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	19	49
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	19	49
3	Q	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	19	49
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	224 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
6	T	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
8	V	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	61
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	61
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
12	Z	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
13	M	228/246 (93%)	219 (96%)	9 (4%)	0	100	100
13	a	228/246 (93%)	221 (97%)	7 (3%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6270/6614 (95%)	6105 (97%)	155 (2%)	10 (0%)	47	78

All (10) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	67	90
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	90
2	B	203/216 (94%)	196 (97%)	7 (3%)	37	71
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	71
3	C	212/226 (94%)	204 (96%)	8 (4%)	33	67
3	Q	212/226 (94%)	204 (96%)	8 (4%)	33	67
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	60
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	60
5	E	190/193 (98%)	181 (95%)	9 (5%)	26	59
5	S	190/193 (98%)	181 (95%)	9 (5%)	26	59
6	F	201/239 (84%)	192 (96%)	9 (4%)	27	60
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	60
7	G	206/210 (98%)	199 (97%)	7 (3%)	37	71
7	U	206/210 (98%)	199 (97%)	7 (3%)	37	71
8	H	181/190 (95%)	176 (97%)	5 (3%)	43	77
8	V	181/190 (95%)	176 (97%)	5 (3%)	43	77
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	87
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	87
10	J	173/175 (99%)	169 (98%)	4 (2%)	50	82
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	76
11	K	171/171 (100%)	165 (96%)	6 (4%)	36	70
11	Y	171/171 (100%)	166 (97%)	5 (3%)	42	76
12	L	185/185 (100%)	179 (97%)	6 (3%)	39	73
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39	73
13	M	196/208 (94%)	190 (97%)	6 (3%)	40	74
13	a	196/208 (94%)	190 (97%)	6 (3%)	40	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	159 (98%)	3 (2%)	57	85
14	b	162/162 (100%)	159 (98%)	3 (2%)	57	85
All	All	5310/5544 (96%)	5140 (97%)	170 (3%)	39	73

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
2	B	50	LYS
2	B	52	THR
2	B	55	LEU
2	B	58	GLN
2	B	114	LEU
2	B	184	LYS
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	203	THR
4	D	20	LEU
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	224	ASP
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	174	THR
5	E	184	ASN

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Mol	Chain	Res	Type
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP
6	F	117	GLN
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	115	LEU
7	G	117	GLN
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	31	CYS
8	H	56	THR
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	53	GLN
11	K	106	ARG
11	K	118	ASP
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	128	VAL
12	L	150	LEU
12	L	167	LYS

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Mol	Chain	Res	Type
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	22	THR
14	N	39	ASP
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	52	THR
2	P	55	LEU
2	P	58	GLN
2	P	114	LEU
2	P	184	LYS
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	203	THR
4	R	20	LEU
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	224	ASP
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	174	THR

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Mol	Chain	Res	Type
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	14	ASP
6	T	117	GLN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	115	LEU
7	U	117	GLN
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	31	CYS
8	V	56	THR
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	23	ARG
10	X	75	LEU
10	X	78	GLN
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	106	ARG
11	Y	118	ASP
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	128	VAL
12	Z	150	LEU

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Mol	Chain	Res	Type
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	22	THR
14	b	39	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	119	GLN
2	B	123	GLN
2	B	176	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	86	ASN
6	F	117	GLN
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	117	GLN
7	G	121	GLN
9	I	37	ASN
10	J	55	GLN

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Mol	Chain	Res	Type
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	70	ASN
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	194	ASN
13	M	213	GLN
1	O	94	HIS
2	P	20	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	117	GLN
7	U	121	GLN
10	X	55	GLN
11	Y	62	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	70	ASN
12	Z	158	ASN
13	a	48	ASN

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Mol	Chain	Res	Type
13	a	102	GLN
13	a	194	ASN
13	a	213	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 19 ligands modelled in this entry, 11 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	MES	Y	303	-	12,12,12	2.16	1 (8%)	14,16,16	1.33	3 (21%)
17	3BV	Y	301	11	54,54,54	1.15	3 (5%)	68,71,71	1.75	13 (19%)
17	3BV	N	201	14	54,54,54	1.30	4 (7%)	68,71,71	1.47	10 (14%)
17	3BV	H	301	8	54,54,54	1.15	3 (5%)	68,71,71	1.49	9 (13%)
17	3BV	b	201	14	54,54,54	1.27	4 (7%)	68,71,71	1.48	10 (14%)
17	3BV	V	301	8	54,54,54	1.13	3 (5%)	68,71,71	1.49	9 (13%)
18	MES	K	303	-	12,12,12	2.17	1 (8%)	14,16,16	1.38	3 (21%)
17	3BV	K	301	11	54,54,54	1.15	3 (5%)	68,71,71	1.74	12 (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
18	MES	Y	303	-	-	0/6/14/14	0/1/1/1
17	3BV	Y	301	11	-	5/59/67/67	0/3/3/3
17	3BV	N	201	14	-	14/59/67/67	0/3/3/3
17	3BV	H	301	8	-	15/59/67/67	0/3/3/3
17	3BV	b	201	14	-	13/59/67/67	0/3/3/3
17	3BV	V	301	8	-	15/59/67/67	0/3/3/3
18	MES	K	303	-	-	0/6/14/14	0/1/1/1
17	3BV	K	301	11	-	5/59/67/67	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	303	MES	C8-S	-7.19	1.67	1.77
18	Y	303	MES	C8-S	-7.16	1.67	1.77
17	N	201	3BV	C51-C47	5.83	1.63	1.53
17	b	201	3BV	C51-C47	5.43	1.63	1.53
17	H	301	3BV	C51-C47	4.67	1.61	1.53
17	b	201	3BV	C32-C33	-4.58	1.40	1.51
17	K	301	3BV	C32-C33	-4.54	1.40	1.51
17	Y	301	3BV	C32-C33	-4.52	1.40	1.51
17	N	201	3BV	C32-C33	-4.52	1.40	1.51
17	V	301	3BV	C51-C47	4.45	1.61	1.53
17	H	301	3BV	C32-C33	-4.39	1.40	1.51
17	K	301	3BV	C51-C47	4.32	1.61	1.53
17	V	301	3BV	C32-C33	-4.28	1.41	1.51
17	Y	301	3BV	C51-C47	4.27	1.61	1.53
17	K	301	3BV	C13-C14	-3.71	1.40	1.51
17	Y	301	3BV	C13-C14	-3.67	1.41	1.51
17	b	201	3BV	C13-C14	-3.66	1.41	1.51
17	N	201	3BV	C13-C14	-3.62	1.41	1.51
17	H	301	3BV	C13-C14	-3.12	1.42	1.51
17	V	301	3BV	C13-C14	-3.09	1.42	1.51
17	N	201	3BV	C59-C51	2.55	1.55	1.52
17	b	201	3BV	C59-C51	2.52	1.55	1.52

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	V	301	3BV	C43-C42-N41	-6.19	102.17	110.18
17	H	301	3BV	C43-C42-N41	-6.13	102.25	110.18
17	b	201	3BV	C43-C42-N41	-6.08	102.32	110.18
17	N	201	3BV	C43-C42-N41	-6.07	102.33	110.18
17	K	301	3BV	C43-C42-N41	-6.01	102.41	110.18
17	Y	301	3BV	C43-C42-N41	-5.94	102.50	110.18
17	K	301	3BV	C7-N4-C5	5.92	120.27	111.09
17	Y	301	3BV	C7-N4-C5	5.86	120.18	111.09
17	N	201	3BV	C58-C51-C59	-4.84	103.52	109.88
17	b	201	3BV	C58-C51-C59	-4.73	103.67	109.88
17	Y	301	3BV	C58-C51-C59	-4.44	104.04	109.88
17	K	301	3BV	C58-C51-C59	-4.12	104.46	109.88
17	H	301	3BV	C25-C24-C23	-4.04	104.33	115.43
17	Y	301	3BV	C6-C5-N4	-3.98	104.07	110.10
17	V	301	3BV	C25-C24-C23	-3.97	104.52	115.43
17	H	301	3BV	C58-C51-C59	-3.95	104.69	109.88
17	V	301	3BV	O1-C6-C5	-3.94	103.12	111.80
17	H	301	3BV	O1-C6-C5	-3.92	103.16	111.80
17	K	301	3BV	C6-C5-N4	-3.90	104.19	110.10
17	V	301	3BV	C58-C51-C59	-3.89	104.77	109.88
17	Y	301	3BV	C33-C32-C31	-3.77	102.98	113.39
17	K	301	3BV	C33-C32-C31	-3.76	103.01	113.39
17	H	301	3BV	C13-C12-C11	-3.24	106.82	113.21
17	V	301	3BV	C13-C12-C11	-3.16	106.98	113.21
17	K	301	3BV	O1-C2-C3	-3.11	104.95	111.80
17	H	301	3BV	C33-C32-C31	-3.10	104.84	113.39
17	b	201	3BV	C33-C32-C31	-3.09	104.86	113.39
17	N	201	3BV	O1-C6-C5	-3.06	105.06	111.80
17	V	301	3BV	C33-C32-C31	-3.05	104.96	113.39
17	b	201	3BV	O1-C6-C5	-3.02	105.14	111.80
17	N	201	3BV	C33-C32-C31	-3.02	105.06	113.39
17	K	301	3BV	C7-N4-C3	-2.97	106.50	111.09
17	Y	301	3BV	O1-C2-C3	-2.95	105.31	111.80
17	b	201	3BV	O1-C2-C3	-2.93	105.34	111.80
17	Y	301	3BV	C7-N4-C3	-2.92	106.56	111.09
17	K	301	3BV	C13-C12-C11	-2.88	107.53	113.21
17	Y	301	3BV	C13-C12-C11	-2.88	107.54	113.21
17	N	201	3BV	O1-C2-C3	-2.85	105.51	111.80
17	V	301	3BV	C6-C5-N4	-2.59	106.17	110.10
17	b	201	3BV	C12-C13-C14	-2.58	104.20	113.18
17	N	201	3BV	C12-C13-C14	-2.57	104.24	113.18
17	Y	301	3BV	O1-C6-C5	-2.55	106.19	111.80
17	K	301	3BV	O1-C6-C5	-2.54	106.20	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	H	301	3BV	C6-C5-N4	-2.53	106.26	110.10
18	Y	303	MES	O1S-S-C8	2.53	109.96	106.92
18	K	303	MES	O1S-S-C8	2.50	109.93	106.92
17	Y	301	3BV	C25-C24-C23	-2.49	108.60	115.43
17	K	301	3BV	C25-C24-C23	-2.46	108.67	115.43
18	K	303	MES	O3S-S-C8	2.43	109.70	105.77
17	N	201	3BV	C25-C24-C23	-2.39	108.86	115.43
18	Y	303	MES	O3S-S-C8	2.36	109.58	105.77
17	b	201	3BV	C25-C24-C23	-2.32	109.04	115.43
17	b	201	3BV	C12-C11-C20	-2.32	104.77	110.20
18	K	303	MES	O2S-S-C8	2.32	109.71	106.92
18	Y	303	MES	O2S-S-C8	2.31	109.69	106.92
17	N	201	3BV	C12-C11-C20	-2.28	104.87	110.20
17	V	301	3BV	O60-C59-C51	-2.22	106.79	111.33
17	K	301	3BV	O60-C59-C51	-2.19	106.85	111.33
17	H	301	3BV	O60-C59-C51	-2.15	106.94	111.33
17	b	201	3BV	C7-N4-C3	-2.14	107.77	111.09
17	Y	301	3BV	O60-C59-C51	-2.13	106.97	111.33
17	N	201	3BV	C7-N4-C3	-2.11	107.82	111.09
17	b	201	3BV	C3-N4-C5	2.08	113.52	108.83
17	Y	301	3BV	C39-C31-N30	-2.05	105.57	111.16
17	V	301	3BV	O1-C2-C3	-2.05	107.28	111.80
17	H	301	3BV	O1-C2-C3	-2.03	107.31	111.80
17	K	301	3BV	C39-C31-N30	-2.02	105.67	111.16
17	N	201	3BV	C3-N4-C5	2.02	113.37	108.83
17	Y	301	3BV	C12-C13-C14	-2.01	106.18	113.18

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	3BV	C8-C7-N4-C3
17	H	301	3BV	N10-C11-C12-C13
17	H	301	3BV	C47-C42-C43-C44
17	H	301	3BV	C42-C47-C51-C58
17	K	301	3BV	C8-C7-N4-C5
17	N	201	3BV	C47-C42-C43-C44
17	N	201	3BV	C42-C47-C51-C58
17	N	201	3BV	C42-C47-C51-C59
17	N	201	3BV	O48-C47-C51-C58
17	V	301	3BV	C8-C7-N4-C3
17	V	301	3BV	N10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	V	301	3BV	C47-C42-C43-C44
17	V	301	3BV	C42-C47-C51-C58
17	Y	301	3BV	C8-C7-N4-C5
17	b	201	3BV	C47-C42-C43-C44
17	b	201	3BV	C42-C47-C51-C58
17	b	201	3BV	C42-C47-C51-C59
17	b	201	3BV	O48-C47-C51-C58
17	H	301	3BV	C20-C11-C12-C13
17	V	301	3BV	C20-C11-C12-C13
17	H	301	3BV	O48-C47-C51-C58
17	V	301	3BV	O48-C47-C51-C58
17	N	201	3BV	O48-C47-C51-C59
17	b	201	3BV	O48-C47-C51-C59
17	V	301	3BV	C42-C43-C44-C46
17	H	301	3BV	C42-C43-C44-C46
17	H	301	3BV	N41-C42-C43-C44
17	K	301	3BV	N41-C42-C43-C44
17	N	201	3BV	N41-C42-C43-C44
17	V	301	3BV	N41-C42-C43-C44
17	Y	301	3BV	N41-C42-C43-C44
17	b	201	3BV	N41-C42-C43-C44
17	N	201	3BV	C8-C7-N4-C5
17	N	201	3BV	C8-C7-N4-C3
17	b	201	3BV	C8-C7-N4-C5
17	b	201	3BV	C8-C7-N4-C3
17	N	201	3BV	C47-C51-C59-O60
17	K	301	3BV	C47-C42-C43-C44
17	Y	301	3BV	C47-C42-C43-C44
17	H	301	3BV	C12-C13-C14-C15
17	V	301	3BV	C12-C13-C14-C15
17	N	201	3BV	N10-C11-C20-N22
17	b	201	3BV	N10-C11-C20-N22
17	H	301	3BV	C12-C13-C14-C19
17	V	301	3BV	C12-C13-C14-C19
17	N	201	3BV	N10-C11-C20-O21
17	b	201	3BV	N10-C11-C20-O21
17	V	301	3BV	N30-C31-C39-O40
17	b	201	3BV	N30-C31-C39-O40
17	H	301	3BV	N30-C31-C39-O40
17	N	201	3BV	N30-C31-C39-O40
17	H	301	3BV	C23-C24-C25-C27
17	V	301	3BV	C23-C24-C25-C27

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Mol	Chain	Res	Type	Atoms
17	H	301	3BV	C23-C24-C25-C26
17	N	201	3BV	N30-C31-C39-N41
17	b	201	3BV	N30-C31-C39-N41
17	V	301	3BV	C23-C24-C25-C26
17	N	201	3BV	N4-C7-C8-O9
17	b	201	3BV	N4-C7-C8-O9
17	H	301	3BV	N30-C31-C39-N41
17	V	301	3BV	N30-C31-C39-N41
17	Y	301	3BV	N30-C31-C39-O40
17	H	301	3BV	C42-C47-C51-C59
17	V	301	3BV	C42-C47-C51-C59
17	K	301	3BV	N30-C31-C39-O40
17	K	301	3BV	N41-C42-C47-C51
17	Y	301	3BV	N41-C42-C47-C51

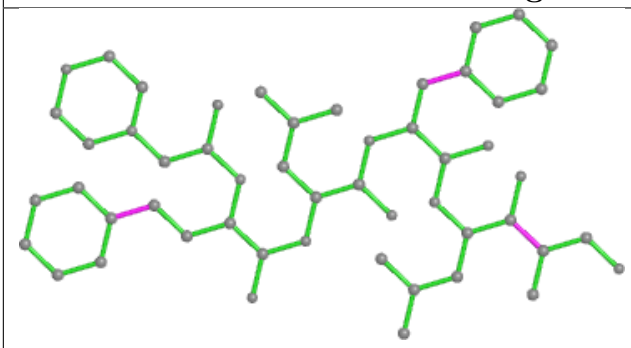
There are no ring outliers.

5 monomers are involved in 9 short contacts:

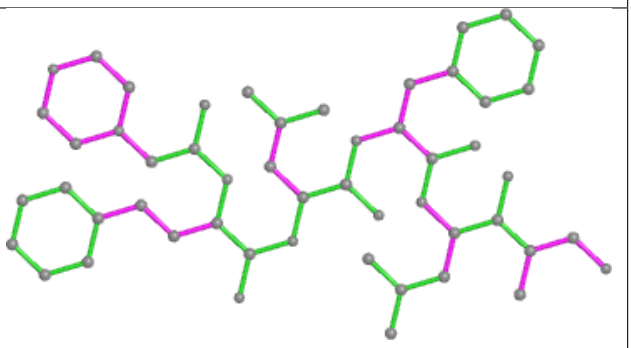
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	301	3BV	2	0
17	N	201	3BV	1	0
17	H	301	3BV	1	0
17	V	301	3BV	1	0
17	K	301	3BV	4	0

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.

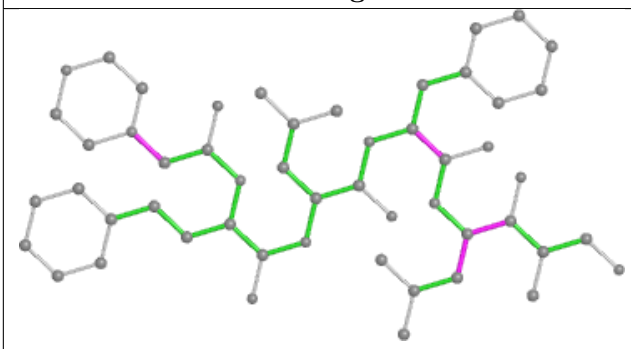
Ligand 3BV Y 301



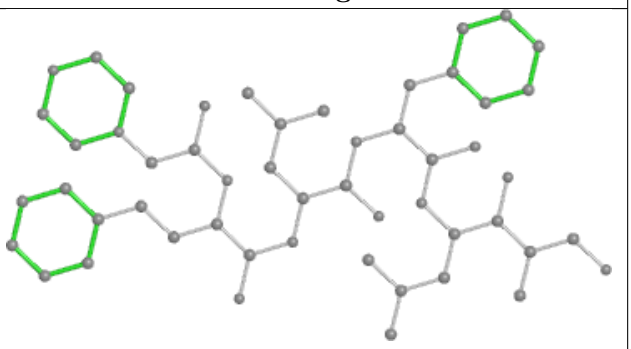
Bond lengths



Bond angles

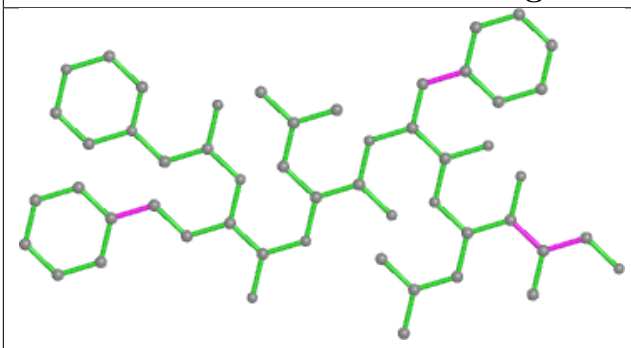


Torsions

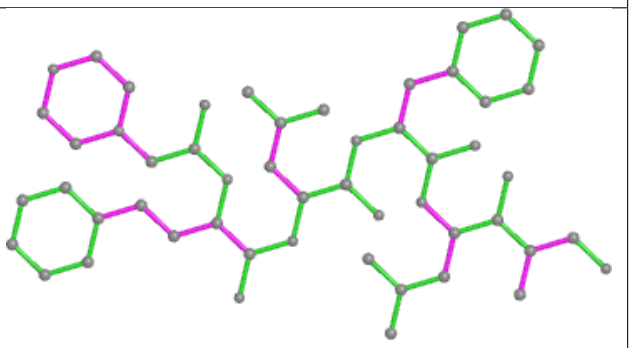


Rings

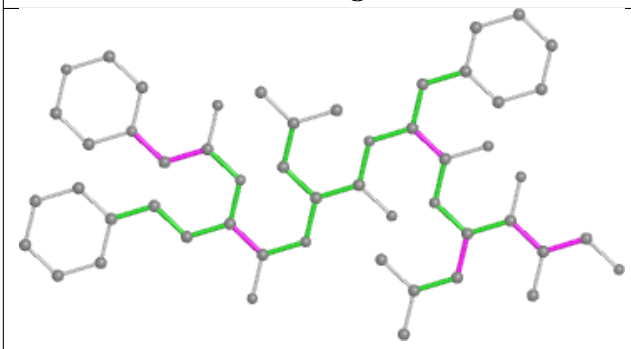
Ligand 3BV N 201



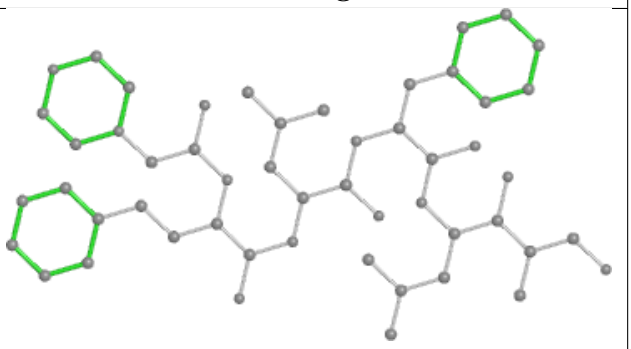
Bond lengths



Bond angles

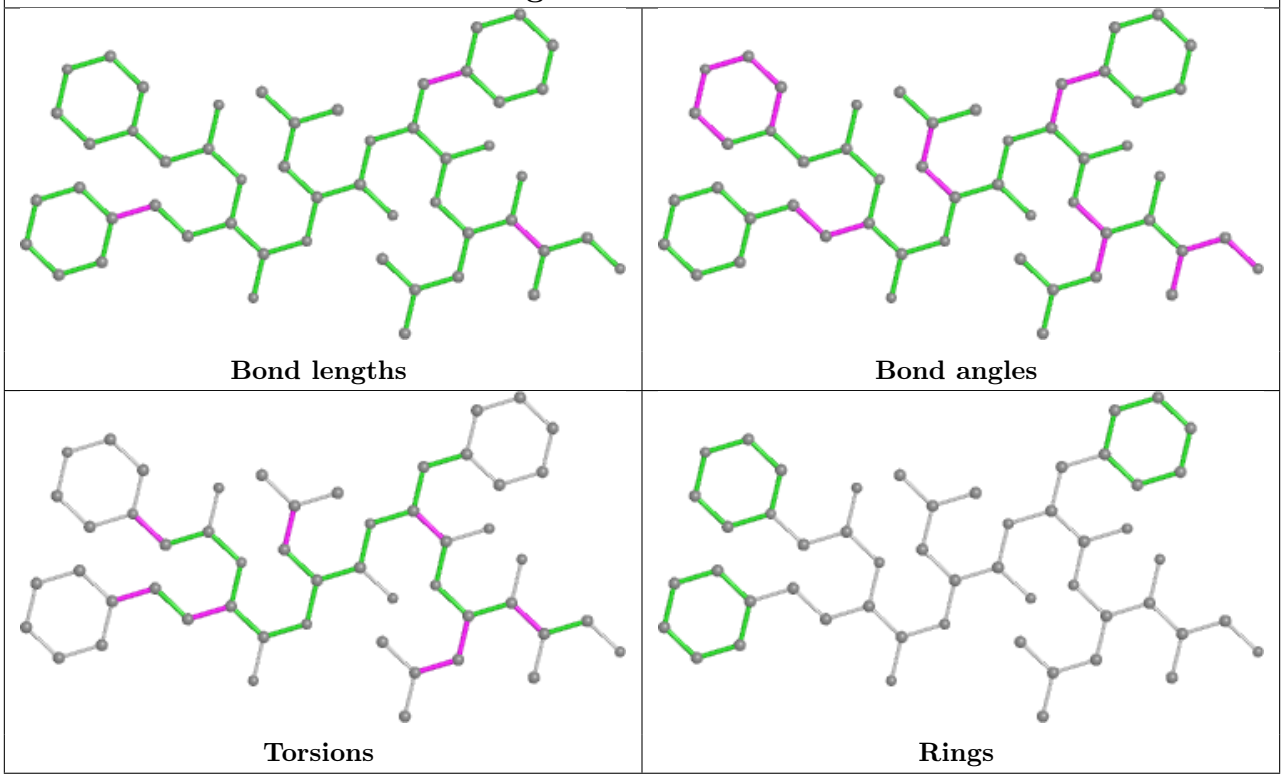


Torsions

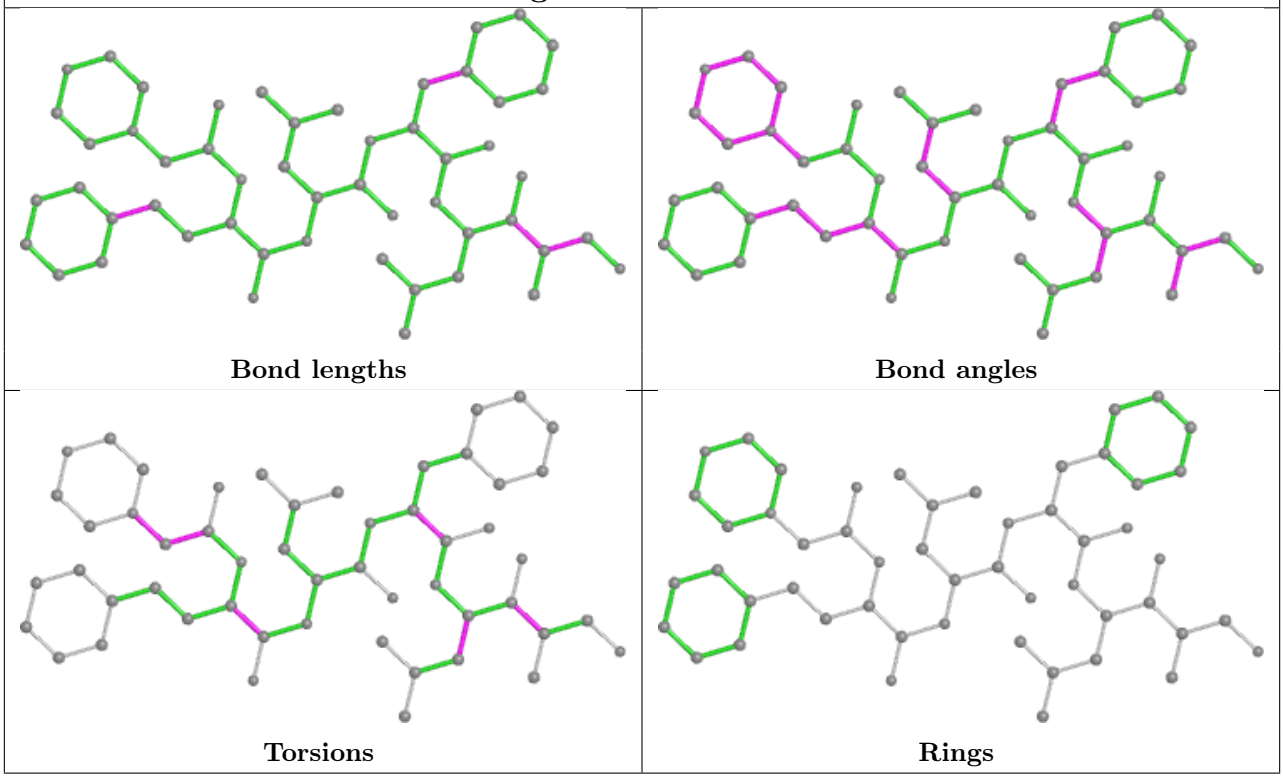


Rings

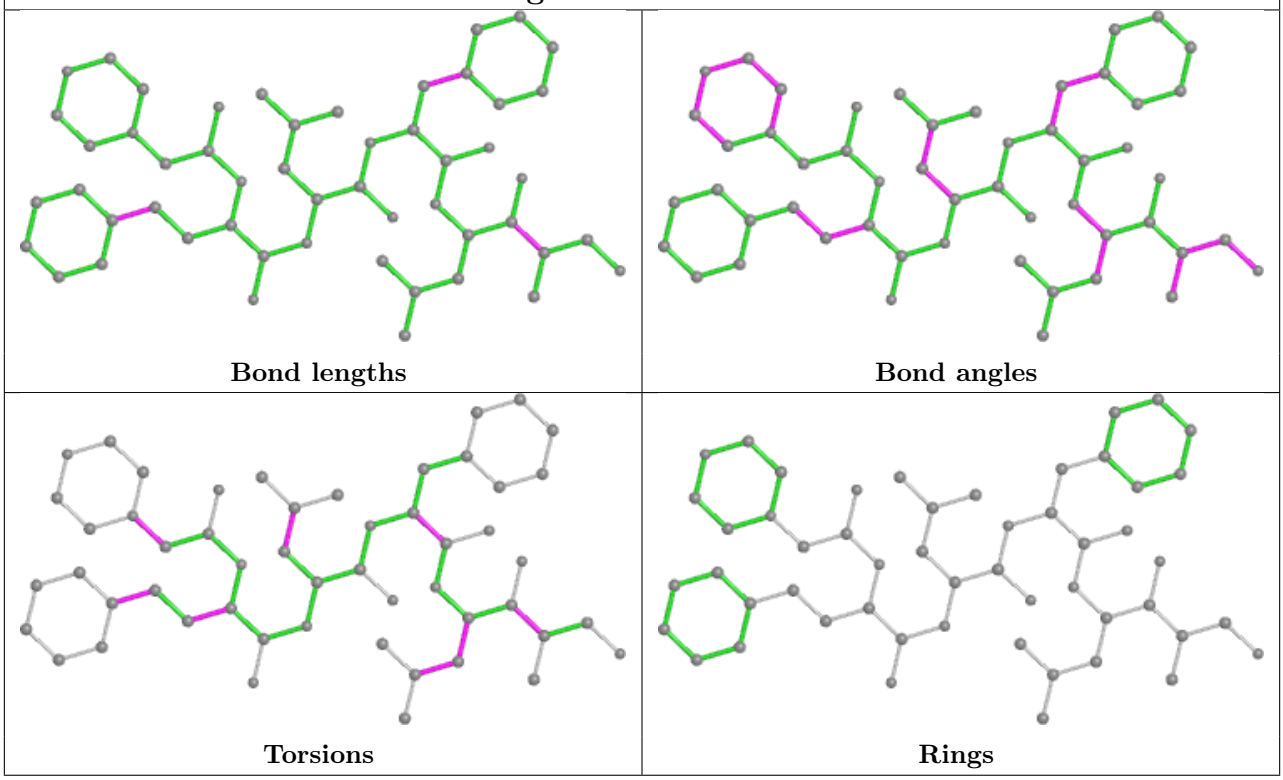
Ligand 3BV H 301



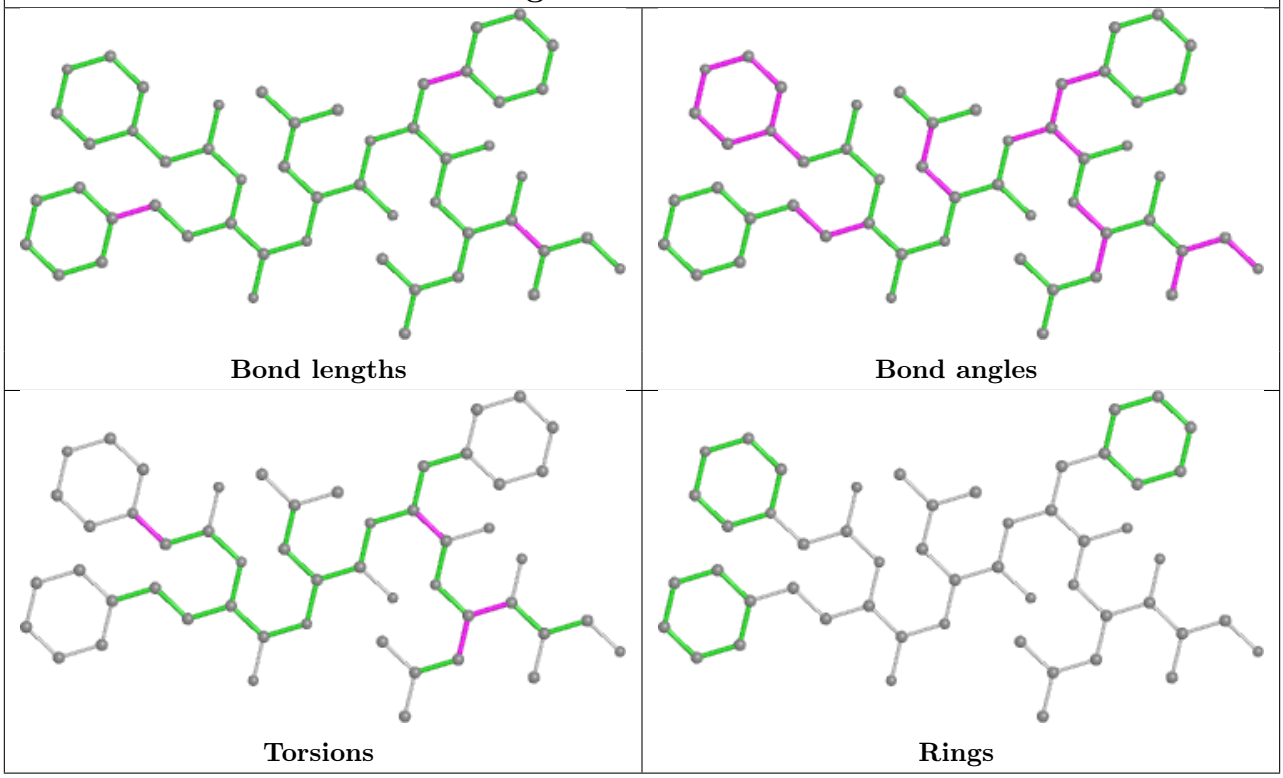
Ligand 3BV b 201



Ligand 3BV V 301



Ligand 3BV K 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.45	4 (1%)	72	66	43, 59, 98, 144	0
1	O	250/250 (100%)	-0.40	6 (2%)	59	49	45, 65, 109, 152	0
2	B	244/258 (94%)	-0.32	13 (5%)	26	17	42, 62, 115, 170	0
2	P	244/258 (94%)	-0.32	10 (4%)	37	27	46, 66, 112, 167	0
3	C	240/254 (94%)	-0.24	13 (5%)	25	17	44, 66, 129, 168	0
3	Q	240/254 (94%)	-0.14	14 (5%)	23	15	48, 79, 157, 202	0
4	D	235/260 (90%)	-0.46	2 (0%)	84	80	48, 68, 99, 143	0
4	R	235/260 (90%)	-0.38	4 (1%)	70	63	53, 74, 111, 157	0
5	E	231/234 (98%)	-0.32	3 (1%)	77	72	52, 74, 110, 152	0
5	S	231/234 (98%)	-0.34	5 (2%)	62	52	49, 71, 111, 143	0
6	F	243/288 (84%)	-0.44	7 (2%)	51	41	43, 67, 122, 150	0
6	T	243/288 (84%)	-0.40	7 (2%)	51	41	38, 66, 118, 155	0
7	G	241/252 (95%)	-0.46	5 (2%)	63	54	43, 63, 108, 161	0
7	U	241/252 (95%)	-0.52	3 (1%)	79	73	41, 60, 97, 133	0
8	H	222/232 (95%)	-0.41	3 (1%)	75	70	45, 59, 105, 154	0
8	V	222/232 (95%)	-0.43	2 (0%)	84	80	43, 61, 98, 142	0
9	I	204/205 (99%)	-0.70	2 (0%)	82	77	39, 54, 90, 110	0
9	W	204/205 (99%)	-0.66	3 (1%)	73	68	39, 57, 94, 114	0
10	J	195/198 (98%)	-0.63	2 (1%)	82	77	38, 54, 83, 125	0
10	X	195/198 (98%)	-0.64	3 (1%)	73	68	40, 57, 86, 129	0
11	K	212/212 (100%)	-0.63	1 (0%)	91	88	41, 58, 92, 113	0
11	Y	212/212 (100%)	-0.62	3 (1%)	75	70	42, 57, 91, 113	0
12	L	222/222 (100%)	-0.59	1 (0%)	91	88	40, 61, 92, 118	0
12	Z	222/222 (100%)	-0.60	1 (0%)	91	88	39, 59, 94, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	230/246 (93%)	-0.60	2 (0%) 84 80	37, 57, 87, 95	0
13	a	230/246 (93%)	-0.63	2 (0%) 84 80	38, 55, 83, 107	0
14	N	196/196 (100%)	-0.71	0 100 100	36, 52, 86, 110	0
14	b	196/196 (100%)	-0.68	1 (0%) 91 88	37, 52, 83, 105	0
All	All	6330/6614 (95%)	-0.48	122 (1%) 66 59	36, 62, 107, 202	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	220	ASN	9.0
8	V	222	ASP	6.9
1	A	1	MET	6.6
8	H	221	CYS	6.4
8	V	221	CYS	6.2
3	C	206	LYS	6.1
10	X	1	MET	5.6
3	Q	50	LEU	5.5
1	O	1	MET	5.5
1	O	249	ALA	5.4
5	S	202	ASP	5.4
2	B	219	ALA	5.4
8	H	222	ASP	5.3
10	J	1	MET	5.3
3	Q	49	THR	5.1
2	P	220	ASN	5.0
2	P	219	ALA	5.0
2	P	51	VAL	4.7
3	Q	239	GLN	4.6
9	W	1	SER	4.4
2	B	221	ASP	4.2
5	E	202	ASP	4.2
2	B	218	GLY	4.1
6	F	202	ASP	4.0
3	C	238	LYS	4.0
2	P	221	ASP	3.9
3	Q	238	LYS	3.8
2	P	222	GLY	3.8
3	Q	206	LYS	3.6
10	J	194	ASP	3.5
2	P	218	GLY	3.4
3	C	225	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
6	F	244	ASN	3.3
3	Q	236	GLN	3.3
3	C	236	GLN	3.3
4	R	125	LEU	3.2
3	C	235	GLU	3.2
3	C	202	GLN	3.2
3	Q	48	SER	3.1
6	T	244	ASN	3.1
7	G	240	ALA	3.1
3	C	239	GLN	3.0
1	A	249	ALA	3.0
1	O	2	THR	3.0
3	C	240	GLU	3.0
6	F	243	ILE	3.0
3	C	205	ALA	2.9
7	G	2	GLY	2.9
3	Q	240	GLU	2.9
2	B	242	GLY	2.9
3	C	49	THR	2.8
7	G	242	GLN	2.8
6	F	181	GLU	2.8
1	O	201	GLU	2.8
3	Q	235	GLU	2.8
9	I	1	SER	2.8
2	P	59	ASP	2.7
6	F	178	HIS	2.7
3	Q	51	LYS	2.7
2	B	51	VAL	2.7
10	X	194	ASP	2.7
1	A	250	LEU	2.7
5	S	54	GLU	2.7
2	P	225	TYR	2.7
6	T	243	ILE	2.7
4	R	242	GLU	2.7
13	a	1	THR	2.6
5	S	233	ILE	2.6
6	T	230	ASP	2.6
2	P	52	THR	2.5
3	Q	225	GLU	2.5
2	B	52	THR	2.5
11	Y	212	GLY	2.5
2	B	203	SER	2.5

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Mol	Chain	Res	Type	RSRZ
11	K	212	GLY	2.5
1	O	231	LYS	2.5
4	D	238	LYS	2.5
5	E	180	LYS	2.5
6	T	205	GLU	2.5
3	Q	180	LYS	2.5
3	Q	141	ASP	2.4
1	A	231	LYS	2.4
7	U	203	ASP	2.4
9	W	133	LYS	2.4
7	G	3	TYR	2.4
7	U	181	LYS	2.4
2	B	217	LYS	2.4
12	Z	210	ASP	2.4
2	B	59	ASP	2.3
13	M	1	THR	2.3
2	B	244	THR	2.3
2	P	182	ASP	2.3
6	T	241	LYS	2.3
4	R	241	ALA	2.3
7	U	2	GLY	2.2
3	C	187	GLU	2.2
4	D	242	GLU	2.2
8	H	207	ARG	2.2
2	B	235	LYS	2.2
9	W	131	GLU	2.2
5	S	3	ASN	2.2
3	C	180	LYS	2.2
5	E	54	GLU	2.2
6	F	201	GLU	2.2
11	Y	147	ASP	2.1
3	Q	202	GLN	2.1
6	F	53	LYS	2.1
13	M	216	ASN	2.1
2	B	222	GLY	2.1
3	C	50	LEU	2.1
9	I	133	LYS	2.1
1	O	248	GLU	2.1
5	S	194	GLU	2.1
6	T	177	ASP	2.1
11	Y	202	GLU	2.1
7	G	179	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
6	T	2	THR	2.1
12	L	1	GLN	2.1
13	a	230	THR	2.0
14	b	105	LYS	2.0
4	R	54	ASP	2.0
10	X	193	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
18	MES	K	303	12/12	0.81	0.47	91,97,118,129	0
18	MES	Y	303	12/12	0.84	0.43	81,86,103,118	0
17	3BV	H	301	52/52	0.88	0.25	62,71,121,124	0
17	3BV	N	201	52/52	0.88	0.24	39,54,132,135	0
17	3BV	K	301	52/52	0.89	0.23	45,59,123,129	0
17	3BV	b	201	52/52	0.89	0.22	42,54,128,132	0
17	3BV	Y	301	52/52	0.90	0.23	43,55,112,116	0
17	3BV	V	301	52/52	0.90	0.26	61,72,119,122	0
16	CL	N	203	1/1	0.93	0.16	57,57,57,57	0
15	MG	Z	301	1/1	0.94	0.28	70,70,70,70	0
16	CL	b	202	1/1	0.94	0.23	67,67,67,67	0
15	MG	I	301	1/1	0.97	0.10	56,56,56,56	0
15	MG	Y	302	1/1	0.98	0.05	49,49,49,49	0
15	MG	G	301	1/1	0.98	0.04	59,59,59,59	0
15	MG	N	202	1/1	0.98	0.07	49,49,49,49	0
16	CL	G	302	1/1	0.99	0.12	46,46,46,46	0
15	MG	K	302	1/1	0.99	0.05	58,58,58,58	0

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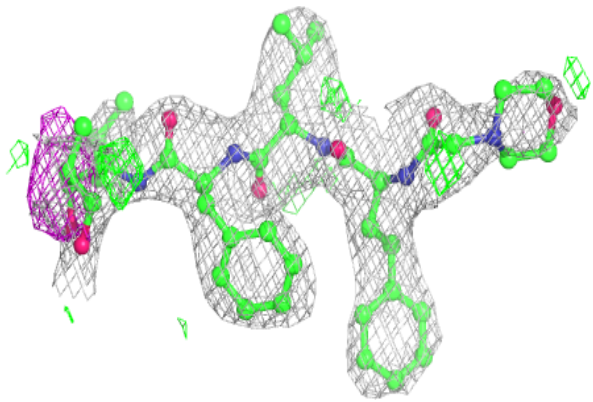
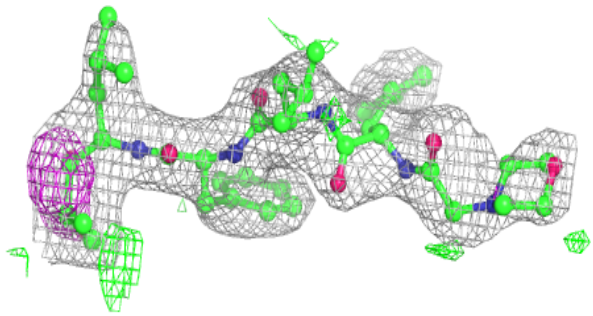
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	CL	U	301	1/1	0.99	0.12	41,41,41,41	0
15	MG	V	302	1/1	0.99	0.07	77,77,77,77	0

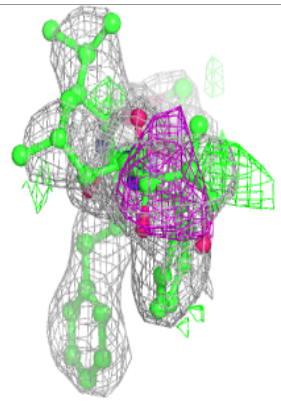
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3BV H 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

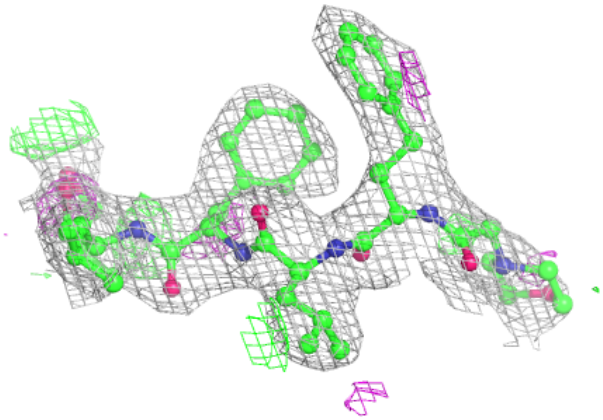


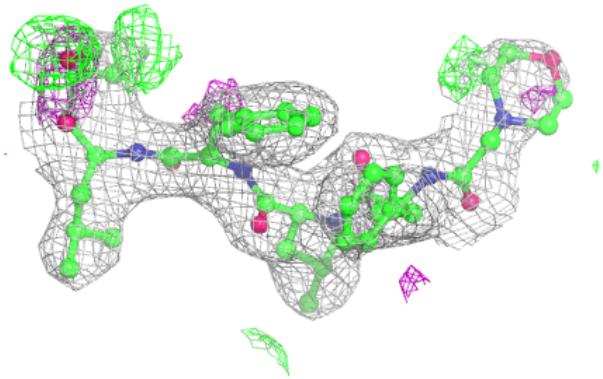


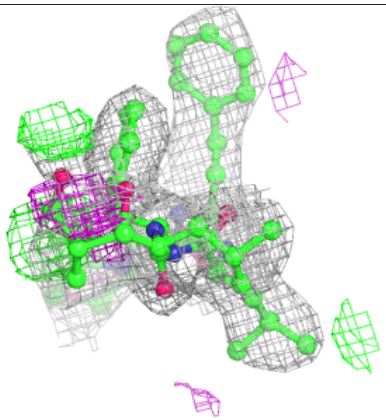


Electron density around 3BV N 201:

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

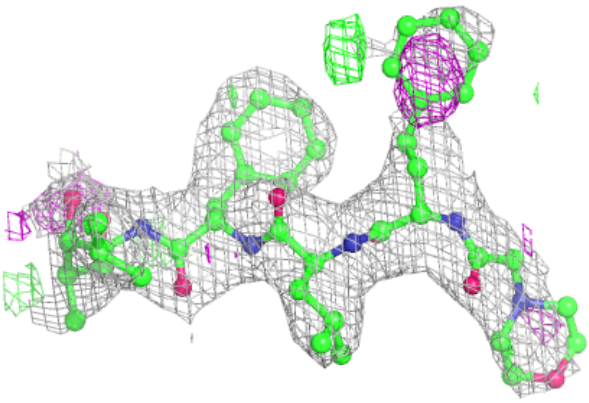


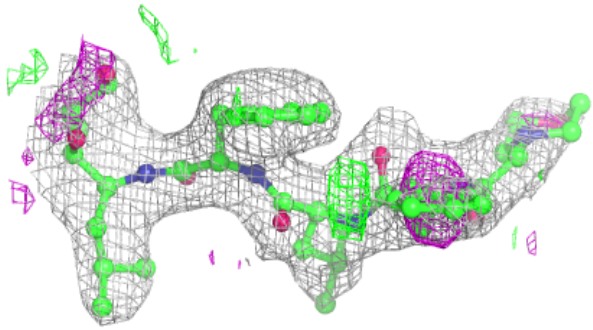


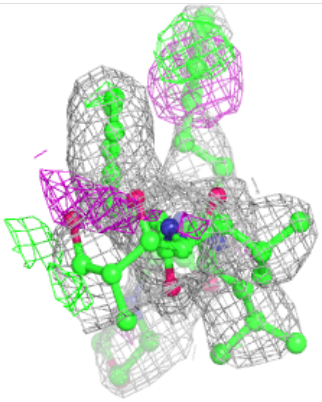


Electron density around 3BV K 301:

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

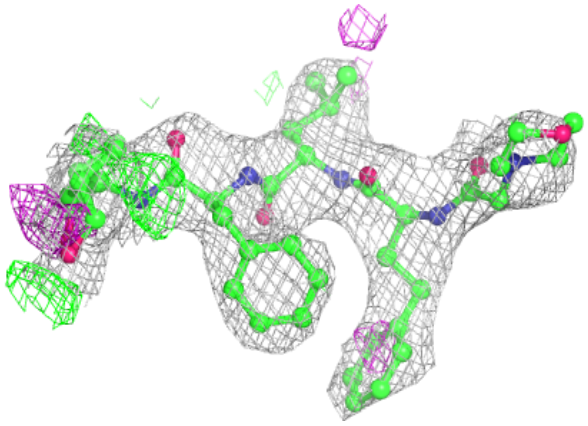


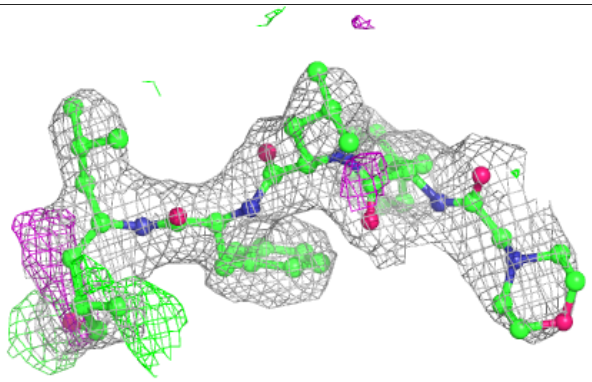


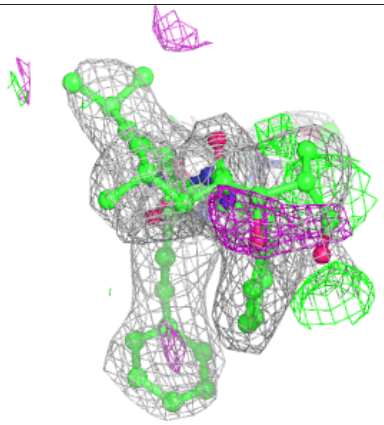


Electron density around 3BV b 201:

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

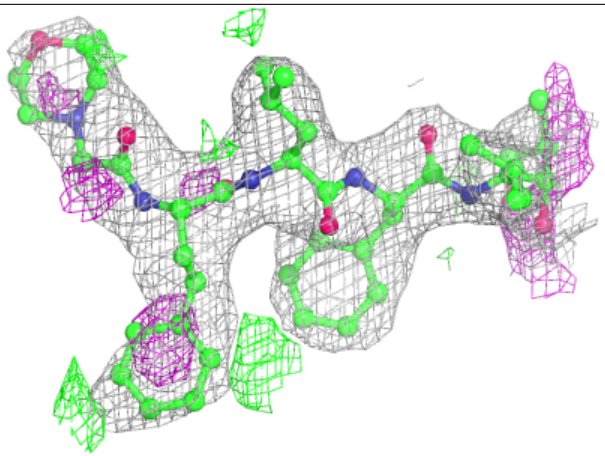


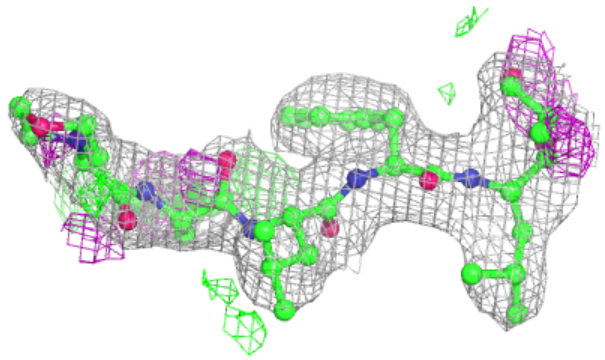




Electron density around 3BV Y 301:

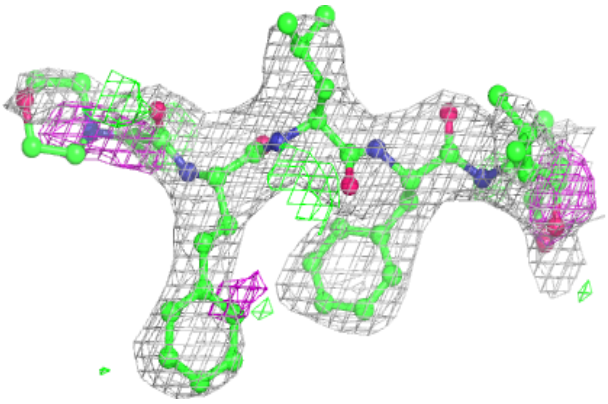
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

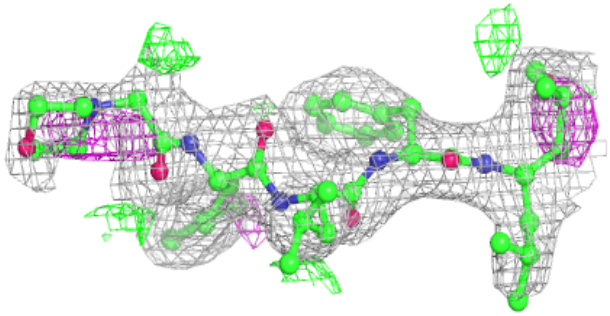


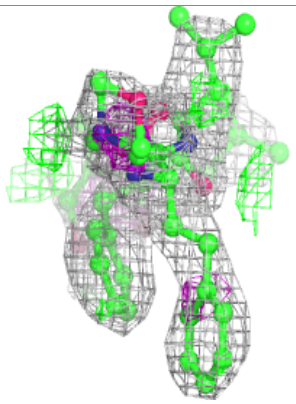


Electron density around 3BV V 301:

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







6.5 Other polymers (i)

There are no such residues in this entry.