Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 11:30 pm GMT

PDB ID	:	5FGG
Title	:	Yeast 20S proteasome beta5-L(-49S)_D17N double mutant in complex with Carfilzomib
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2015-12-20
Resolution	:	2.70 Å(reported)

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

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

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

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

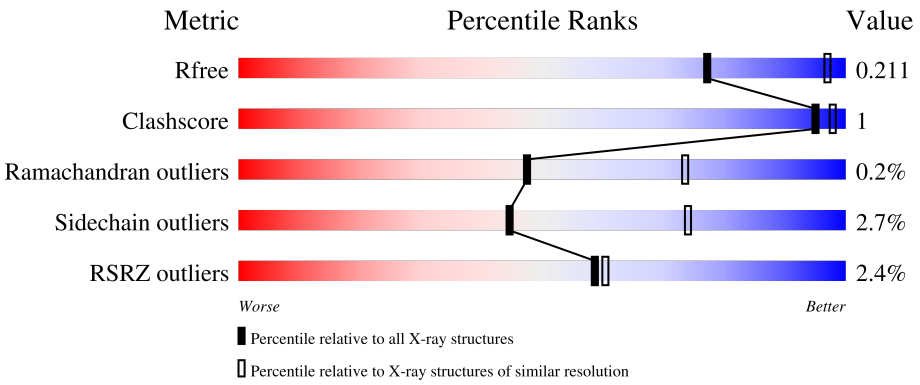
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	250	3% 99%
1	O	250	2% 98%
2	B	258	5% 90% • • 5%
2	P	258	3% 90% • • 5%
3	C	254	6% 90% • • 6%

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

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 50084 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	1906	1214	320	364	8	0	0	0

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	212	1644	1045	281	311	7	0	0	0
11	Y	212	1644	1045	281	311	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	17	ASN	ASP	engineered mutation	UNP P30656
Y	17	ASN	ASP	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
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	1832	1159	315	351	7	0	1	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

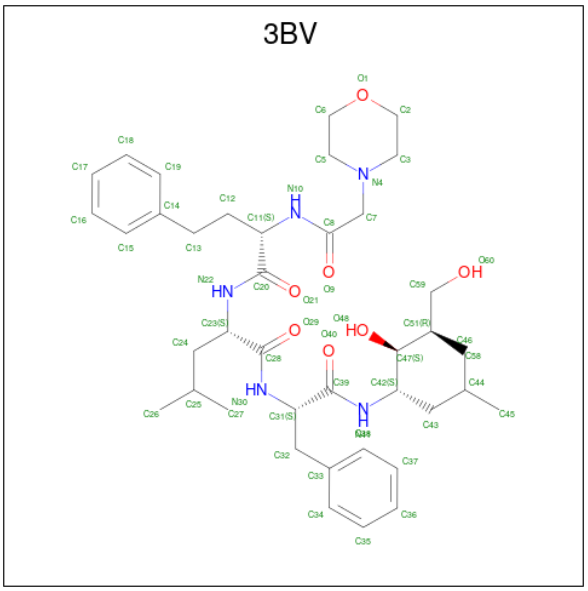
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

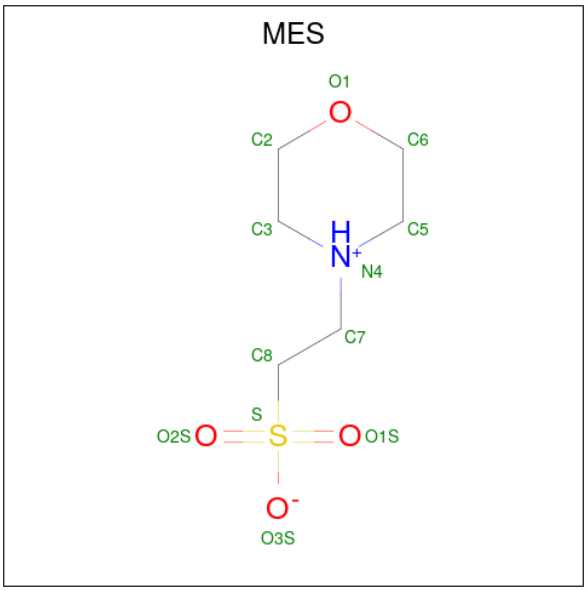
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
16	G	1	1	1	0	0
			Total	Cl		
16	N	1	1	1	0	0
			Total	Cl		
16	U	1	1	1	0	0
			Total	Cl		
16	b	1	1	1	0	0

- 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	H	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
18	K	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
18	V	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	18	18	18	0	0
			Total	O		
19	B	20	20	20	0	0
			Total	O		
19	C	12	12	12	0	0
			Total	O		
19	D	16	16	16	0	0
			Total	O		
19	E	8	8	8	0	0
			Total	O		
19	F	18	18	18	0	0
			Total	O		
19	G	14	14	14	0	0
			Total	O		
19	H	17	17	17	0	0

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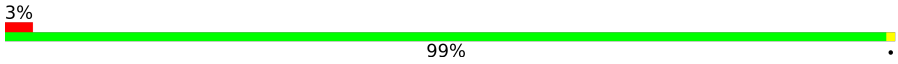
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
19	I	8	8	8	0	0
			Total	O		
19	J	15	15	15	0	0
			Total	O		
19	K	13	13	13	0	0
			Total	O		
19	L	14	14	14	0	0
			Total	O		
19	M	28	28	28	0	0
			Total	O		
19	N	14	14	14	0	0
			Total	O		
19	O	15	15	15	0	0
			Total	O		
19	P	15	15	15	0	0
			Total	O		
19	Q	11	11	11	0	0
			Total	O		
19	R	10	10	10	0	0
			Total	O		
19	S	8	8	8	0	0
			Total	O		
19	T	11	11	11	0	0
			Total	O		
19	U	18	18	18	0	0
			Total	O		
19	V	22	22	22	0	0
			Total	O		
19	W	11	11	11	0	0
			Total	O		
19	X	12	12	12	0	0
			Total	O		
19	Y	10	10	10	0	0
			Total	O		
19	Z	13	13	13	0	0
			Total	O		
19	a	20	20	20	0	0
			Total	O		
19	b	18	18	18	0	0

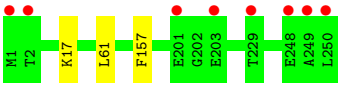
3 Residue-property plots (i)

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

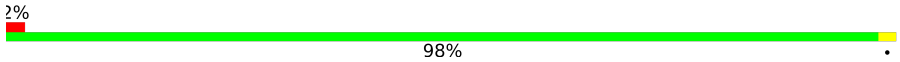
Chain A:





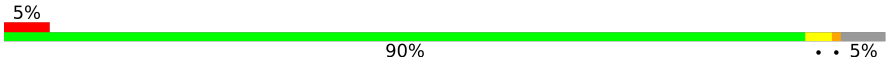
• Molecule 1: Proteasome subunit alpha type-2

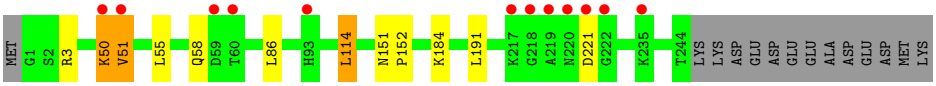
Chain O:



• Molecule 2: Proteasome subunit alpha type-3

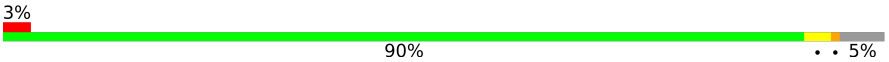
Chain B:

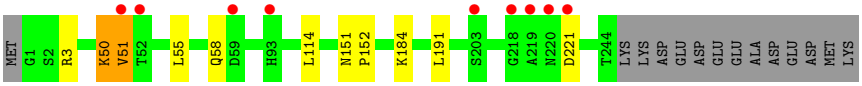




• Molecule 2: Proteasome subunit alpha type-3

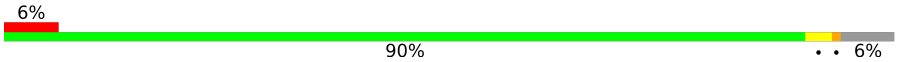
Chain P:

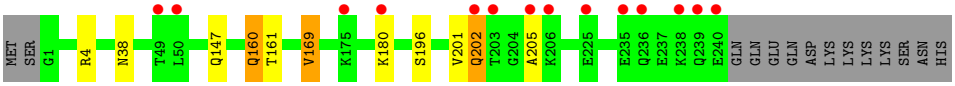




• Molecule 3: Proteasome subunit alpha type-4

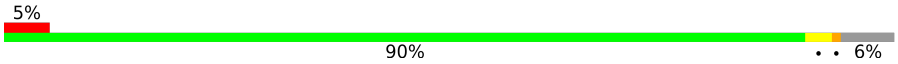
Chain C:

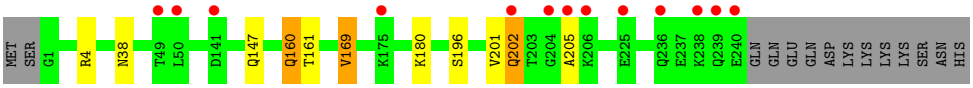




• Molecule 3: Proteasome subunit alpha type-4

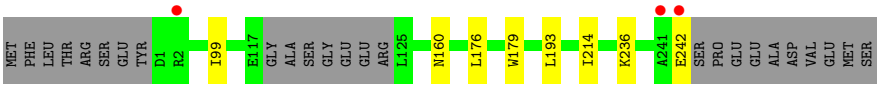
Chain Q:





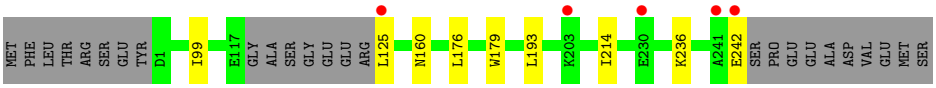
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



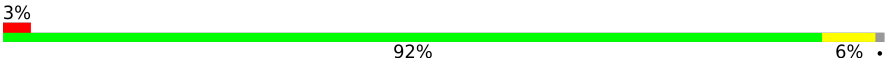
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



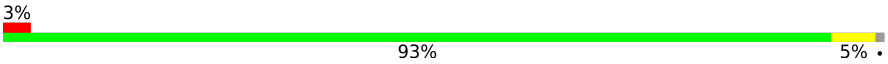
• Molecule 5: Proteasome subunit alpha type-6

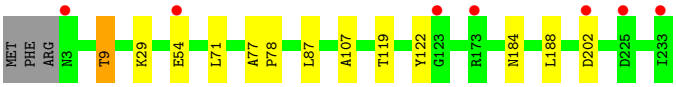
Chain E:



• Molecule 5: Proteasome subunit alpha type-6

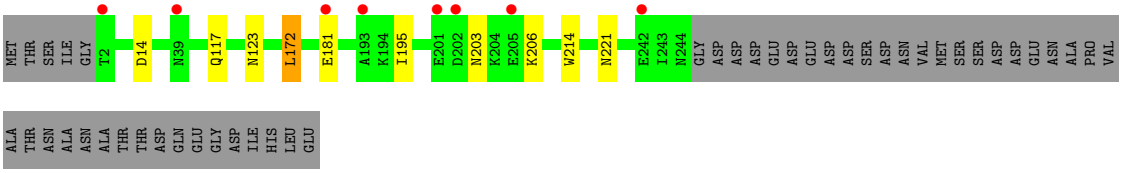
Chain S:





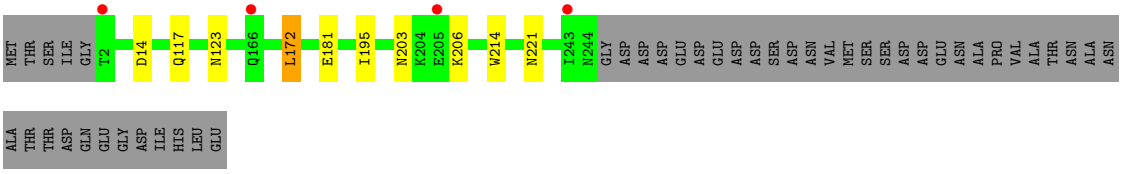
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



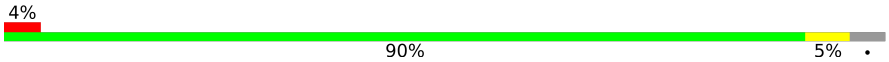
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



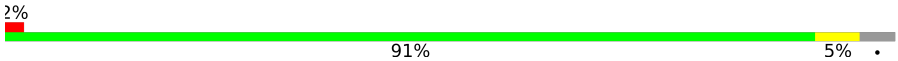
• Molecule 7: Proteasome subunit alpha type-1

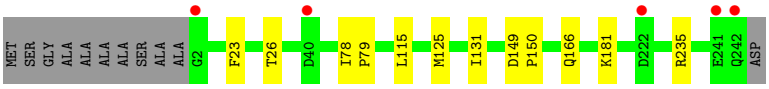
Chain G:



• Molecule 7: Proteasome subunit alpha type-1

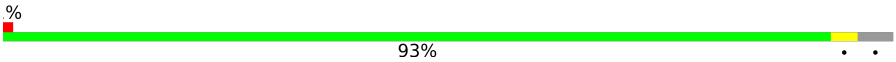
Chain U:

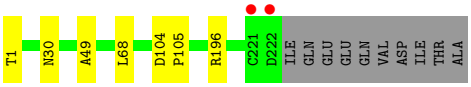




• Molecule 8: Proteasome subunit beta type-2

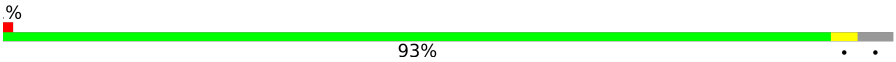
Chain H:

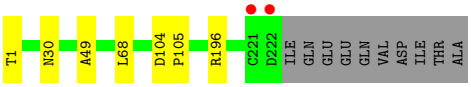




• Molecule 8: Proteasome subunit beta type-2

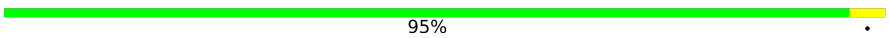
Chain V:





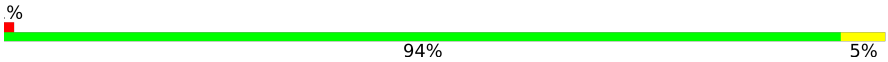
• Molecule 9: Proteasome subunit beta type-3

Chain I:



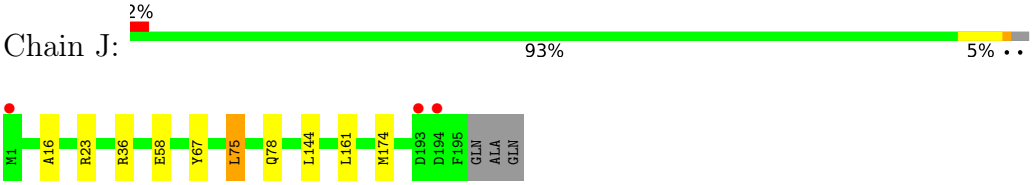
• Molecule 9: Proteasome subunit beta type-3

Chain W:



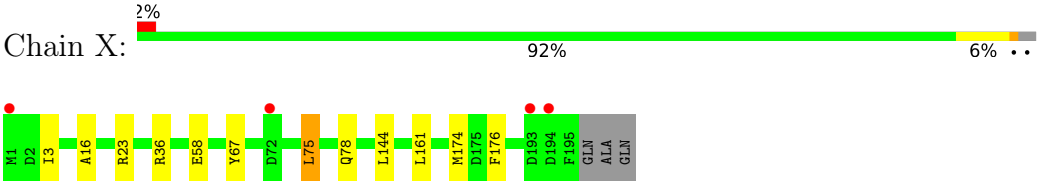
• Molecule 10: Proteasome subunit beta type-4

Chain J:



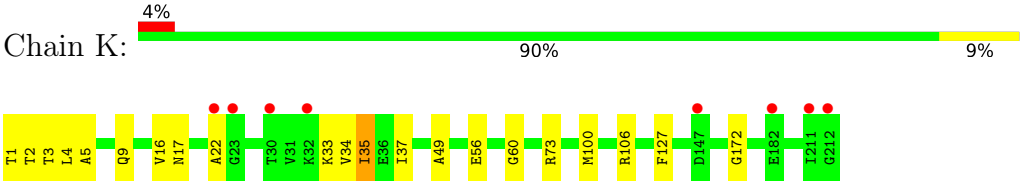
• Molecule 10: Proteasome subunit beta type-4

Chain X:



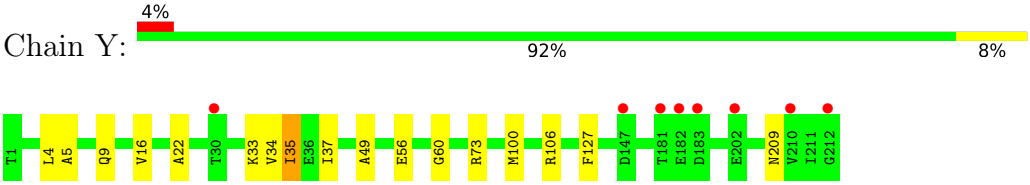
• Molecule 11: Proteasome subunit beta type-5

Chain K:



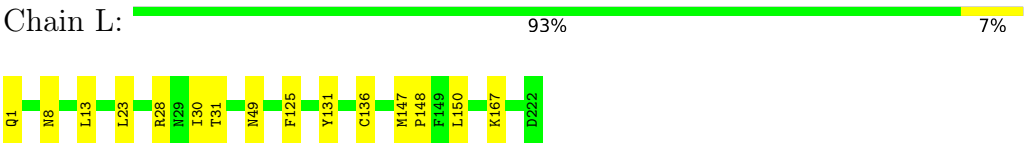
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



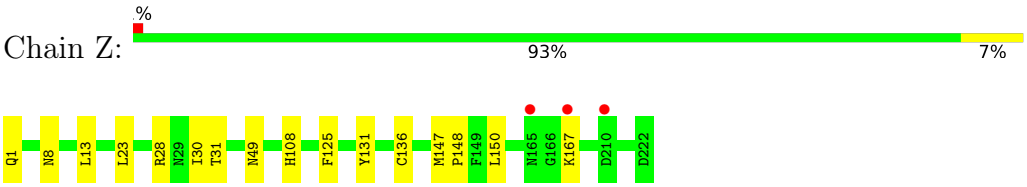
• Molecule 12: Proteasome subunit beta type-6

Chain L:



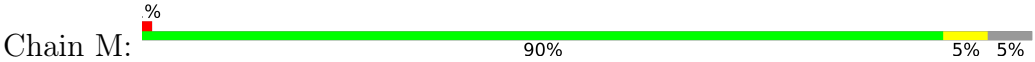
• Molecule 12: Proteasome subunit beta type-6

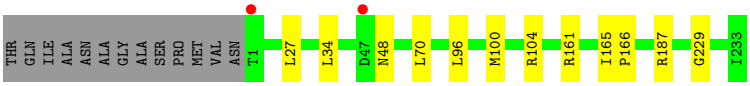
Chain Z:



• Molecule 13: Proteasome subunit beta type-7

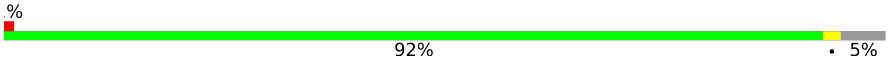
Chain M:

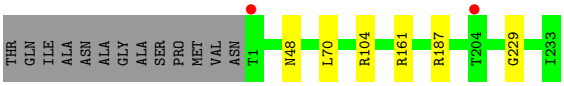




• Molecule 13: Proteasome subunit beta type-7

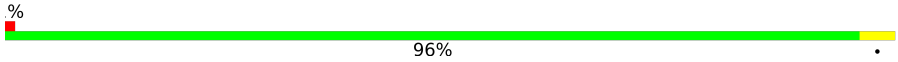
Chain a:

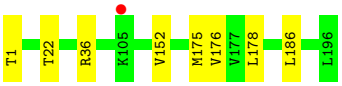




• Molecule 14: Proteasome subunit beta type-1

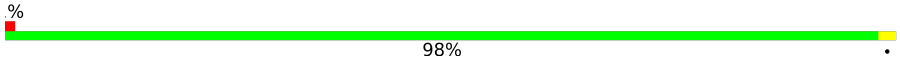
Chain N:

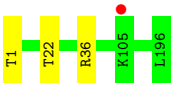




• Molecule 14: Proteasome subunit beta type-1

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	134.33Å 300.47Å 144.29Å 90.00° 112.69° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.4 (15.00-2.70) 97.4 (15.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.189 , 0.208 0.193 , 0.211	Depositor DCC
R_{free} test set	13930 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	55.0	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.0	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	50084	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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, CL, 3BV, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.26	0/1952	0.46	0/2642
1	O	0.26	0/1952	0.46	0/2642
2	B	0.25	0/1934	0.48	0/2618
2	P	0.25	0/1934	0.48	0/2618
3	C	0.26	0/1910	0.50	0/2586
3	Q	0.26	0/1910	0.50	0/2586
4	D	0.25	0/1837	0.46	0/2475
4	R	0.25	0/1837	0.46	0/2475
5	E	0.25	0/1800	0.46	0/2433
5	S	0.25	0/1800	0.46	0/2433
6	F	0.26	0/1932	0.45	0/2609
6	T	0.26	0/1932	0.45	0/2609
7	G	0.26	0/1945	0.47	0/2634
7	U	0.26	0/1944	0.47	0/2632
8	H	0.26	0/1715	0.52	1/2326 (0.0%)
8	V	0.27	0/1715	0.53	1/2326 (0.0%)
9	I	0.29	0/1611	0.54	0/2174
9	W	0.29	0/1611	0.53	0/2174
10	J	0.25	0/1589	0.48	0/2142
10	X	0.25	0/1589	0.48	0/2142
11	K	0.27	0/1681	0.52	0/2274
11	Y	0.26	0/1681	0.52	0/2274
12	L	0.28	0/1795	0.51	0/2420
12	Z	0.28	0/1795	0.51	0/2420
13	M	0.27	0/1855	0.54	0/2514
13	a	0.27	0/1866	0.54	0/2528
14	N	0.26	0/1541	0.52	1/2087 (0.0%)
14	b	0.26	0/1541	0.52	1/2087 (0.0%)
All	All	0.26	0/50204	0.49	4/67880 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	V	1	THR	N-CA-C	6.14	127.58	111.00
14	N	1	THR	N-CA-C	5.94	127.04	111.00
8	H	1	THR	N-CA-C	5.83	126.74	111.00
14	b	1	THR	N-CA-C	5.69	126.36	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	0	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	4	0
2	P	1904	0	1904	3	0
3	C	1881	0	1895	5	0
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	1	0
4	R	1813	0	1797	1	0
5	E	1773	0	1775	5	0
5	S	1773	0	1775	4	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	5	0
7	U	1906	0	1901	4	0
8	H	1684	0	1685	2	0
8	V	1684	0	1685	2	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	5	0
10	J	1561	0	1569	3	0
10	X	1561	0	1569	4	0
11	K	1644	0	1595	13	0
11	Y	1644	0	1595	11	0
12	L	1757	0	1711	6	0
12	Z	1757	0	1711	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1824	0	1832	3	0
13	a	1832	0	1845	0	0
14	N	1512	0	1478	3	0
14	b	1512	0	1478	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	Z	1	0	0	0	0
15	b	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	3	0
17	K	52	0	59	7	0
17	N	52	0	58	1	0
17	V	52	0	59	4	0
17	Y	52	0	59	7	0
17	b	52	0	59	0	0
18	H	12	0	13	1	0
18	K	12	0	13	0	0
18	V	12	0	13	1	0
18	Y	12	0	13	0	0
19	A	18	0	0	0	0
19	B	20	0	0	0	0
19	C	12	0	0	0	0
19	D	16	0	0	0	0
19	E	8	0	0	0	0
19	F	18	0	0	0	0
19	G	14	0	0	1	0
19	H	17	0	0	0	0
19	I	8	0	0	0	0
19	J	15	0	0	0	0
19	K	13	0	0	0	0
19	L	14	0	0	0	0
19	M	28	0	0	0	0
19	N	14	0	0	0	0
19	O	15	0	0	0	0
19	P	15	0	0	0	0
19	Q	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	R	10	0	0	0	0
19	S	8	0	0	0	0
19	T	11	0	0	0	0
19	U	18	0	0	0	0
19	V	22	0	0	0	0
19	W	11	0	0	0	0
19	X	12	0	0	0	0
19	Y	10	0	0	0	0
19	Z	13	0	0	0	0
19	a	20	0	0	0	0
19	b	18	0	0	0	0
All	All	50084	0	49474	111	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 (111) 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)
17:V:301:3BV:O60	18:V:302:MES:O1S	2.03	0.77
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.81	0.61
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.82	0.61
14:N:152:VAL:HA	14:N:175:MET:HE1	1.83	0.60
17:Y:301:3BV:O9	17:Y:301:3BV:H2	2.03	0.59
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.85	0.59
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.85	0.58
17:K:301:3BV:O9	17:K:301:3BV:H2	2.03	0.57
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.41	0.55
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.41	0.54
3:C:201:VAL:O	3:C:202:GLN:CB	2.57	0.53
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.57	0.52
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.92	0.51
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.50
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.93	0.50
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.93	0.50
17:N:201:3BV:H21	17:N:201:3BV:H17	1.77	0.50
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.42	0.49
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.95	0.49
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.43	0.49
7:U:23:PHE:O	7:U:26:THR:HB	2.12	0.49
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.95	0.49
8:H:49:ALA:HA	17:H:301:3BV:H50	1.95	0.48
11:K:5:ALA:HB3	11:K:100:MET:CE	2.43	0.48
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.96	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.95	0.48
11:Y:35:ILE:HG21	11:Y:56:GLU:HB3	1.96	0.48
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.96	0.48
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.43	0.48
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.44	0.48
17:H:301:3BV:H2	17:H:301:3BV:O9	2.14	0.47
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.95	0.47
11:K:35:ILE:HG21	11:K:56:GLU:HB3	1.95	0.47
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.97	0.47
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.43	0.47
11:K:49:ALA:HA	17:K:301:3BV:H50	1.98	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.96	0.46
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.46
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.96	0.46
17:K:301:3BV:H44	17:K:301:3BV:H53	1.74	0.46
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.98	0.46
11:Y:49:ALA:HA	17:Y:301:3BV:H50	1.97	0.46
13:M:96:LEU:O	13:M:100:MET:HG2	2.16	0.45
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.49	0.45
11:Y:33:LYS:HZ1	17:Y:301:3BV:H58	1.82	0.44
11:K:22:ALA:HB1	17:K:301:3BV:H1	1.98	0.44
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.44
7:G:122:ARG:HD2	19:G:412:HOH:O	2.17	0.44
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.00	0.44
7:G:78:ILE:N	7:G:79:PRO:CD	2.81	0.44
12:L:8:ASN:HA	12:L:30:ILE:O	2.18	0.44
17:K:301:3BV:H62	17:K:301:3BV:H55	1.66	0.43
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.00	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.48	0.43
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.48	0.43
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.01	0.43
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.18	0.43
2:B:50:LYS:O	2:B:51:VAL:C	2.57	0.43
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.83	0.43
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.54	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.54	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:3:ARG:NH1	5:S:122:TYR:OH	2.52	0.43
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.43
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.84	0.42
3:C:201:VAL:HG13	3:C:202:GLN:N	2.34	0.42
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.01	0.42
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.50	0.42
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.01	0.42
11:Y:22:ALA:HB1	17:Y:301:3BV:H1	1.99	0.42
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.34	0.42
12:L:147:MET:N	12:L:148:PRO:HD2	2.34	0.42
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.00	0.42
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.54	0.42
2:P:50:LYS:O	2:P:51:VAL:C	2.58	0.42
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.50	0.42
2:B:3:ARG:NH1	5:E:122:TYR:OH	2.52	0.42
8:V:49:ALA:HA	17:V:301:3BV:H50	2.02	0.42
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	2.02	0.42
12:L:28:ARG:HG2	12:L:30:ILE:HG23	2.02	0.42
5:E:9:THR:HG21	5:E:119:THR:HA	2.02	0.42
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.34	0.42
14:N:175:MET:HB2	14:N:186:LEU:HB2	2.01	0.41
11:K:16:VAL:HG21	11:K:34:VAL:HG23	2.02	0.41
12:Z:28:ARG:HG2	12:Z:30:ILE:HG23	2.02	0.41
7:G:26:THR:HG21	7:G:131:ILE:HD12	2.01	0.41
11:K:17:ASN:HD22	11:K:172:GLY:H	1.68	0.41
2:B:86:LEU:HB3	2:B:114:LEU:HD21	2.02	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
11:K:1:THR:HG22	11:K:2:THR:N	2.35	0.41
11:K:33:LYS:HZ1	17:K:301:3BV:H58	1.84	0.41
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.02	0.41
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	2.02	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
1:O:119:GLN:O	1:O:122:THR:HB	2.21	0.41
17:V:301:3BV:O60	17:V:301:3BV:O48	2.35	0.41
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.56	0.41
17:Y:301:3BV:O9	17:Y:301:3BV:C5	2.68	0.41
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.52	0.41
11:Y:33:LYS:NZ	17:Y:301:3BV:H58	2.36	0.41
17:V:301:3BV:H19	9:W:125:LEU:HD13	2.02	0.40
17:Y:301:3BV:O1	12:Z:108:HIS:HE1	2.04	0.40
11:K:33:LYS:NZ	17:K:301:3BV:H58	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:9:THR:HG21	5:S:119:THR:HA	2.02	0.40
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.53	0.40
11:K:1:THR:CG2	11:K:3:THR:HG23	2.51	0.40
3:C:161:THR:HG21	3:C:169:VAL:HG13	2.02	0.40
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.56	0.40
17:H:301:3BV:O60	18:H:302:MES:O1S	2.40	0.40
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
2	B	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	19	43
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	19	43
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	19	43
3	Q	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	19	43
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	234 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	4 (2%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	219 (95%)	11 (5%)	1 (0%)	34	60
13	a	232/246 (94%)	220 (95%)	11 (5%)	1 (0%)	34	60
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	6277/6614 (95%)	6102 (97%)	165 (3%)	10 (0%)	47	73

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
3	C	205	ALA
3	Q	205	ALA
2	B	221	ASP
2	P	221	ASP
13	M	229	GLY
13	a	229	GLY

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	67	86
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	86
2	B	203/216 (94%)	197 (97%)	6 (3%)	41	70
2	P	203/216 (94%)	197 (97%)	6 (3%)	41	70
3	C	212/226 (94%)	206 (97%)	6 (3%)	43	73
3	Q	212/226 (94%)	206 (97%)	6 (3%)	43	73
4	D	194/215 (90%)	188 (97%)	6 (3%)	40	69
4	R	194/215 (90%)	187 (96%)	7 (4%)	35	64
5	E	190/193 (98%)	183 (96%)	7 (4%)	34	63
5	S	190/193 (98%)	183 (96%)	7 (4%)	34	63
6	F	201/239 (84%)	192 (96%)	9 (4%)	27	55
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	55
7	G	206/210 (98%)	201 (98%)	5 (2%)	49	77
7	U	206/210 (98%)	201 (98%)	5 (2%)	49	77
8	H	181/190 (95%)	178 (98%)	3 (2%)	60	84
8	V	181/190 (95%)	178 (98%)	3 (2%)	60	84
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	84
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	84
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	71
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	71
11	K	169/169 (100%)	164 (97%)	5 (3%)	41	70
11	Y	169/169 (100%)	164 (97%)	5 (3%)	41	70
12	L	185/185 (100%)	179 (97%)	6 (3%)	39	68
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39	68
13	M	199/208 (96%)	194 (98%)	5 (2%)	47	76
13	a	200/208 (96%)	195 (98%)	5 (2%)	47	76
14	N	162/162 (100%)	160 (99%)	2 (1%)	71	88
14	b	162/162 (100%)	160 (99%)	2 (1%)	71	88
All	All	5313/5540 (96%)	5170 (97%)	143 (3%)	44	74

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
2	B	50	LYS
2	B	55	LEU
2	B	58	GLN
2	B	114	LEU
2	B	184	LYS
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
4	D	99	ILE
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP
6	F	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	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
8	H	30	ASN

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Mol	Chain	Res	Type
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	23	ARG
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	73	ARG
11	K	106	ARG
12	L	1	GLN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	136	CYS
12	L	167	LYS
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	22	THR
14	N	36	ARG
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	55	LEU
2	P	58	GLN
2	P	114	LEU
2	P	184	LYS
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL

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Mol	Chain	Res	Type
3	Q	180	LYS
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	14	ASP
6	T	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	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
8	V	30	ASN
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

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Mol	Chain	Res	Type
11	Y	35	ILE
11	Y	73	ARG
11	Y	106	ARG
12	Z	1	GLN
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	136	CYS
12	Z	167	LYS
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	22	THR
14	b	36	ARG

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
3	C	38	ASN
3	C	147	GLN
3	C	160	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	120	GLN
5	E	184	ASN
6	F	86	ASN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	117	GLN
7	G	121	GLN
8	H	66	HIS

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Mol	Chain	Res	Type
8	H	86	HIS
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	70	ASN
12	L	108	HIS
12	L	158	ASN
12	L	159	GLN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	91	HIS
4	R	146	GLN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	184	ASN
6	T	86	ASN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	117	GLN
7	U	121	GLN
8	V	86	HIS
10	X	55	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	70	ASN

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Mol	Chain	Res	Type
12	Z	108	HIS
12	Z	158	ASN
12	Z	159	GLN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 12 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
17	3BV	b	201	14	54,54,54	1.42	4 (7%)	68,71,71	1.42	5 (7%)
17	3BV	V	301	8	54,54,54	1.32	3 (5%)	68,71,71	1.55	8 (11%)
18	MES	K	303	-	12,12,12	2.14	1 (8%)	14,16,16	1.36	3 (21%)
18	MES	Y	302	-	12,12,12	2.14	1 (8%)	14,16,16	1.30	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	3BV	H	301	8	54,54,54	1.35	3 (5%)	68,71,71	1.42	6 (8%)
18	MES	V	302	-	12,12,12	2.14	1 (8%)	14,16,16	1.50	3 (21%)
17	3BV	N	201	14	54,54,54	1.40	4 (7%)	68,71,71	1.54	9 (13%)
18	MES	H	302	-	12,12,12	2.12	1 (8%)	14,16,16	1.42	3 (21%)
17	3BV	K	301	11	54,54,54	1.24	3 (5%)	68,71,71	1.83	14 (20%)
17	3BV	Y	301	11	54,54,54	1.23	3 (5%)	68,71,71	1.82	13 (19%)

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
17	3BV	b	201	14	-	11/59/67/67	0/3/3/3
17	3BV	V	301	8	-	14/59/67/67	0/3/3/3
18	MES	K	303	-	-	0/6/14/14	0/1/1/1
18	MES	Y	302	-	-	0/6/14/14	0/1/1/1
17	3BV	H	301	8	-	13/59/67/67	0/3/3/3
18	MES	V	302	-	-	0/6/14/14	0/1/1/1
17	3BV	N	201	14	-	11/59/67/67	0/3/3/3
18	MES	H	302	-	-	5/6/14/14	0/1/1/1
17	3BV	K	301	11	-	7/59/67/67	0/3/3/3
17	3BV	Y	301	11	-	7/59/67/67	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	302	MES	C8-S	-7.08	1.67	1.77
18	K	303	MES	C8-S	-7.02	1.67	1.77
18	Y	302	MES	C8-S	-7.01	1.67	1.77
18	H	302	MES	C8-S	-6.99	1.67	1.77
17	b	201	3BV	C32-C33	-6.29	1.36	1.51
17	H	301	3BV	C32-C33	-6.13	1.36	1.51
17	V	301	3BV	C32-C33	-6.08	1.36	1.51
17	N	201	3BV	C32-C33	-5.91	1.37	1.51
17	Y	301	3BV	C51-C47	5.17	1.62	1.53
17	K	301	3BV	C51-C47	5.05	1.62	1.53
17	K	301	3BV	C32-C33	-4.99	1.39	1.51
17	Y	301	3BV	C32-C33	-4.90	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	201	3BV	C13-C14	-4.75	1.37	1.51
17	N	201	3BV	C13-C14	-4.48	1.38	1.51
17	H	301	3BV	C13-C14	-4.43	1.38	1.51
17	V	301	3BV	C13-C14	-4.29	1.39	1.51
17	N	201	3BV	C51-C47	4.08	1.60	1.53
17	K	301	3BV	C13-C14	-4.00	1.40	1.51
17	Y	301	3BV	C13-C14	-3.98	1.40	1.51
17	b	201	3BV	C51-C47	3.57	1.59	1.53
17	N	201	3BV	O48-C47	-2.98	1.36	1.43
17	V	301	3BV	O48-C47	-2.41	1.37	1.43
17	H	301	3BV	C51-C47	2.32	1.57	1.53
17	b	201	3BV	O48-C47	-2.09	1.38	1.43

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	201	3BV	C43-C42-N41	-7.47	100.52	110.18
17	V	301	3BV	C43-C42-N41	-7.17	100.91	110.18
17	b	201	3BV	C43-C42-N41	-7.12	100.97	110.18
17	H	301	3BV	C43-C42-N41	-6.94	101.20	110.18
17	Y	301	3BV	C43-C42-N41	-6.62	101.63	110.18
17	K	301	3BV	C43-C42-N41	-6.60	101.65	110.18
17	V	301	3BV	C58-C51-C59	-5.18	103.07	109.88
17	N	201	3BV	C58-C51-C59	-4.96	103.36	109.88
17	Y	301	3BV	C33-C32-C31	-4.76	100.25	113.39
17	K	301	3BV	C33-C32-C31	-4.76	100.27	113.39
17	Y	301	3BV	C58-C51-C59	-4.67	103.74	109.88
17	K	301	3BV	C58-C51-C59	-4.54	103.91	109.88
17	K	301	3BV	C25-C24-C23	-4.29	103.64	115.43
17	Y	301	3BV	C25-C24-C23	-4.23	103.79	115.43
17	H	301	3BV	C58-C51-C59	-3.75	104.96	109.88
18	V	302	MES	O1S-S-C8	3.67	111.34	106.92
17	K	301	3BV	C7-N4-C5	3.65	116.75	111.09
17	Y	301	3BV	C7-N4-C5	3.63	116.72	111.09
17	K	301	3BV	C44-C43-C42	-3.60	108.67	115.84
17	Y	301	3BV	C44-C43-C42	-3.59	108.70	115.84
17	K	301	3BV	C6-C5-N4	-3.52	104.77	110.10
17	H	301	3BV	C3-N4-C5	3.34	116.34	108.83
17	V	301	3BV	C12-C11-N10	-3.28	104.23	110.88
17	Y	301	3BV	C6-C5-N4	-3.27	105.14	110.10
18	H	302	MES	O2S-S-C8	3.19	110.76	106.92
17	Y	301	3BV	O1-C6-C5	-3.18	104.78	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	K	301	3BV	C13-C12-C11	-3.17	106.95	113.21
17	Y	301	3BV	C13-C12-C11	-3.16	106.98	113.21
17	K	301	3BV	O1-C6-C5	-3.06	105.06	111.80
18	K	303	MES	O3S-S-C8	3.06	110.72	105.77
17	N	201	3BV	C7-N4-C5	-2.91	106.58	111.09
18	Y	302	MES	O3S-S-C8	2.91	110.47	105.77
17	N	201	3BV	C44-C43-C42	2.91	121.63	115.84
17	b	201	3BV	C58-C51-C59	-2.89	106.08	109.88
17	V	301	3BV	C3-N4-C5	2.87	115.28	108.83
17	K	301	3BV	O1-C2-C3	-2.85	105.51	111.80
17	Y	301	3BV	O1-C2-C3	-2.79	105.65	111.80
17	N	201	3BV	C12-C11-C20	-2.78	103.71	110.20
17	H	301	3BV	C12-C11-N10	-2.68	105.45	110.88
18	H	302	MES	O1S-S-C8	2.66	110.12	106.92
18	V	302	MES	O3S-S-C8	2.60	109.97	105.77
17	K	301	3BV	C3-N4-C5	2.56	114.58	108.83
17	V	301	3BV	C12-C11-C20	-2.47	104.43	110.20
17	Y	301	3BV	C3-N4-C5	2.46	114.38	108.83
17	K	301	3BV	C7-N4-C3	-2.40	107.37	111.09
17	H	301	3BV	C44-C43-C42	2.38	120.57	115.84
17	V	301	3BV	C33-C32-C31	-2.37	106.86	113.39
17	Y	301	3BV	C12-C13-C14	-2.34	105.06	113.18
17	K	301	3BV	C12-C13-C14	-2.29	105.23	113.18
17	Y	301	3BV	C7-N4-C3	-2.24	107.63	111.09
17	b	201	3BV	C7-N4-C3	-2.22	107.65	111.09
17	b	201	3BV	C12-C11-N10	-2.22	106.38	110.88
17	b	201	3BV	C24-C23-N22	-2.21	105.49	110.58
17	V	301	3BV	C2-C3-N4	2.21	113.45	110.10
17	N	201	3BV	C12-C11-N10	-2.18	106.46	110.88
18	V	302	MES	O2S-S-C8	2.17	109.53	106.92
17	H	301	3BV	C20-C11-N10	-2.17	105.25	111.16
17	V	301	3BV	C25-C24-C23	-2.16	109.48	115.43
18	K	303	MES	O2S-S-C8	2.15	109.51	106.92
18	Y	302	MES	O2S-S-C8	2.15	109.50	106.92
17	N	201	3BV	C3-N4-C5	2.13	113.63	108.83
17	N	201	3BV	C12-C13-C14	-2.10	105.88	113.18
18	K	303	MES	O1S-S-C8	2.08	109.42	106.92
17	N	201	3BV	O1-C6-C5	-2.05	107.27	111.80
17	K	301	3BV	C39-C31-N30	-2.02	105.65	111.16
18	H	302	MES	O3S-S-C8	2.01	109.02	105.77

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	3BV	N41-C42-C43-C44
17	H	301	3BV	C42-C47-C51-C58
17	K	301	3BV	C8-C7-N4-C5
17	K	301	3BV	C47-C42-C43-C44
17	N	201	3BV	N41-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	C47-C42-C43-C44
17	V	301	3BV	C42-C47-C51-C58
17	V	301	3BV	C42-C47-C51-C59
17	Y	301	3BV	C8-C7-N4-C5
17	Y	301	3BV	C47-C42-C43-C44
17	b	201	3BV	N41-C42-C43-C44
17	b	201	3BV	C42-C47-C51-C58
17	b	201	3BV	C42-C47-C51-C59
17	H	301	3BV	N10-C11-C12-C13
17	H	301	3BV	C20-C11-C12-C13
17	H	301	3BV	C42-C43-C44-C45
17	H	301	3BV	C42-C43-C44-C46
18	H	302	MES	C7-C8-S-O3S
17	H	301	3BV	O48-C47-C51-C58
17	V	301	3BV	O48-C47-C51-C59
17	b	201	3BV	O48-C47-C51-C58
17	V	301	3BV	C42-C43-C44-C46
17	N	201	3BV	O48-C47-C51-C59
17	V	301	3BV	O48-C47-C51-C58
17	b	201	3BV	O48-C47-C51-C59
17	N	201	3BV	N4-C7-C8-O9
17	N	201	3BV	N4-C7-C8-N10
18	H	302	MES	C8-C7-N4-C3
17	K	301	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	N10-C11-C20-O21
17	b	201	3BV	N30-C31-C39-O40
17	V	301	3BV	N10-C11-C12-C13
17	N	201	3BV	C42-C43-C44-C46
17	K	301	3BV	C42-C43-C44-C46
17	b	201	3BV	N30-C31-C39-N41
17	Y	301	3BV	C42-C43-C44-C46
17	K	301	3BV	C8-C7-N4-C3

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Mol	Chain	Res	Type	Atoms
17	Y	301	3BV	C8-C7-N4-C3
17	b	201	3BV	N10-C11-C20-N22
17	V	301	3BV	C42-C43-C44-C45
17	H	301	3BV	C42-C47-C51-C59
18	H	302	MES	C7-C8-S-O1S
18	H	302	MES	C7-C8-S-O2S
17	H	301	3BV	C47-C42-C43-C44
17	N	201	3BV	C47-C42-C43-C44
17	b	201	3BV	C47-C42-C43-C44
17	N	201	3BV	N30-C31-C39-O40
17	N	201	3BV	N30-C31-C39-N41
18	H	302	MES	C8-C7-N4-C5
17	V	301	3BV	N30-C31-C39-O40
17	H	301	3BV	N30-C31-C39-O40
17	H	301	3BV	C12-C13-C14-C15
17	H	301	3BV	C12-C13-C14-C19
17	V	301	3BV	N30-C31-C39-N41
17	H	301	3BV	N30-C31-C39-N41
17	b	201	3BV	C42-C43-C44-C46
17	K	301	3BV	N10-C11-C20-O21
17	Y	301	3BV	N10-C11-C20-O21
17	V	301	3BV	C12-C13-C14-C19
17	K	301	3BV	N41-C42-C47-C51
17	Y	301	3BV	N41-C42-C47-C51
17	V	301	3BV	C12-C13-C14-C15
17	V	301	3BV	N10-C11-C20-O21

There are no ring outliers.

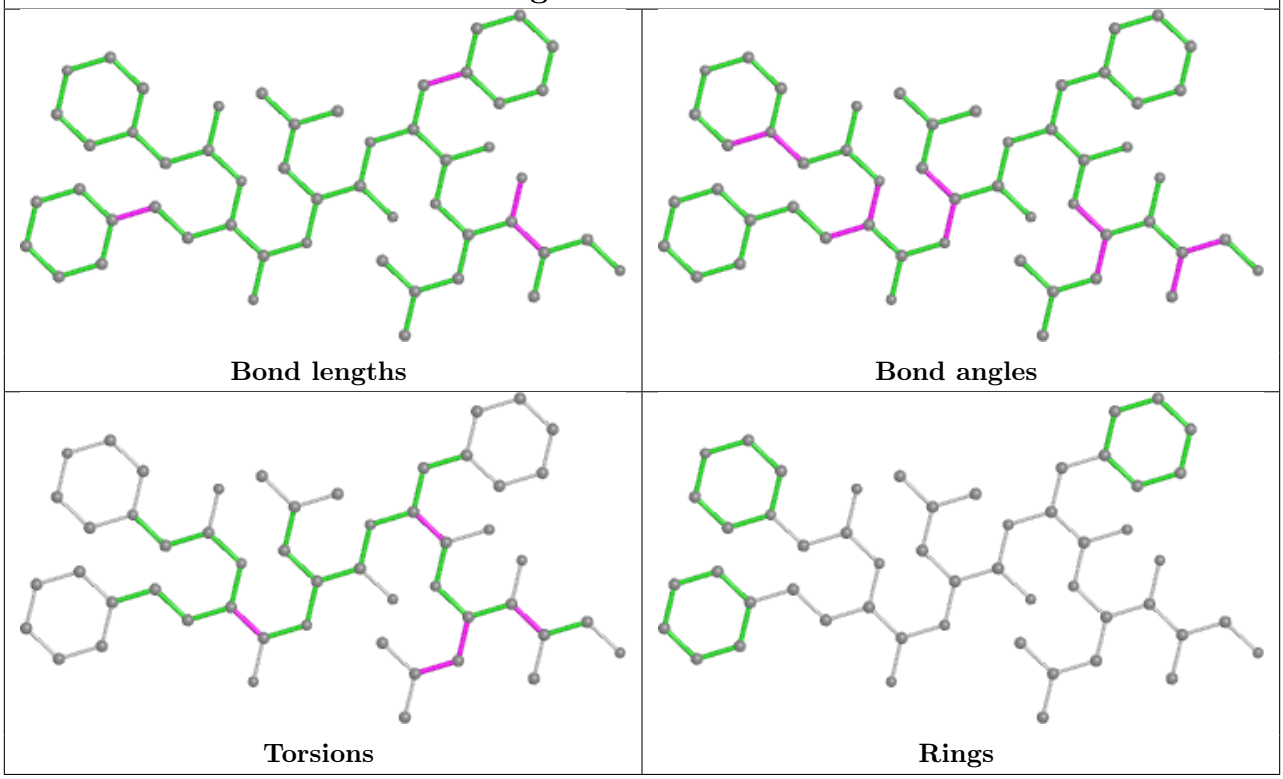
7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	V	301	3BV	4	0
17	H	301	3BV	3	0
18	V	302	MES	1	0
17	N	201	3BV	1	0
18	H	302	MES	1	0
17	K	301	3BV	7	0
17	Y	301	3BV	7	0

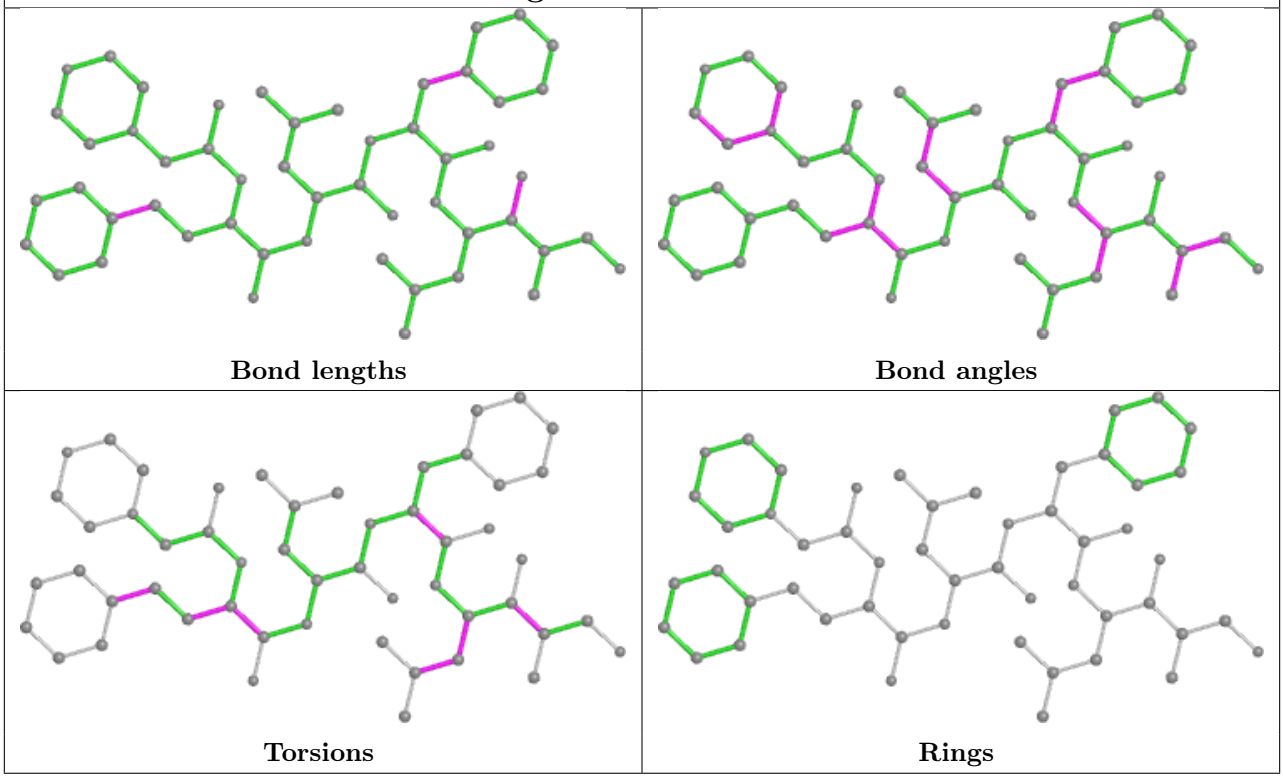
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

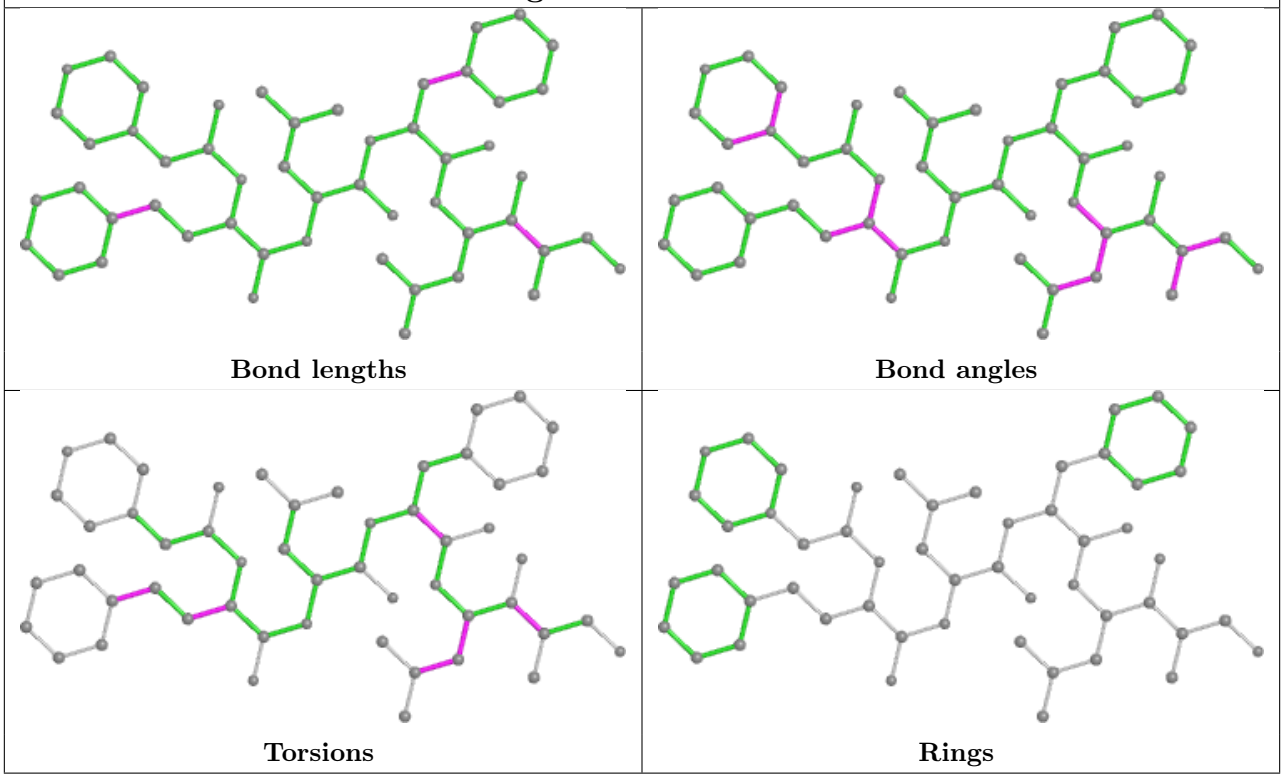
Ligand 3BV b 201



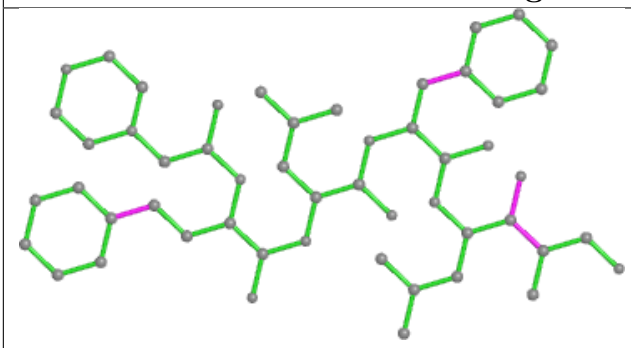
Ligand 3BV V 301



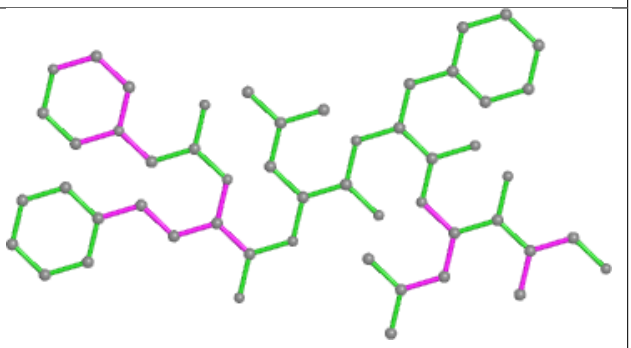
Ligand 3BV H 301



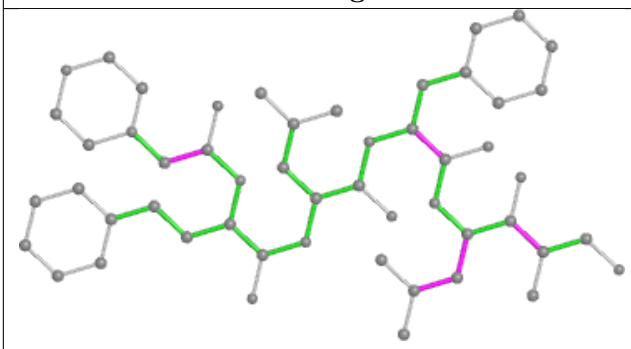
Ligand 3BV N 201



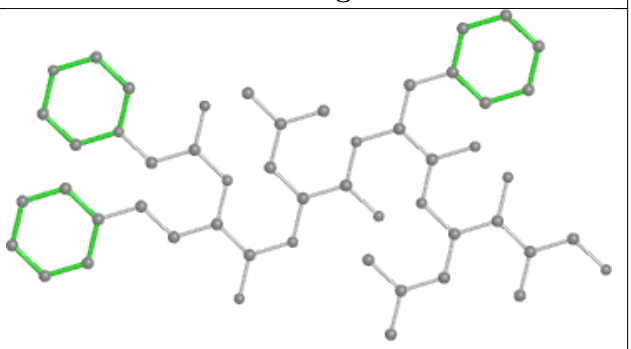
Bond lengths



Bond angles

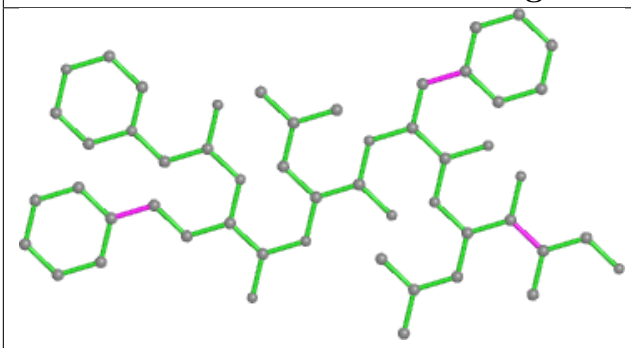


Torsions

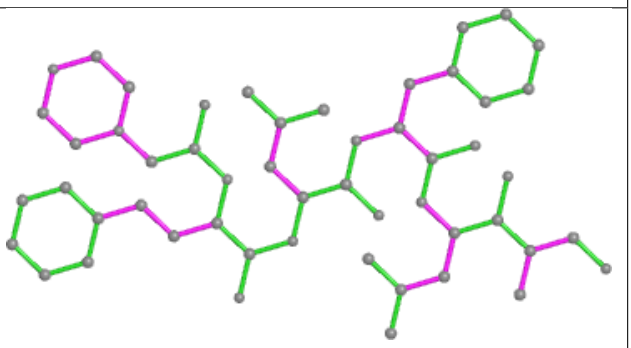


Rings

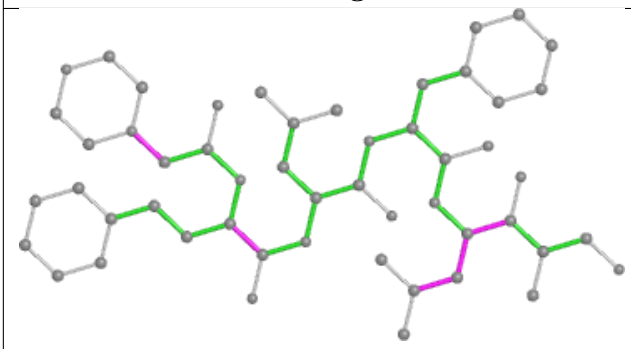
Ligand 3BV K 301



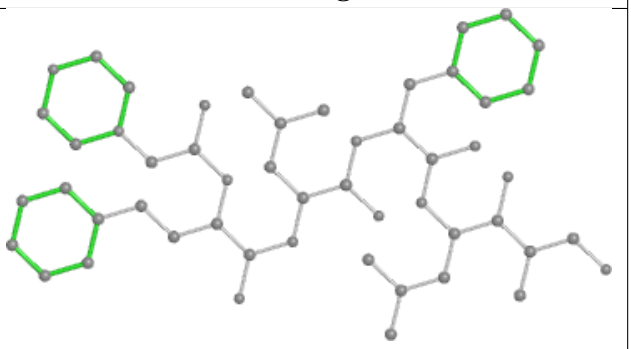
Bond lengths



Bond angles

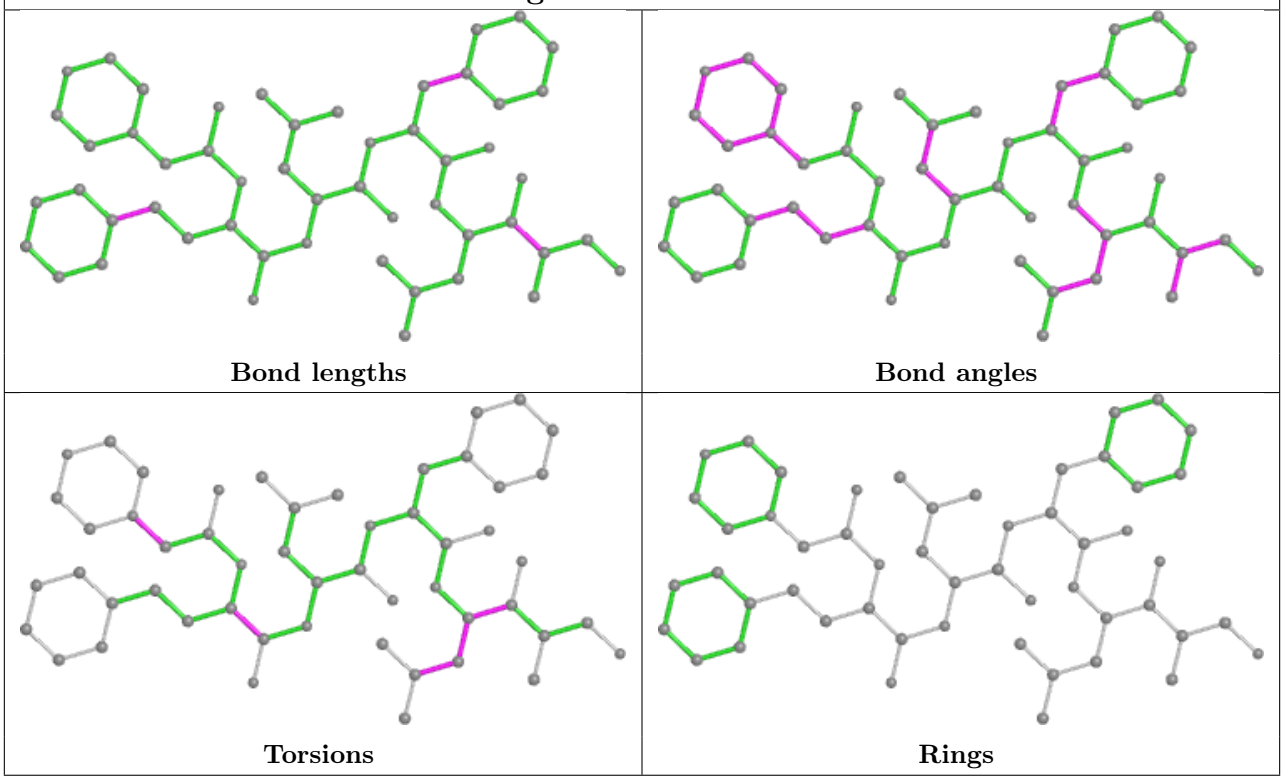


Torsions



Rings

Ligand 3BV Y 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%)	-0.30	8 (3%)	47	48	37, 52, 92, 149	0
1	O	250/250 (100%)	-0.26	6 (2%)	59	60	39, 58, 104, 145	0
2	B	244/258 (94%)	-0.22	12 (4%)	29	28	37, 58, 106, 158	0
2	P	244/258 (94%)	-0.24	9 (3%)	41	41	39, 60, 106, 155	0
3	C	240/254 (94%)	-0.06	14 (5%)	23	22	36, 61, 129, 165	0
3	Q	240/254 (94%)	-0.01	13 (5%)	25	24	42, 69, 144, 181	0
4	D	235/260 (90%)	-0.31	3 (1%)	77	78	38, 61, 91, 136	0
4	R	235/260 (90%)	-0.14	5 (2%)	63	65	51, 70, 107, 147	0
5	E	231/234 (98%)	-0.16	7 (3%)	50	51	42, 64, 104, 144	0
5	S	231/234 (98%)	-0.13	7 (3%)	50	51	45, 70, 113, 144	0
6	F	243/288 (84%)	-0.33	8 (3%)	46	46	38, 59, 108, 136	0
6	T	243/288 (84%)	-0.25	4 (1%)	72	74	39, 67, 121, 160	0
7	G	241/252 (95%)	-0.28	9 (3%)	41	41	36, 55, 97, 150	0
7	U	241/252 (95%)	-0.38	5 (2%)	63	65	32, 55, 89, 130	0
8	H	222/232 (95%)	-0.51	2 (0%)	84	85	37, 50, 88, 123	0
8	V	222/232 (95%)	-0.46	2 (0%)	84	85	36, 52, 89, 129	0
9	I	204/205 (99%)	-0.63	1 (0%)	91	92	35, 52, 82, 103	0
9	W	204/205 (99%)	-0.54	2 (0%)	82	83	34, 53, 80, 106	0
10	J	195/198 (98%)	-0.41	3 (1%)	73	76	34, 53, 84, 119	0
10	X	195/198 (98%)	-0.41	4 (2%)	63	65	36, 55, 81, 127	0
11	K	212/212 (100%)	-0.14	8 (3%)	40	39	43, 63, 95, 119	0
11	Y	212/212 (100%)	-0.12	8 (3%)	40	39	45, 64, 98, 121	0
12	L	222/222 (100%)	-0.47	0	100	100	31, 53, 88, 122	0
12	Z	222/222 (100%)	-0.41	3 (1%)	75	77	35, 55, 91, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.55	2 (0%)	84	85	33, 50, 74, 82	0
13	a	233/246 (94%)	-0.55	2 (0%)	84	85	34, 51, 75, 87	0
14	N	196/196 (100%)	-0.58	1 (0%)	91	92	30, 47, 81, 102	0
14	b	196/196 (100%)	-0.57	1 (0%)	91	92	34, 47, 79, 104	0
All	All	6336/6614 (95%)	-0.33	149 (2%)	59	60	30, 57, 102, 181	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	7.5
10	J	1	MET	7.3
2	B	220	ASN	6.9
2	P	51	VAL	6.8
3	C	206	LYS	6.4
10	X	1	MET	6.4
1	O	1	MET	5.8
2	B	221	ASP	5.5
11	Y	212	GLY	5.3
4	R	241	ALA	5.3
2	P	219	ALA	5.3
9	W	1	SER	5.0
8	V	222	ASP	5.0
5	S	202	ASP	4.9
2	P	220	ASN	4.8
5	E	202	ASP	4.7
2	B	218	GLY	4.7
13	a	1	THR	4.6
3	Q	238	LYS	4.5
2	P	221	ASP	4.3
3	C	238	LYS	4.2
3	C	49	THR	4.2
2	B	219	ALA	4.2
9	I	1	SER	4.1
1	O	250	LEU	4.1
11	K	212	GLY	4.1
3	C	239	GLN	4.1
3	C	235	GLU	4.1
8	H	222	ASP	3.9
3	Q	239	GLN	3.9
3	C	225	GLU	3.7
6	F	202	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
10	X	194	ASP	3.7
3	Q	240	GLU	3.7
3	Q	206	LYS	3.6
2	P	218	GLY	3.6
10	X	193	ASP	3.5
11	K	23	GLY	3.4
11	K	147	ASP	3.4
3	Q	50	LEU	3.4
7	G	179	LYS	3.3
2	B	51	VAL	3.3
3	Q	205	ALA	3.2
10	J	194	ASP	3.2
11	Y	147	ASP	3.2
5	E	233	ILE	3.2
2	B	59	ASP	3.1
11	K	32	LYS	3.1
1	O	249	ALA	3.1
3	Q	202	GLN	3.1
12	Z	165	ASN	3.1
1	O	52	SER	3.1
5	E	54	GLU	3.1
2	P	203	SER	3.0
6	F	205	GLU	3.0
1	A	248	GLU	3.0
7	U	242	GLN	3.0
1	O	201	GLU	3.0
11	K	182	GLU	3.0
5	S	3	ASN	3.0
2	P	59	ASP	3.0
3	Q	141	ASP	3.0
8	H	221	CYS	3.0
11	K	22	ALA	3.0
13	M	47	ASP	2.9
2	P	52	THR	2.9
6	T	2	THR	2.9
5	S	233	ILE	2.9
1	A	249	ALA	2.9
3	C	236	GLN	2.9
5	S	173	ARG	2.9
3	Q	49	THR	2.8
11	K	211	ILE	2.8
4	R	242	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
3	Q	175	LYS	2.8
5	S	54	GLU	2.8
8	V	221	CYS	2.8
4	R	230	GLU	2.7
7	U	2	GLY	2.7
1	A	201	GLU	2.7
14	b	105	LYS	2.7
3	C	50	LEU	2.7
11	Y	182	GLU	2.7
6	F	181	GLU	2.6
4	D	242	GLU	2.6
7	U	222	ASP	2.6
1	A	2	THR	2.6
1	A	250	LEU	2.6
4	R	203	LYS	2.6
13	M	1	THR	2.6
11	Y	202	GLU	2.6
3	C	202	GLN	2.5
3	C	240	GLU	2.5
3	Q	236	GLN	2.5
11	Y	30	THR	2.5
3	C	205	ALA	2.5
7	G	242	GLN	2.5
1	A	203	GLU	2.5
2	B	222	GLY	2.4
3	Q	204	GLY	2.4
2	B	60	THR	2.4
3	C	175	LYS	2.4
7	G	188	GLU	2.4
11	K	30	THR	2.4
7	G	3	TYR	2.4
5	E	201	ARG	2.4
7	G	222	ASP	2.4
12	Z	167	LYS	2.4
14	N	105	LYS	2.4
4	D	241	ALA	2.3
6	F	2	THR	2.3
7	G	180	SER	2.3
3	C	180	LYS	2.3
6	T	205	GLU	2.3
6	T	166	GLN	2.3
13	a	204	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	235	LYS	2.3
2	P	93	HIS	2.3
12	Z	210	ASP	2.3
3	Q	225	GLU	2.2
4	D	2	ARG	2.2
5	S	123	GLY	2.2
7	U	241	GLU	2.2
10	J	193	ASP	2.2
5	E	163	ARG	2.2
11	Y	181	THR	2.2
11	Y	183	ASP	2.2
9	W	133	LYS	2.2
6	F	201	GLU	2.2
7	G	68	ARG	2.2
11	Y	210	VAL	2.2
1	A	229	THR	2.2
3	C	203	THR	2.1
5	E	123	GLY	2.1
5	E	217	LYS	2.1
6	F	39	ASN	2.1
5	S	225	ASP	2.1
7	U	40	ASP	2.1
4	R	125	LEU	2.1
2	B	217	LYS	2.1
6	T	243	ILE	2.1
2	B	50	LYS	2.1
1	O	248	GLU	2.1
6	F	193	ALA	2.0
6	F	242	GLU	2.0
7	G	240	ALA	2.0
7	G	230	GLU	2.0
2	B	93	HIS	2.0
10	X	72	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)

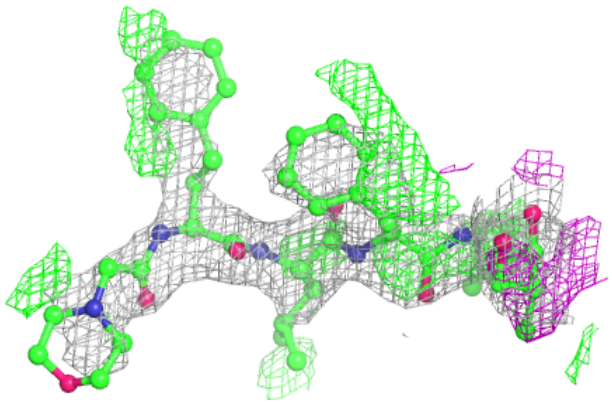
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

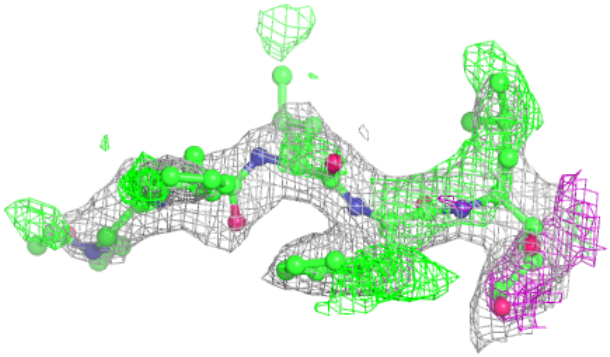
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	3BV	K	301	52/52	0.72	0.37	43,56,111,115	48
17	3BV	Y	301	52/52	0.74	0.36	42,56,111,114	48
18	MES	V	302	12/12	0.83	0.37	73,78,102,106	0
18	MES	H	302	12/12	0.85	0.35	70,75,90,101	0
18	MES	K	303	12/12	0.86	0.53	47,50,94,101	0
17	3BV	N	201	52/52	0.86	0.23	40,54,134,140	0
18	MES	Y	302	12/12	0.86	0.49	46,50,88,93	0
15	MG	G	301	1/1	0.87	0.14	51,51,51,51	0
15	MG	I	301	1/1	0.87	0.16	65,65,65,65	0
15	MG	L	301	1/1	0.87	0.16	62,62,62,62	0
17	3BV	b	201	52/52	0.87	0.22	42,55,133,140	0
17	3BV	V	301	52/52	0.89	0.20	51,61,107,114	0
17	3BV	H	301	52/52	0.90	0.20	49,59,110,113	0
15	MG	b	202	1/1	0.90	0.15	30,30,30,30	0
15	MG	Z	301	1/1	0.93	0.21	62,62,62,62	0
15	MG	I	302	1/1	0.96	0.07	62,62,62,62	0
15	MG	N	202	1/1	0.96	0.08	51,51,51,51	0
16	CL	N	203	1/1	0.98	0.05	49,49,49,49	0
16	CL	b	203	1/1	0.98	0.05	50,50,50,50	0
15	MG	K	302	1/1	0.98	0.07	60,60,60,60	0
16	CL	U	301	1/1	0.99	0.14	44,44,44,44	0
16	CL	G	302	1/1	0.99	0.13	41,41,41,41	0

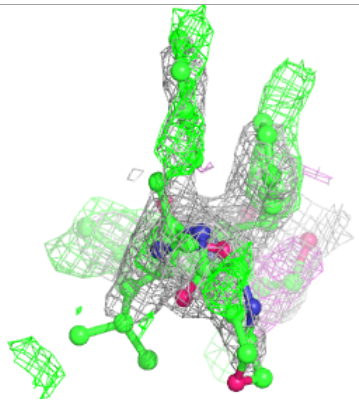
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3BV 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)

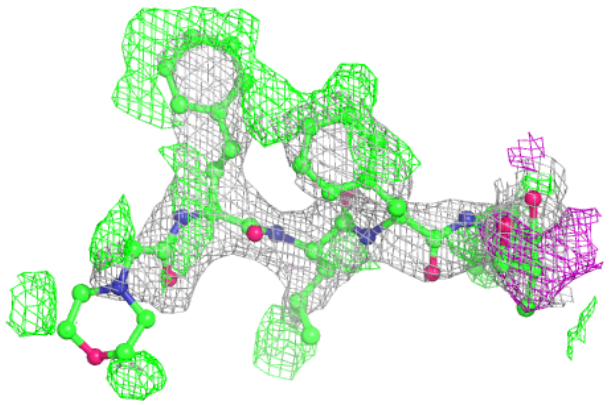


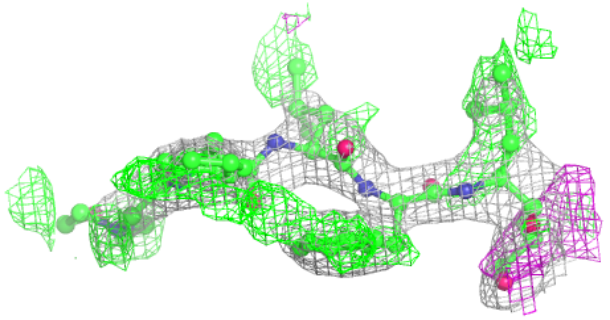


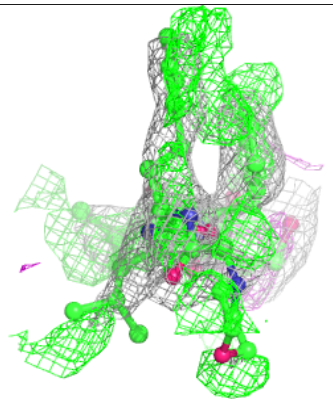


Electron density around 3BV Y 301:

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

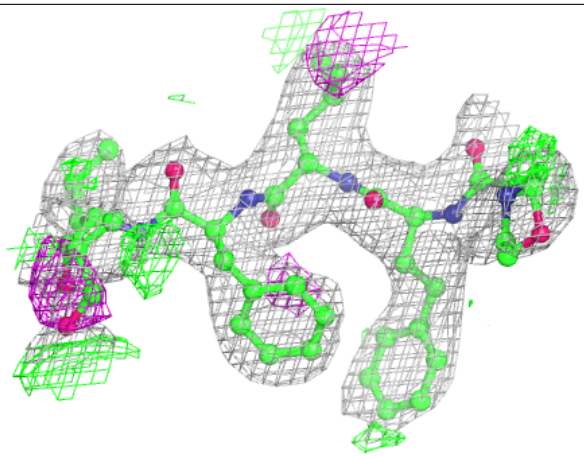


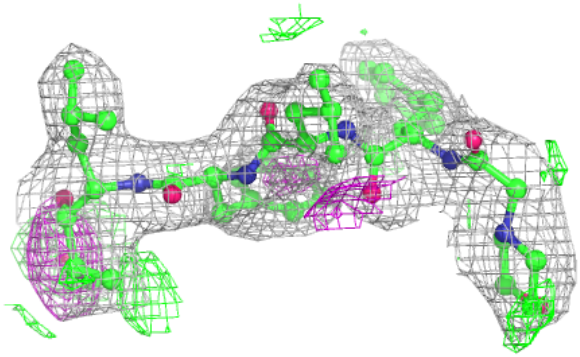


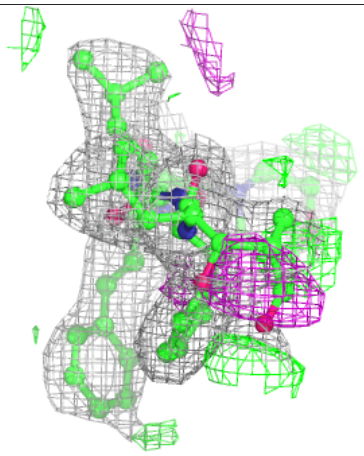


Electron density around 3BV N 201:

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

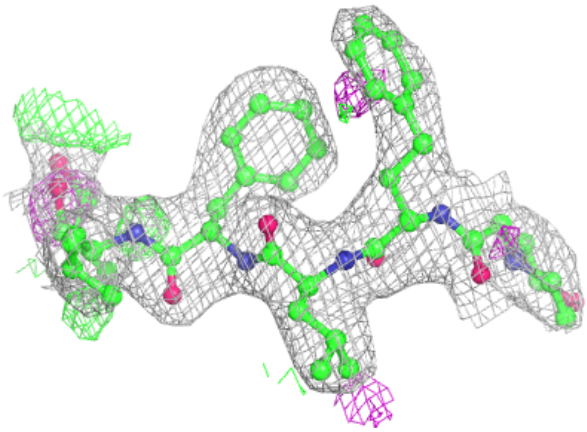


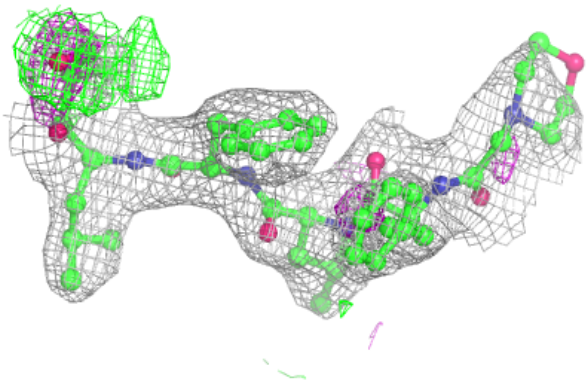


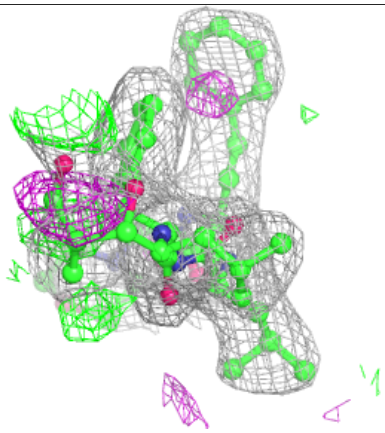


Electron density around 3BV b 201:

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

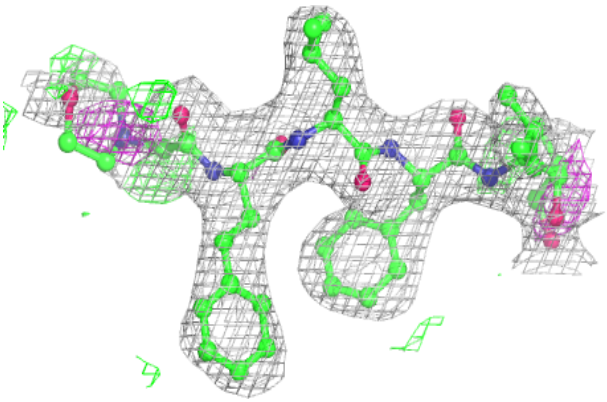


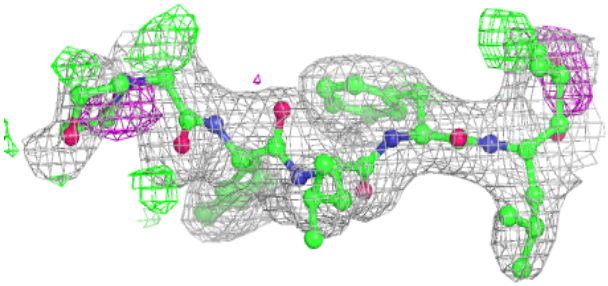


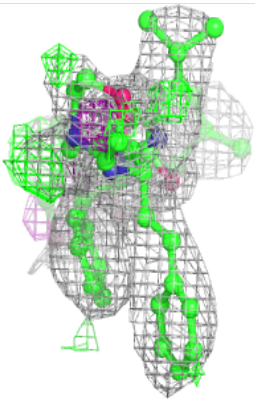


Electron density around 3BV V 301:

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

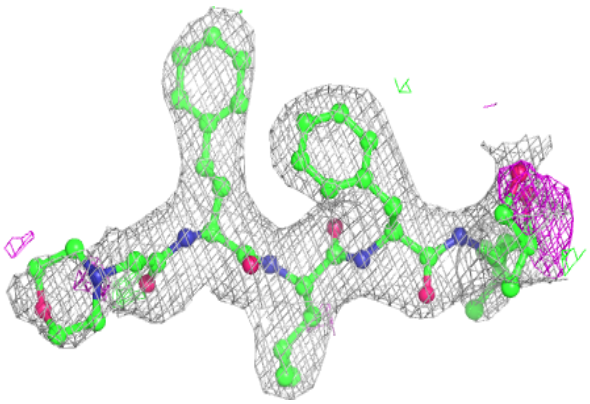


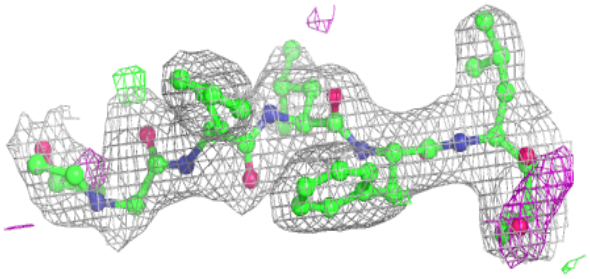


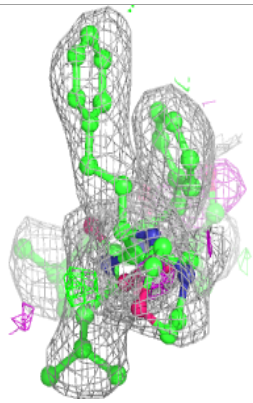


Electron density around 3BV H 301:

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







6.5 Other polymers (i)

There are no such residues in this entry.