



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:12 PM UTC

PDB ID : 5L67 / pdb_00005l67
Title : Yeast 20S proteasome with mouse beta5i (1-138) and mouse beta6 (97-111; 118-133) in complex with PR-924
Authors : Groll, M.; Huber, E.M.
Deposited on : 2016-05-28
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

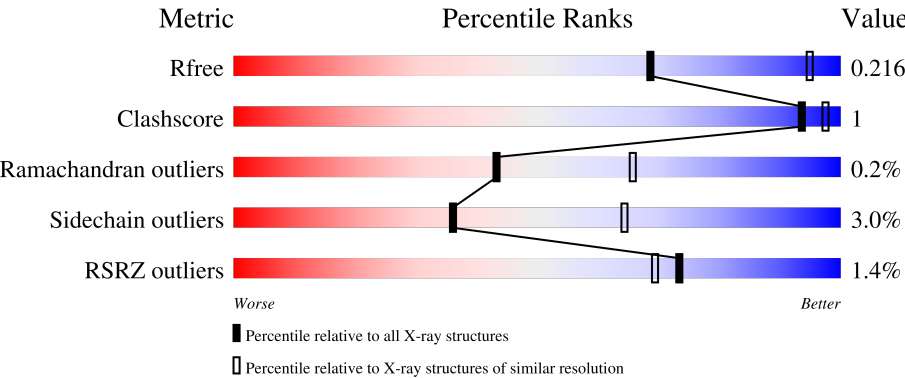
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	98%
1	O	250	% 98%
2	B	258	3% 87% 7% 5%
2	P	258	2% 88% 7% 5%
3	C	254	3% 87% 6% 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	211	
11	Y	211	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 50030 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			

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

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

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

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

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

- Molecule 11 is a protein called Proteasome subunit beta type-8,Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1645	1039	281	313	12			
11	Y	211	Total	C	N	O	S	0	0	0
			1645	1039	281	313	12			

- Molecule 12 is a protein called Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	1	0
			1832	1159	315	351	7			
13	a	233	Total	C	N	O	S	0	2	0
			1840	1164	318	351	7			

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

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

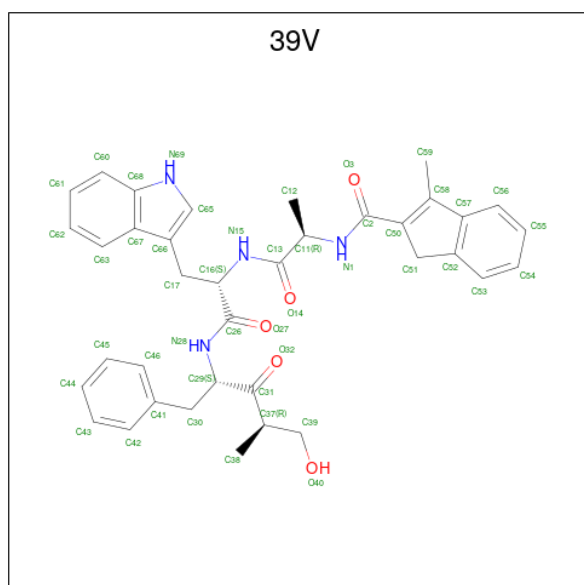
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

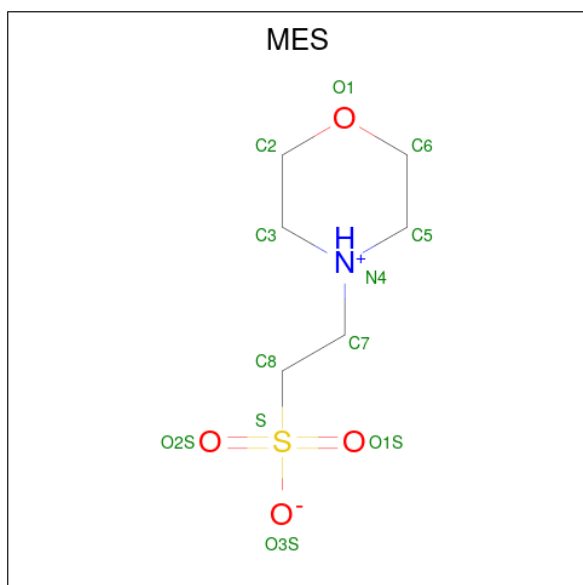
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is N-[(3-methyl-1H-inden-2-yl)carbonyl]-D-alanyl-N-[(2S,4R)-5-hydroxy-4-methyl-3-oxo-1-phenylpentan-2-yl]-L-tryptophanamide (CCD ID: 39V) (formula: $C_{37}H_{40}N_4O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	K	1	Total	C	N	O	0	0
			46	37	4	5		
17	Y	1	Total	C	N	O	0	0
			46	37	4	5		

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	29	Total	O	0	0
			29	29		
19	B	17	Total	O	0	0
			17	17		
19	C	18	Total	O	0	0
			18	18		
19	D	14	Total	O	0	0
			14	14		
19	E	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	F	16	Total O 16 16	0	0
19	G	20	Total O 20 20	0	0
19	H	27	Total O 27 27	0	0
19	I	20	Total O 20 20	0	0
19	J	16	Total O 16 16	0	0
19	K	12	Total O 12 12	0	0
19	L	18	Total O 18 18	0	0
19	M	27	Total O 27 27	0	0
19	N	15	Total O 15 15	0	0
19	O	16	Total O 16 16	0	0
19	P	16	Total O 16 16	0	0
19	Q	6	Total O 6 6	0	0
19	R	16	Total O 16 16	0	0
19	S	12	Total O 12 12	0	0
19	T	10	Total O 10 10	0	0
19	U	23	Total O 23 23	0	0
19	V	26	Total O 26 26	0	0
19	W	17	Total O 17 17	0	0
19	X	15	Total O 15 15	0	0
19	Y	18	Total O 18 18	0	0
19	Z	15	Total O 15 15	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	a	28	Total	O	0	0
			28	28		
19	b	21	Total	O	0	0
			21	21		

3 Residue-property plots

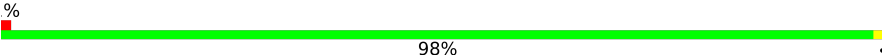
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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:  98% .



- Molecule 1: Proteasome subunit alpha type-2

Chain O:  98% .



- Molecule 2: Proteasome subunit alpha type-3

Chain B:  3% 87% 7% 5%



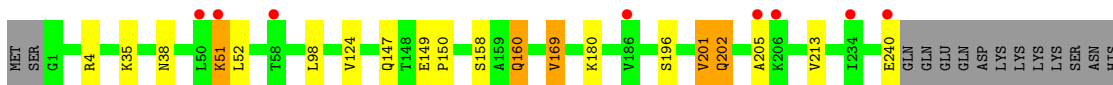
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  2% 88% 7% 5%



- Molecule 3: Proteasome subunit alpha type-4

Chain C:  3% 87% 6% 6%



- Molecule 3: Proteasome subunit alpha type-4

MET	SER	G1	Y2	D3	R4	K35	N38	T49	L50	K51	L52	L98	D141	Q147	T148	E149	P150	S158	A159	Q160	V169	K175	K180	S196	V201	Q202	T203	G204	A205	V213	K238	Q239	E240	GLN	GLN	GLU	GLN	GLN	ASP	LYS	LYS	LYS	LYS	SER	ASN	HIS
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- Chain D: 2% 85% 5% 10%

MET	PHE	LEU	THR	ARG	SER	GLU	TYR	D11	L20	L40	H89	T90	H91	L98	L113	GLY	ALA	SER	GLY	GLU	GLU	GLU	ARG	L125	L160	GL167	L176	W179	L193	I214	L235	K236	A241	E242	SER	PRO	PRO	GLU	GLU	ALA	ASP	VAL	GLU	GLU	MET	SER
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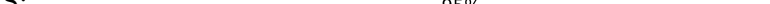
- Chain R: 

[illegible]

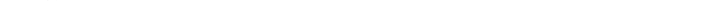
MET
SER

- Chain E: 96%

MET PHE ARG N3 T9 F12 K29 L55 L71 Y122 L188 I233

- Chain S:  95%

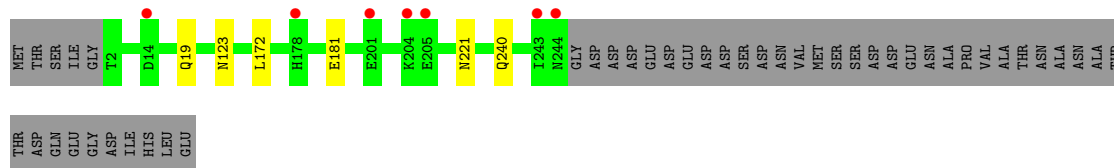
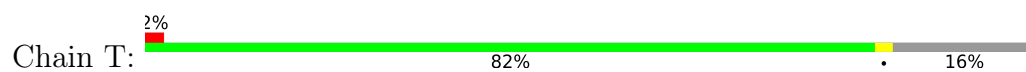
Sequence logo for the 1000th iteration. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows amino acid positions from 1 to 19. The sequence is: MET (grey), PHE (grey), ARG (grey), N3 (green), T9 (yellow), F12 (green), K29 (green), L55 (yellow), L71 (yellow), A77 (yellow), P78 (yellow), L96 (green), L188 (yellow), I233 (green). Red dots are above MET and L96.

- Chain F:  82% 16% 2%

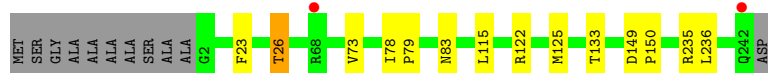
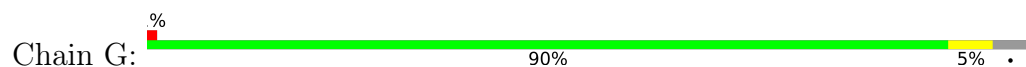
MET	THR	SER	ILE	GLY	T2	Q19	M123	L172	E181	D202	C215	I243	N244	GLY	ASP	ASP	ASP	GLU	ASP	ASP	ASP	ASP	ASP	ASN	ASN	VAL	VAL	ALA	ALA	VAL	ALA	THR	THR	ASP	GLN	GLY	GLY
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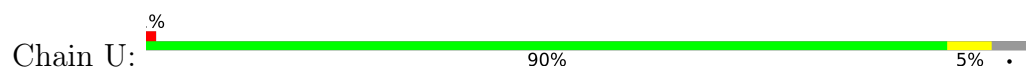
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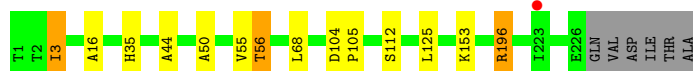
- Molecule 7: Proteasome subunit alpha type-1



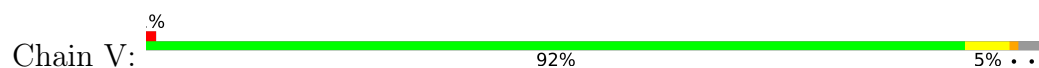
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2



- Molecule 9: Proteasome subunit beta type-3

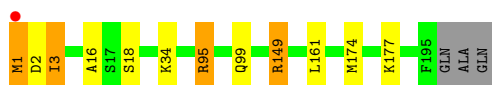
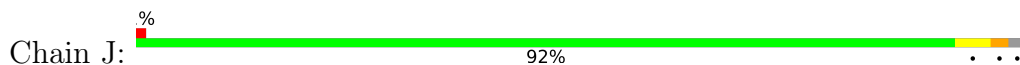


- Molecule 9: Proteasome subunit beta type-3

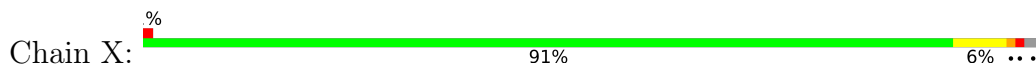




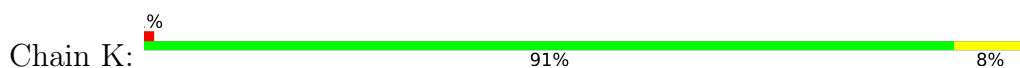
- Molecule 10: Proteasome subunit beta type-4



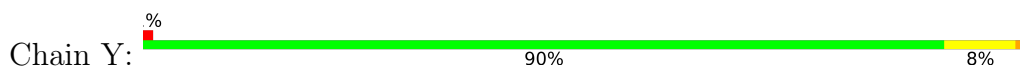
- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-8,Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-8,Proteasome subunit beta type-5



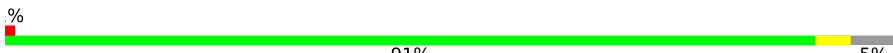
- Molecule 12: Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6

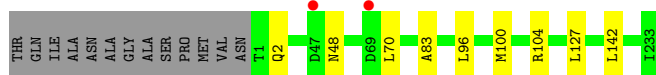


- Molecule 12: Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6



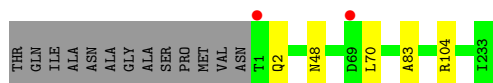
- Molecule 13: Proteasome subunit beta type-7

Chain M:  91% 5%



- Molecule 13: Proteasome subunit beta type-7

Chain a:  93% 5%



- Molecule 14: Proteasome subunit beta type-1

Chain N:  94% 5%



- Molecule 14: Proteasome subunit beta type-1

Chain b:  94% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.56Å 300.68Å 145.63Å 90.00° 112.94° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (15.00-2.60) 98.3 (15.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.191 , 0.213 0.195 , 0.216	Depositor DCC
R_{free} test set	16111 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50030	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 39V, CL, MES, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.40	0/1952	0.68	0/2642
1	O	0.40	0/1952	0.69	0/2642
2	B	0.40	0/1934	0.67	0/2618
2	P	0.40	0/1934	0.67	0/2618
3	C	0.40	0/1910	0.69	1/2586 (0.0%)
3	Q	0.40	0/1910	0.69	1/2586 (0.0%)
4	D	0.40	0/1837	0.65	0/2475
4	R	0.39	0/1837	0.65	0/2475
5	E	0.40	0/1800	0.65	0/2433
5	S	0.40	0/1800	0.65	0/2433
6	F	0.40	0/1932	0.69	0/2609
6	T	0.40	0/1932	0.70	0/2609
7	G	0.40	0/1945	0.67	0/2634
7	U	0.40	0/1945	0.67	0/2634
8	H	0.36	0/1750	0.66	0/2373
8	V	0.36	0/1750	0.67	0/2373
9	I	0.34	0/1611	0.69	0/2174
9	W	0.34	0/1611	0.69	0/2174
10	J	0.40	0/1589	0.83	6/2142 (0.3%)
10	X	0.39	0/1589	0.82	6/2142 (0.3%)
11	K	0.39	1/1681 (0.1%)	0.77	4/2268 (0.2%)
11	Y	0.40	1/1681 (0.1%)	0.76	4/2268 (0.2%)
12	L	0.36	0/1802	0.78	3/2430 (0.1%)
12	Z	0.38	0/1802	0.75	5/2430 (0.2%)
13	M	0.37	0/1866	0.67	0/2528
13	a	0.37	0/1877	0.67	0/2542
14	N	0.35	0/1541	0.67	1/2087 (0.0%)
14	b	0.35	0/1541	0.67	1/2087 (0.0%)
All	All	0.39	2/50311 (0.0%)	0.70	32/68012 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	2
10	X	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	1	THR	CB-OG1	-6.21	1.33	1.43
11	K	1	THR	CB-OG1	-5.55	1.34	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	100	ARG	NE-CZ-NH2	11.97	129.97	119.20
12	L	100	ARG	NE-CZ-NH1	-11.35	110.15	121.50
10	J	149	ARG	NE-CZ-NH1	-11.09	110.41	121.50
10	X	95	ARG	NE-CZ-NH1	-11.06	110.44	121.50
10	X	95	ARG	NE-CZ-NH2	10.37	128.53	119.20
10	J	149	ARG	NE-CZ-NH2	10.32	128.49	119.20
10	X	149	ARG	NE-CZ-NH2	-10.04	110.16	119.20
10	J	95	ARG	NE-CZ-NH2	-9.91	110.28	119.20
12	Z	100	ARG	NE-CZ-NH2	-9.80	110.38	119.20
11	K	73	ARG	CG-CD-NE	9.73	133.41	112.00
10	X	149	ARG	CD-NE-CZ	9.16	137.23	124.40
10	J	149	ARG	CD-NE-CZ	9.03	137.05	124.40
12	Z	100	ARG	CD-NE-CZ	9.02	137.03	124.40
10	J	95	ARG	CD-NE-CZ	8.85	136.78	124.40
11	Y	73	ARG	CG-CD-NE	8.82	131.40	112.00
12	L	100	ARG	CD-NE-CZ	8.66	136.52	124.40
10	X	95	ARG	CD-NE-CZ	8.50	136.30	124.40
12	Z	100	ARG	NE-CZ-NH1	8.28	129.78	121.50
10	J	95	ARG	NE-CZ-NH1	6.62	128.12	121.50
10	X	149	ARG	NE-CZ-NH1	6.39	127.89	121.50
11	Y	1	THR	CB-CA-C	-5.98	95.94	109.10
11	K	1	THR	N-CA-C	5.84	127.35	111.00
11	Y	1	THR	CA-CB-CG2	5.75	120.28	110.50
3	Q	201	VAL	N-CA-C	5.65	116.38	110.62
3	C	201	VAL	N-CA-C	5.61	116.34	110.62
11	K	1	THR	CA-CB-CG2	5.34	119.58	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	1	THR	N-CA-C	5.28	125.78	111.00
11	K	73	ARG	CB-CG-CD	5.17	123.20	111.30
14	b	115	LEU	N-CA-C	5.09	117.22	111.11
12	Z	103	PHE	CA-C-N	5.04	124.98	119.78
12	Z	103	PHE	C-N-CA	5.04	124.98	119.78
14	N	115	LEU	N-CA-C	5.02	117.14	111.11

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	149	ARG	Sidechain
10	J	95	ARG	Sidechain
10	X	149	ARG	Sidechain

5.2 Too-close contacts

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	7	0
2	P	1904	0	1904	6	0
3	C	1881	0	1895	8	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	4	0
8	H	1719	0	1719	10	0
8	V	1719	0	1719	6	0
9	I	1581	0	1574	10	0
9	W	1581	0	1574	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	1561	0	1569	4	0
10	X	1561	0	1569	6	0
11	K	1645	0	1589	12	0
11	Y	1645	0	1589	15	0
12	L	1764	0	1716	6	0
12	Z	1764	0	1716	6	0
13	M	1832	0	1845	2	0
13	a	1840	0	1858	0	0
14	N	1512	0	1481	5	0
14	b	1512	0	1481	5	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	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	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	K	46	0	39	9	0
17	Y	46	0	39	8	0
18	K	12	0	13	2	0
18	Y	12	0	13	0	0
19	A	29	0	0	0	0
19	B	17	0	0	1	0
19	C	18	0	0	0	0
19	D	14	0	0	0	0
19	E	9	0	0	0	0
19	F	16	0	0	0	0
19	G	20	0	0	0	0
19	H	27	0	0	0	0
19	I	20	0	0	0	0
19	J	16	0	0	0	0
19	K	12	0	0	0	0
19	L	18	0	0	0	0
19	M	27	0	0	0	0
19	N	15	0	0	0	0
19	O	16	0	0	0	0
19	P	16	0	0	1	0
19	Q	6	0	0	0	0
19	R	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	S	12	0	0	0	0
19	T	10	0	0	0	0
19	U	23	0	0	0	0
19	V	26	0	0	0	0
19	W	17	0	0	0	0
19	X	15	0	0	0	0
19	Y	18	0	0	0	0
19	Z	15	0	0	0	0
19	a	28	0	0	0	0
19	b	21	0	0	0	0
All	All	50030	0	49271	139	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 (139) 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:Y:302:39V:H9	12:Z:124:SER:OG	1.66	0.96
11:K:31:MET:HE1	17:K:301:39V:H7	1.66	0.78
11:Y:73:ARG:HB2	11:Y:73:ARG:HH11	1.48	0.77
17:K:301:39V:H9	12:L:124:SER:OG	1.86	0.75
11:K:73:ARG:HH11	11:K:73:ARG:HB2	1.59	0.67
12:L:100:ARG:HD2	12:L:105:TYR:CE2	2.33	0.64
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.31	0.64
11:K:208:ASN:O	9:W:38:LYS:NZ	2.34	0.60
11:Y:31:MET:HE1	17:Y:302:39V:H7	1.84	0.60
14:b:152:VAL:HA	14:b:175:MET:HE1	1.85	0.58
12:Z:100:ARG:HD3	12:Z:105:TYR:CE2	2.39	0.57
12:L:100:ARG:HD2	12:L:105:TYR:CZ	2.39	0.57
17:K:301:39V:O32	17:K:301:39V:O40	2.22	0.56
14:N:152:VAL:HA	14:N:175:MET:HE1	1.85	0.56
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.87	0.56
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.87	0.56
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.89	0.55
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.89	0.54
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.38	0.54
2:B:93:HIS:HB3	19:B:301:HOH:O	2.07	0.53
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.38	0.53
17:Y:302:39V:C59	17:Y:302:39V:H1	2.22	0.52
8:H:3:ILE:HG21	8:H:44:ALA:HB1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:3:ILE:HG21	8:V:44:ALA:HB1	1.93	0.51
4:R:89:VAL:HG12	11:Y:61:LYS:HG3	1.93	0.51
11:Y:1:THR:HG22	11:Y:2:THR:N	2.24	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.51
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.93	0.50
2:P:50:LYS:O	2:P:51:VAL:C	2.54	0.50
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.93	0.50
8:H:3:ILE:HG21	8:H:44:ALA:CB	2.42	0.50
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.50
7:U:23:PHE:O	7:U:26:THR:HB	2.11	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.49
2:B:50:LYS:O	2:B:51:VAL:C	2.55	0.49
11:K:36:GLU:OE1	11:K:184:TRP:CH2	2.66	0.49
8:V:3:ILE:HG21	8:V:44:ALA:CB	2.42	0.49
11:Y:36:GLU:OE1	11:Y:184:TRP:CH2	2.65	0.49
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.96	0.48
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.96	0.48
11:Y:27:SER:HB2	17:Y:302:39V:H11	1.96	0.47
3:C:201:VAL:O	3:C:202:GLN:HB3	2.14	0.47
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.79	0.47
11:Y:1:THR:CG2	11:Y:2:THR:N	2.78	0.47
11:Y:33:LYS:HE2	17:Y:302:39V:C42	2.45	0.47
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.79	0.46
2:P:93:HIS:HB3	19:P:301:HOH:O	2.13	0.46
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.15	0.46
17:Y:302:39V:H5	12:Z:130:SER:OG	2.15	0.46
9:I:148:MET:HE2	9:I:172:ASN:HB2	1.98	0.46
17:K:301:39V:H1	17:K:301:39V:C59	2.28	0.46
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.51	0.45
9:W:148:MET:HE2	9:W:172:ASN:HB2	1.98	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.45
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.97	0.45
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.82	0.45
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.99	0.45
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.97	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.45
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.97	0.45
14:b:35:THR:HG21	14:b:45:ARG:HE	1.82	0.45
11:K:33:LYS:HE2	17:K:301:39V:C42	2.47	0.45
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.81	0.45
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.99	0.44
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.97	0.44
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.98	0.44
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.99	0.44
11:Y:104:TRP:CE2	11:Y:181:GLU:HB3	2.52	0.44
4:D:89:VAL:HG12	11:K:61:LYS:HG3	2.00	0.44
11:K:104:TRP:CE2	11:K:181:GLU:HB3	2.52	0.44
3:C:51:LYS:O	3:C:52:LEU:HB2	2.18	0.44
14:N:35:THR:HG21	14:N:45:ARG:HE	1.83	0.44
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.18	0.43
17:K:301:39V:O40	18:K:303:MES:O3S	2.35	0.43
14:N:133:PHE:HA	14:b:132:THR:O	2.19	0.43
12:L:8:ASN:HA	12:L:30:ILE:O	2.18	0.43
11:K:40:TYR:CD2	11:K:73:ARG:NE	2.86	0.43
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.01	0.43
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.99	0.43
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.18	0.43
11:Y:73:ARG:HH11	11:Y:73:ARG:CB	2.26	0.43
11:K:20:ALA:HB3	11:K:28:SER:HB3	2.00	0.43
10:X:148:TYR:O	10:X:149:ARG:HD3	2.18	0.43
11:Y:20:ALA:HB3	11:Y:28:SER:HB3	2.01	0.43
11:Y:144:LYS:HB2	11:Y:147:LEU:HD13	2.01	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.01	0.43
2:B:217:LYS:C	2:B:219:ALA:H	2.27	0.43
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.01	0.43
17:K:301:39V:C65	17:K:301:39V:N15	2.81	0.43
5:S:12:PHE:H	6:T:19:GLN:HE22	1.67	0.43
17:Y:302:39V:C65	17:Y:302:39V:N15	2.82	0.42
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.01	0.42
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.49	0.42
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.01	0.42
11:K:31:MET:HE1	17:K:301:39V:C56	2.40	0.42
11:K:144:LYS:HB2	11:K:147:LEU:HD13	2.01	0.42
11:Y:12:VAL:HG13	11:Y:179:VAL:HB	2.01	0.42
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.50	0.42
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.02	0.42
11:K:12:VAL:HG13	11:K:179:VAL:HB	2.01	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.49	0.42
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.01	0.42
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.02	0.42
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.42
2:P:217:LYS:C	2:P:219:ALA:H	2.28	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.02	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.55	0.42
5:E:12:PHE:H	6:F:19:GLN:HE22	1.68	0.41
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.20	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.50	0.41
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.02	0.41
10:J:177:LYS:NZ	10:X:169:GLU:O	2.53	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.02	0.41
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.02	0.41
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.56	0.41
2:B:145:TYR:OH	2:B:217:LYS:N	2.54	0.41
2:P:145:TYR:OH	2:P:217:LYS:N	2.54	0.41
8:H:196:ARG:NH2	9:I:150:GLU:O	2.54	0.41
11:Y:36:GLU:OE1	11:Y:184:TRP:CZ2	2.74	0.41
3:C:35:LYS:HG2	3:C:158:SER:O	2.20	0.41
8:H:3:ILE:HG23	8:H:16:ALA:HB2	2.02	0.41
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.56	0.41
17:K:301:39V:O40	18:K:303:MES:S	2.79	0.41
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.51	0.41
17:Y:302:39V:C59	17:Y:302:39V:N1	2.83	0.41
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.51	0.40
13:M:96:LEU:O	13:M:100:MET:HG2	2.22	0.40
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.36	0.40
5:S:77:ALA:N	5:S:78:PRO:CD	2.85	0.40
10:X:1:MET:N	10:X:48:GLY:O	2.54	0.40
7:G:73:VAL:HG12	7:G:133:THR:HB	2.03	0.40
8:H:3:ILE:HG21	8:H:3:ILE:HD13	1.92	0.40
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.03	0.40
8:V:3:ILE:HG23	8:V:16:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	30	51
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	30	51
2	B	242/258 (94%)	235 (97%)	4 (2%)	3 (1%)	10	23
2	P	242/258 (94%)	234 (97%)	5 (2%)	3 (1%)	10	23
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	34
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	34
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	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%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
11	Y	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	232/246 (94%)	224 (97%)	7 (3%)	1 (0%)	30	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	233/246 (95%)	225 (97%)	7 (3%)	1 (0%)	30	51
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6285/6612 (95%)	6135 (98%)	136 (2%)	14 (0%)	43	66

All (14) 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
1	A	2	THR
2	B	218	GLY
2	B	222	GLY
1	O	2	THR
2	P	218	GLY
2	P	222	GLY
3	C	205	ALA
3	Q	205	ALA
13	a	83	ALA
13	M	83	ALA

5.3.2 Protein sidechains ⓘ

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%)	205 (98%)	4 (2%)	50	75
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	75
2	B	203/216 (94%)	197 (97%)	6 (3%)	36	64
2	P	203/216 (94%)	197 (97%)	6 (3%)	36	64
3	C	212/226 (94%)	202 (95%)	10 (5%)	23	48
3	Q	212/226 (94%)	202 (95%)	10 (5%)	23	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	194/215 (90%)	184 (95%)	10 (5%)	21	44
4	R	194/215 (90%)	184 (95%)	10 (5%)	21	44
5	E	190/193 (98%)	185 (97%)	5 (3%)	40	68
5	S	190/193 (98%)	185 (97%)	5 (3%)	40	68
6	F	201/239 (84%)	196 (98%)	5 (2%)	42	69
6	T	201/239 (84%)	196 (98%)	5 (2%)	42	69
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	60
7	U	206/210 (98%)	199 (97%)	7 (3%)	32	60
8	H	185/190 (97%)	179 (97%)	6 (3%)	34	62
8	V	185/190 (97%)	179 (97%)	6 (3%)	34	62
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	78
9	W	172/173 (99%)	169 (98%)	3 (2%)	53	78
10	J	173/175 (99%)	168 (97%)	5 (3%)	37	65
10	X	173/175 (99%)	168 (97%)	5 (3%)	37	65
11	K	172/172 (100%)	165 (96%)	7 (4%)	27	54
11	Y	172/172 (100%)	165 (96%)	7 (4%)	27	54
12	L	186/186 (100%)	180 (97%)	6 (3%)	34	62
12	Z	186/186 (100%)	180 (97%)	6 (3%)	34	62
13	M	200/208 (96%)	196 (98%)	4 (2%)	48	74
13	a	201/208 (97%)	197 (98%)	4 (2%)	48	74
14	N	162/162 (100%)	159 (98%)	3 (2%)	50	75
14	b	162/162 (100%)	159 (98%)	3 (2%)	50	75
All	All	5331/5548 (96%)	5169 (97%)	162 (3%)	36	64

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	55	LEU
2	B	79	LEU
2	B	102	ASN

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Mol	Chain	Res	Type
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	98	LEU
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	213	VAL
3	C	240	GLU
4	D	20	LEU
4	D	40	LEU
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	188	LEU
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	221	ASN
6	F	240	GLN
7	G	26	THR
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	3	ILE
8	H	55	VAL

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Mol	Chain	Res	Type
8	H	56	THR
8	H	68	LEU
8	H	153	LYS
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
10	J	1	MET
10	J	2	ASP
10	J	3	ILE
10	J	99	GLN
10	J	174	MET
11	K	4	LEU
11	K	12	VAL
11	K	31	MET
11	K	73	ARG
11	K	88	LEU
11	K	124	GLN
11	K	147	LEU
12	L	23	LEU
12	L	49	ASN
12	L	119	LYS
12	L	128	VAL
12	L	132	GLN
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
14	N	9	LYS
14	N	119	VAL
14	N	178	LEU
1	O	1	MET
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	55	LEU
2	P	79	LEU
2	P	102	ASN
2	P	113	ARG
2	P	191	LEU
2	P	238	LEU

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Mol	Chain	Res	Type
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	98	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	213	VAL
3	Q	240	GLU
4	R	20	LEU
4	R	40	LEU
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	188	LEU
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	221	ASN
6	T	240	GLN
7	U	26	THR
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	3	ILE
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	153	LYS

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Mol	Chain	Res	Type
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
10	X	1	MET
10	X	2	ASP
10	X	3	ILE
10	X	99	GLN
10	X	174	MET
11	Y	4	LEU
11	Y	12	VAL
11	Y	31	MET
11	Y	73	ARG
11	Y	88	LEU
11	Y	124	GLN
11	Y	147	LEU
12	Z	23	LEU
12	Z	49	ASN
12	Z	119	LYS
12	Z	128	VAL
12	Z	132	GLN
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
14	b	9	LYS
14	b	119	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	93	HIS
2	B	123	GLN
2	B	124	HIS
2	B	220	ASN
3	C	17	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN

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Mol	Chain	Res	Type
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	180	HIS
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	123	ASN
7	G	114	ASN
7	G	121	GLN
7	G	175	ASN
8	H	35	HIS
8	H	165	ASN
9	I	63	ASN
9	I	203	GLN
10	J	63	ASN
11	K	32	ASN
11	K	142	ASN
11	K	175	ASN
12	L	49	ASN
12	L	79	HIS
12	L	158	ASN
12	L	197	GLN
13	M	48	ASN
13	M	62	HIS
13	M	108	ASN
14	N	38	HIS
14	N	141	ASN
2	P	93	HIS
2	P	123	GLN
2	P	124	HIS
2	P	220	ASN
3	Q	17	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN

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Mol	Chain	Res	Type
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	123	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	175	ASN
8	V	35	HIS
8	V	86	HIS
9	W	63	ASN
10	X	63	ASN
11	Y	32	ASN
11	Y	132	ASN
11	Y	142	ASN
11	Y	175	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	158	ASN
12	Z	197	GLN
13	a	48	ASN
13	a	62	HIS
13	a	108	ASN
13	a	149	HIS
14	b	38	HIS
14	b	141	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	39V	K	301	11	48,50,50	3.73	17 (35%)	61,70,70	1.63	10 (16%)
18	MES	K	303	-	12,12,12	2.39	1 (8%)	15,16,16	1.26	3 (20%)
18	MES	Y	303	-	12,12,12	2.32	1 (8%)	15,16,16	1.12	1 (6%)
17	39V	Y	302	11	48,50,50	3.79	16 (33%)	61,70,70	1.59	8 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	39V	K	301	11	-	13/42/54/54	0/5/5/5
18	MES	K	303	-	-	5/6/14/14	0/1/1/1
18	MES	Y	303	-	-	0/6/14/14	0/1/1/1
17	39V	Y	302	11	-	12/42/54/54	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	302	39V	O32-C31	12.06	1.40	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	301	39V	C51-C50	-11.35	1.36	1.51
17	Y	302	39V	C51-C50	-11.16	1.37	1.51
17	K	301	39V	O32-C31	10.72	1.38	1.21
18	K	303	MES	C8-S	-8.11	1.66	1.77
17	K	301	39V	C67-C66	-8.07	1.30	1.44
17	Y	302	39V	C67-C68	-8.01	1.31	1.41
18	Y	303	MES	C8-S	-7.82	1.66	1.77
17	Y	302	39V	C67-C66	-7.67	1.31	1.44
17	K	301	39V	C67-C68	-7.33	1.32	1.41
17	K	301	39V	C57-C58	-7.10	1.31	1.44
17	Y	302	39V	C51-C52	-7.00	1.38	1.50
17	K	301	39V	C51-C52	-6.85	1.38	1.50
17	Y	302	39V	C57-C58	-6.78	1.31	1.44
17	Y	302	39V	C63-C67	-5.45	1.31	1.39
17	K	301	39V	C63-C67	-5.42	1.31	1.39
17	K	301	39V	C57-C52	-5.35	1.32	1.39
17	K	301	39V	C56-C57	-5.16	1.32	1.39
17	Y	302	39V	C57-C52	-5.09	1.32	1.39
17	Y	302	39V	C30-C41	-4.88	1.39	1.51
17	Y	302	39V	C56-C57	-4.87	1.32	1.39
17	K	301	39V	C30-C41	-4.83	1.39	1.51
17	K	301	39V	C53-C52	-4.61	1.32	1.39
17	K	301	39V	C60-C68	-4.59	1.32	1.39
17	Y	302	39V	C60-C68	-4.58	1.32	1.39
17	Y	302	39V	C53-C52	-4.41	1.32	1.39
17	K	301	39V	C68-N69	-3.56	1.32	1.37
17	K	301	39V	C65-C66	-3.49	1.31	1.36
17	Y	302	39V	C68-N69	-3.43	1.32	1.37
17	Y	302	39V	C65-N69	-3.28	1.31	1.37
17	Y	302	39V	C65-C66	-3.10	1.32	1.36
17	K	301	39V	C65-N69	-3.04	1.32	1.37
17	Y	302	39V	C50-C58	-2.29	1.31	1.36
17	K	301	39V	C37-C31	2.08	1.58	1.52
17	K	301	39V	C29-C31	2.01	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	39V	O32-C31-C37	-5.96	110.54	121.30
17	Y	302	39V	O32-C31-C37	-5.14	112.01	121.30
17	K	301	39V	C30-C29-N28	-4.05	102.44	110.83
17	Y	302	39V	C66-C65-N69	-3.79	106.14	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	302	39V	C30-C29-N28	-3.79	102.99	110.83
17	Y	302	39V	C67-C66-C65	3.73	109.98	106.16
17	K	301	39V	C67-C66-C65	3.66	109.91	106.16
17	K	301	39V	C66-C65-N69	-3.11	106.89	110.31
18	K	303	MES	O1S-S-C8	2.90	111.11	106.73
17	K	301	39V	C63-C67-C68	2.74	121.68	118.84
17	K	301	39V	C16-C17-C66	-2.73	108.27	113.44
17	Y	302	39V	C16-C17-C66	-2.59	108.54	113.44
17	Y	302	39V	C62-C61-C60	-2.58	117.05	120.24
17	Y	302	39V	C52-C51-C50	2.41	104.65	102.72
18	K	303	MES	O3S-S-C8	2.36	110.61	106.00
17	K	301	39V	C52-C51-C50	2.32	104.58	102.72
18	Y	303	MES	O1S-S-C8	2.29	110.19	106.73
17	Y	302	39V	C12-C11-N1	-2.28	106.19	110.38
17	K	301	39V	C12-C11-N1	-2.26	106.23	110.38
17	K	301	39V	C17-C16-N15	-2.19	106.45	110.64
17	K	301	39V	C59-C58-C57	-2.13	121.00	124.76
18	K	303	MES	O2S-S-O1S	-2.11	106.96	113.82

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	301	39V	C29-C31-C37-C38
17	K	301	39V	O32-C31-C37-C38
17	K	301	39V	C31-C37-C39-O40
17	K	301	39V	C38-C37-C39-O40
17	Y	302	39V	O32-C31-C37-C38
18	K	303	MES	C8-C7-N4-C3
18	K	303	MES	C7-C8-S-O1S
18	K	303	MES	C7-C8-S-O3S
17	K	301	39V	C29-C30-C41-C42
17	K	301	39V	C29-C30-C41-C46
17	Y	302	39V	C29-C30-C41-C42
17	Y	302	39V	C29-C30-C41-C46
17	Y	302	39V	C29-C31-C37-C38
17	K	301	39V	N1-C11-C13-N15
17	Y	302	39V	N1-C11-C13-N15
18	K	303	MES	C7-C8-S-O2S
17	K	301	39V	C30-C29-C31-O32
17	Y	302	39V	C30-C29-C31-O32
17	K	301	39V	N1-C11-C13-O14

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Mol	Chain	Res	Type	Atoms
17	Y	302	39V	N1-C11-C13-O14
17	Y	302	39V	N15-C16-C26-O27
17	K	301	39V	N28-C29-C31-C37
17	Y	302	39V	N28-C29-C31-C37
17	Y	302	39V	N15-C16-C26-N28
18	K	303	MES	N4-C7-C8-S
17	K	301	39V	N15-C16-C26-O27
17	Y	302	39V	O3-C2-C50-C58
17	K	301	39V	N15-C16-C26-N28
17	K	301	39V	N28-C29-C30-C41
17	Y	302	39V	C12-C11-C13-O14

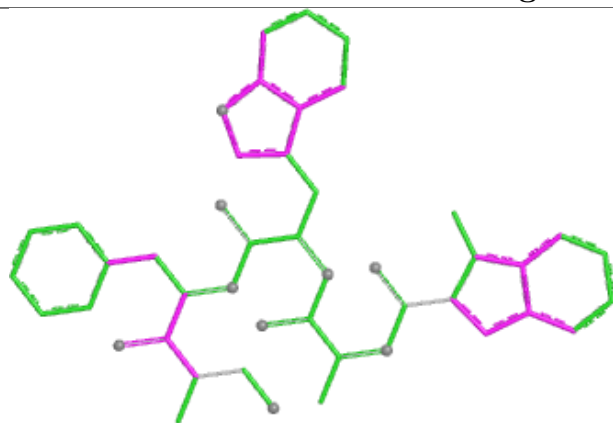
There are no ring outliers.

3 monomers are involved in 17 short contacts:

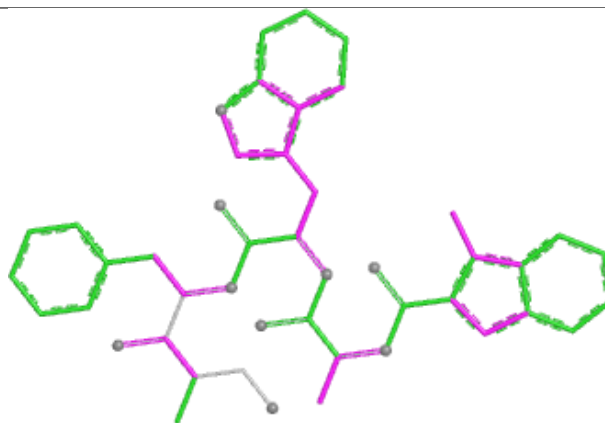
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	301	39V	9	0
18	K	303	MES	2	0
17	Y	302	39V	8	0

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 than 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.

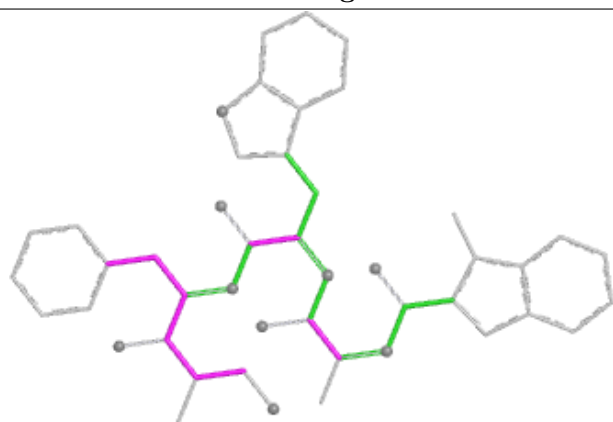
Ligand 39V K 301



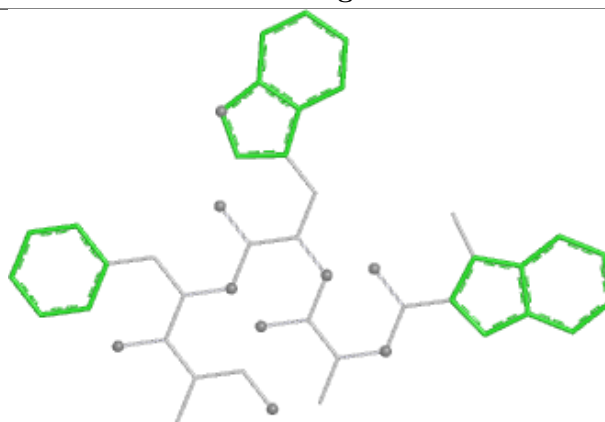
Bond lengths



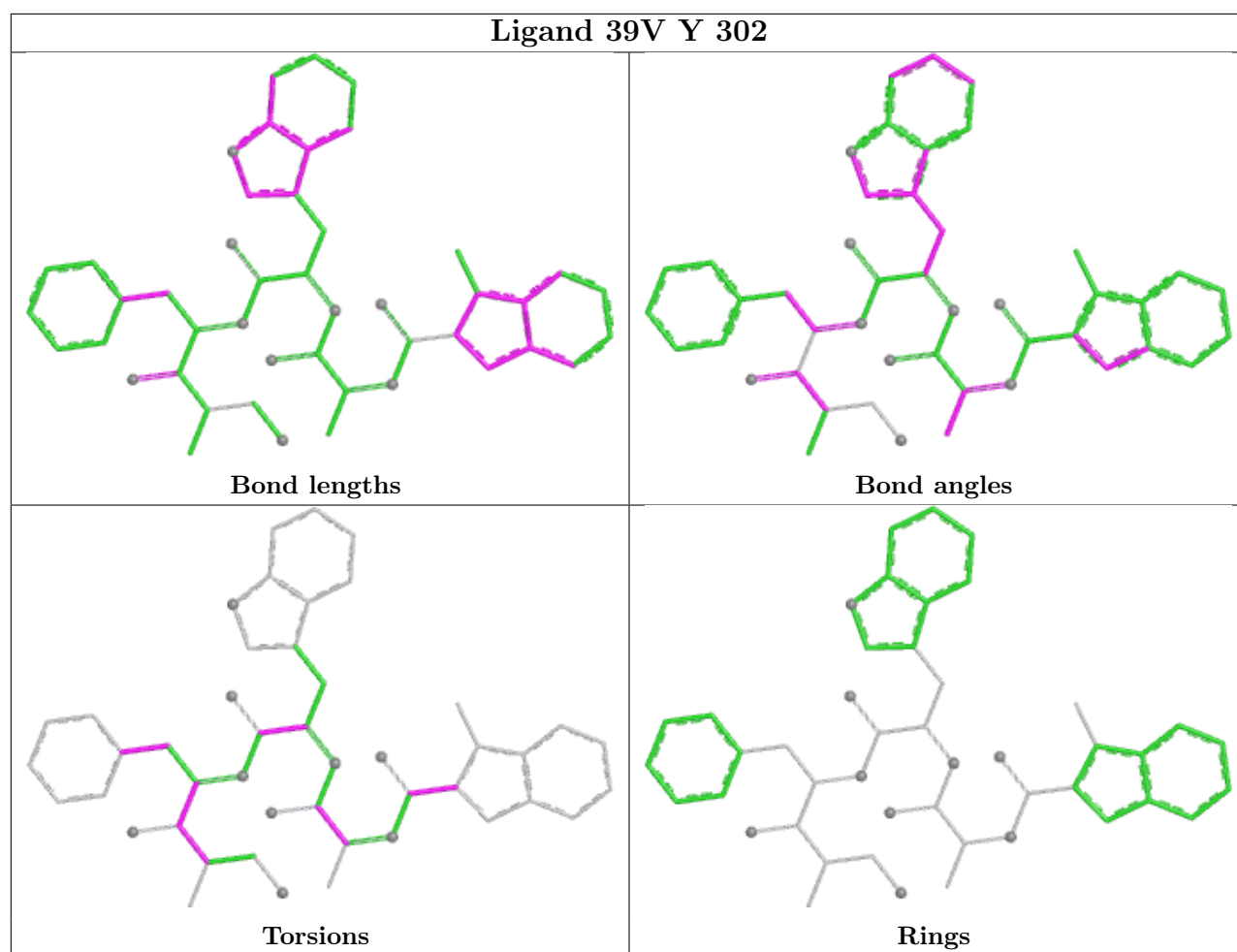
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.39	1 (0%) 88 86	36, 54, 89, 125	0
1	O	250/250 (100%)	-0.32	3 (1%) 76 73	41, 58, 102, 134	0
2	B	244/258 (94%)	-0.13	7 (2%) 53 48	40, 60, 102, 157	0
2	P	244/258 (94%)	-0.18	6 (2%) 58 52	43, 62, 106, 155	0
3	C	240/254 (94%)	0.00	8 (3%) 49 43	39, 65, 134, 168	0
3	Q	240/254 (94%)	0.10	11 (4%) 37 32	29, 74, 157, 197	0
4	D	235/260 (90%)	-0.18	4 (1%) 69 64	44, 63, 95, 130	0
4	R	235/260 (90%)	-0.03	8 (3%) 48 42	53, 71, 112, 143	0
5	E	231/234 (98%)	-0.17	1 (0%) 88 86	46, 64, 102, 144	0
5	S	231/234 (98%)	-0.10	2 (0%) 81 78	49, 70, 109, 141	0
6	F	243/288 (84%)	-0.29	3 (1%) 76 73	40, 60, 108, 136	0
6	T	243/288 (84%)	-0.18	7 (2%) 53 48	38, 66, 120, 154	0
7	G	241/252 (95%)	-0.35	2 (0%) 82 80	38, 55, 92, 150	0
7	U	241/252 (95%)	-0.36	2 (0%) 82 80	41, 55, 90, 130	0
8	H	226/232 (97%)	-0.36	1 (0%) 88 86	39, 53, 86, 145	0
8	V	226/232 (97%)	-0.32	2 (0%) 81 78	40, 55, 87, 163	0
9	I	204/205 (99%)	-0.52	1 (0%) 87 85	38, 53, 85, 105	0
9	W	204/205 (99%)	-0.51	1 (0%) 87 85	40, 54, 84, 109	0
10	J	195/198 (98%)	-0.40	1 (0%) 87 85	38, 56, 81, 124	0
10	X	195/198 (98%)	-0.39	2 (1%) 79 76	41, 57, 84, 134	0
11	K	211/211 (100%)	-0.22	2 (0%) 81 78	46, 62, 93, 118	0
11	Y	211/211 (100%)	-0.18	2 (0%) 81 78	45, 63, 93, 122	0
12	L	222/222 (100%)	-0.18	3 (1%) 73 69	44, 60, 104, 133	0
12	Z	222/222 (100%)	-0.17	2 (0%) 81 78	44, 62, 106, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.45	2 (0%) 81 78	31, 54, 79, 96	1 (0%)
13	a	233/246 (94%)	-0.43	2 (0%) 81 78	32, 55, 80, 99	2 (0%)
14	N	196/196 (100%)	-0.50	0 100 100	38, 50, 79, 107	0
14	b	196/196 (100%)	-0.51	0 100 100	38, 50, 80, 108	0
All	All	6342/6612 (95%)	-0.27	86 (1%) 73 69	29, 59, 103, 197	3 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	5.4
12	L	174	TYR	5.1
2	B	218	GLY	4.9
10	J	1	MET	4.7
12	Z	174	TYR	4.7
3	Q	50	LEU	4.0
4	R	113	LEU	3.8
2	P	51	VAL	3.8
3	Q	205	ALA	3.6
2	P	218	GLY	3.5
4	R	112	ALA	3.5
13	a	1	THR	3.5
4	D	241	ALA	3.4
2	P	219	ALA	3.3
6	T	204	LYS	3.2
6	T	243	ILE	3.2
2	B	219	ALA	3.1
3	C	205	ALA	3.1
6	F	215	CYS	3.1
9	W	1	SER	3.1
8	V	223	ILE	3.0
6	T	14	ASP	3.0
1	O	1	MET	2.9
8	H	223	ILE	2.9
7	G	68	ARG	2.8
2	B	222	GLY	2.8
3	C	234	ILE	2.7
4	D	113	LEU	2.7
3	Q	240	GLU	2.7
3	C	240	GLU	2.7
3	Q	175	LYS	2.7
3	C	50	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
6	T	201	GLU	2.7
4	R	116	GLY	2.6
10	X	195	PHE	2.6
8	V	224	GLN	2.6
3	C	51	LYS	2.6
1	O	53	SER	2.6
2	B	51	VAL	2.6
6	T	205	GLU	2.5
11	Y	208	ASN	2.5
3	Q	51	LYS	2.4
3	Q	49	THR	2.4
6	F	202	ASP	2.4
2	B	1	GLY	2.4
11	K	146	ASP	2.4
4	R	117	GLU	2.4
4	R	125	LEU	2.4
2	P	1	GLY	2.4
5	E	122	TYR	2.4
9	I	1	SER	2.3
3	C	186	VAL	2.3
2	P	52	THR	2.3
1	A	1	MET	2.3
3	Q	38	ASN	2.3
3	Q	141	ASP	2.3
2	B	217	LYS	2.2
6	T	244	ASN	2.2
12	L	165	ASN	2.2
4	R	114	ARG	2.2
3	C	206	LYS	2.2
4	R	238	LYS	2.2
11	Y	146	ASP	2.2
13	M	69	ASP	2.2
1	O	4	ARG	2.2
2	B	220	ASN	2.2
7	U	24	LYS	2.2
4	D	167	GLY	2.2
13	a	69	ASP	2.2
6	F	243	ILE	2.2
2	P	220	ASN	2.1
3	Q	238	LYS	2.1
4	D	117	GLU	2.1
7	G	242	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	58	THR	2.1
7	U	179	LYS	2.1
5	S	96	LEU	2.1
12	Z	166	GLY	2.1
4	R	239	GLU	2.1
5	S	3	ASN	2.1
3	Q	3	ASP	2.0
12	L	164	THR	2.0
13	M	47	ASP	2.0
6	T	178	HIS	2.0
3	Q	204	GLY	2.0
11	K	40	TYR	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 oligosaccharides 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	Y	303	12/12	0.74	0.33	58,61,66,67	12
18	MES	K	303	12/12	0.80	0.32	61,63,68,70	12
17	39V	Y	302	46/46	0.80	0.15	57,67,82,84	0
17	39V	K	301	46/46	0.82	0.14	54,66,78,83	0
15	MG	Y	301	1/1	0.89	0.16	80,80,80,80	0
15	MG	Z	301	1/1	0.93	0.07	64,64,64,64	0
15	MG	K	302	1/1	0.96	0.08	56,56,56,56	0
15	MG	I	301	1/1	0.97	0.06	63,63,63,63	0
15	MG	G	301	1/1	0.97	0.04	60,60,60,60	0
15	MG	J	201	1/1	0.98	0.07	56,56,56,56	0
15	MG	L	301	1/1	0.98	0.05	63,63,63,63	0

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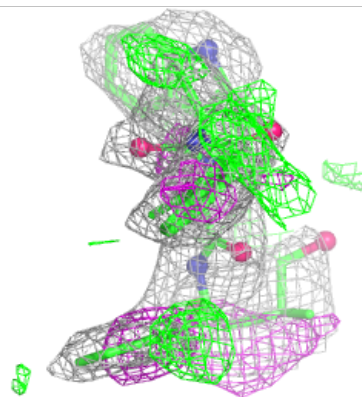
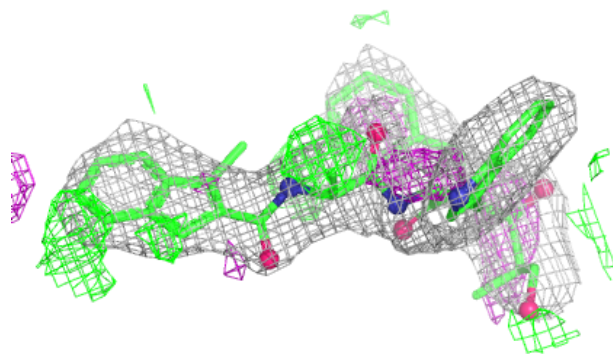
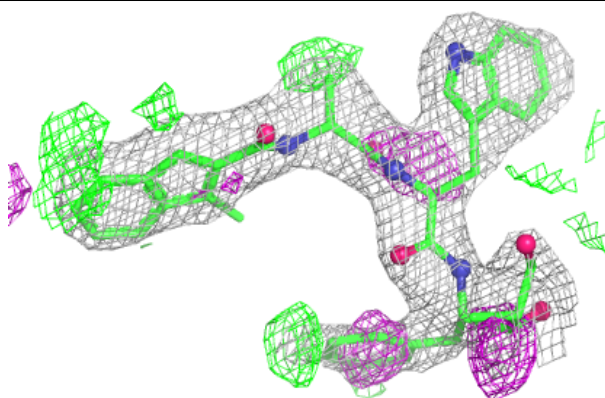
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	N	201	1/1	0.98	0.04	55,55,55,55	0
16	CL	G	302	1/1	0.99	0.07	43,43,43,43	0
16	CL	U	301	1/1	0.99	0.07	44,44,44,44	0
15	MG	I	302	1/1	0.99	0.07	59,59,59,59	0

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.

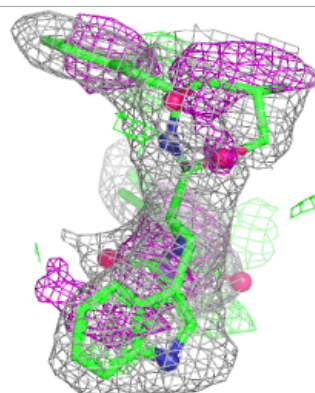
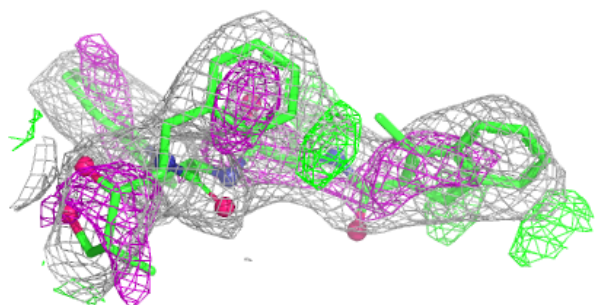
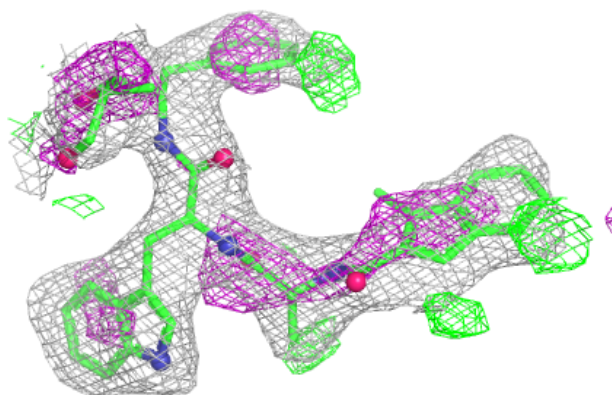
Electron density around 39V Y 302:

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 39V K 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.