



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 01:35 PM UTC

PDB ID : 9FT1 / pdb_00009ft1
Title : Yeast 20S proteasome in complex with epoxyketone inhibitor 9
Authors : Maurits, E.; Huber, E.M.; Dekker, P.M.; Wang, X.; Heinemeyer, W.; Florea, B.I.; Groll, M.; Overkleeft, H.S.
Deposited on : 2024-06-23
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

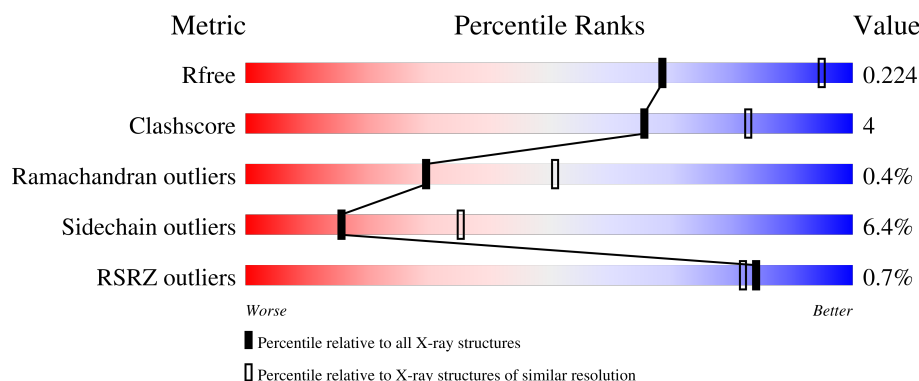
1 Overall quality at a glance

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	% 92% 7% .
1	O	250	91% 8% .
2	B	258	2% 79% 14% 5%
2	P	258	3% 81% 13% 5%
3	C	254	% 82% 10% 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	231	
8	V	231	
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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	MES	b	201	-	-	X	X

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49970 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	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	7			
8	V	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	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-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			

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

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

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

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

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

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

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

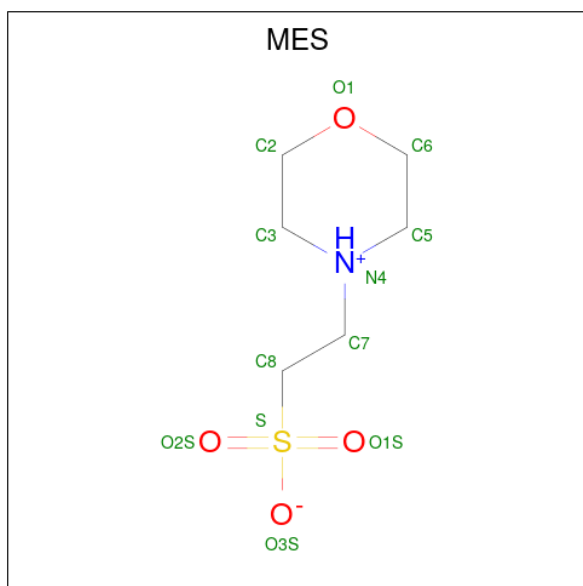
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	H	1	Total	Mg	0	0
			1	1		

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

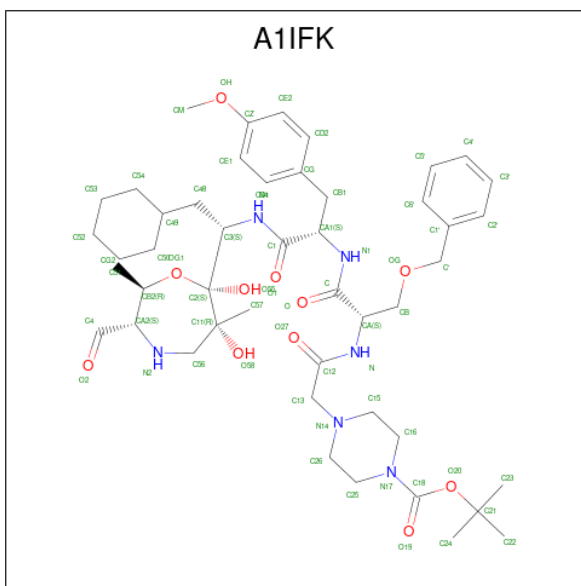
- Molecule 16 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
16	J	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
16	V	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
16	X	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
16	b	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 17 is tert-butyl 4-[2-[[[(2S)-1-[[[(2S)-1-[[[(1S)-2-cyclohexyl-1-[(2R,3S,6R,7S)-3-meth

anoyl-2,6-dimethyl-6,7-bis(oxidanyl)-1,4-oxazepan-7-yl]ethyl]amino]-3-(4-methoxyphenyl)-1-oxidanylidene-propan-2-yl]amino]-1-oxidanylidene-3-phenylmethoxy-propan-2-yl]amino]-2-oxidanylidene-ethyl]piperazine-1-carboxylate (CCD ID: A1IFK) (formula: $C_{47}H_{70}N_6O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			64	47	6	11		
17	K	1	Total	C	N	O	0	0
			64	47	6	11		
17	V	1	Total	C	N	O	0	0
			64	47	6	11		
17	Y	1	Total	C	N	O	0	0
			64	47	6	11		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	14	Total	O	0	0
			14	14		
18	B	14	Total	O	0	0
			14	14		
18	C	11	Total	O	0	0
			11	11		
18	D	11	Total	O	0	0
			11	11		
18	E	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	F	11	Total O 11 11	0	0
18	G	13	Total O 13 13	0	0
18	H	18	Total O 18 18	0	0
18	I	17	Total O 17 17	0	0
18	J	19	Total O 19 19	0	0
18	K	18	Total O 18 18	0	0
18	L	22	Total O 22 22	0	0
18	M	16	Total O 16 16	0	0
18	N	14	Total O 14 14	0	0
18	O	15	Total O 15 15	0	0
18	P	11	Total O 11 11	0	0
18	Q	8	Total O 8 8	0	0
18	R	7	Total O 7 7	0	0
18	S	5	Total O 5 5	0	0
18	T	7	Total O 7 7	0	0
18	U	20	Total O 20 20	0	0
18	V	10	Total O 10 10	0	0
18	W	16	Total O 16 16	0	0
18	X	15	Total O 15 15	0	0
18	Y	15	Total O 15 15	0	0
18	Z	14	Total O 14 14	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	a	15	Total	O	0	0
			15	15		
18	b	18	Total	O	0	0
			18	18		

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.

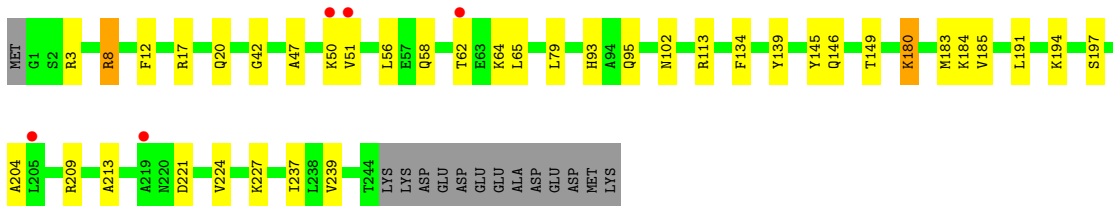
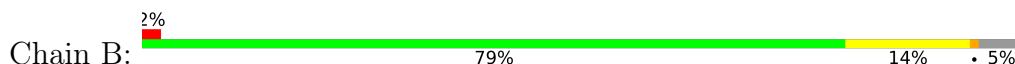
- Molecule 1: Proteasome subunit alpha type-2



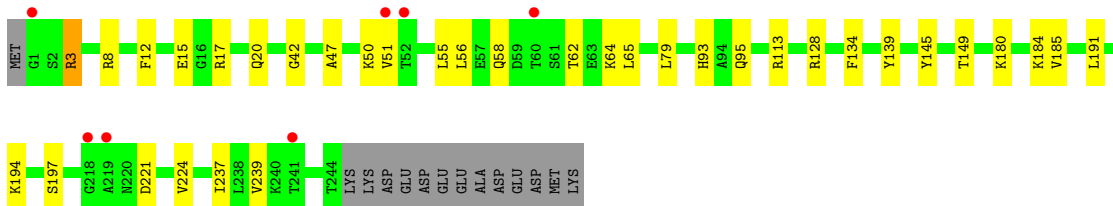
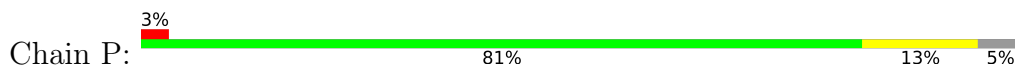
- Molecule 1: Proteasome subunit alpha type-2



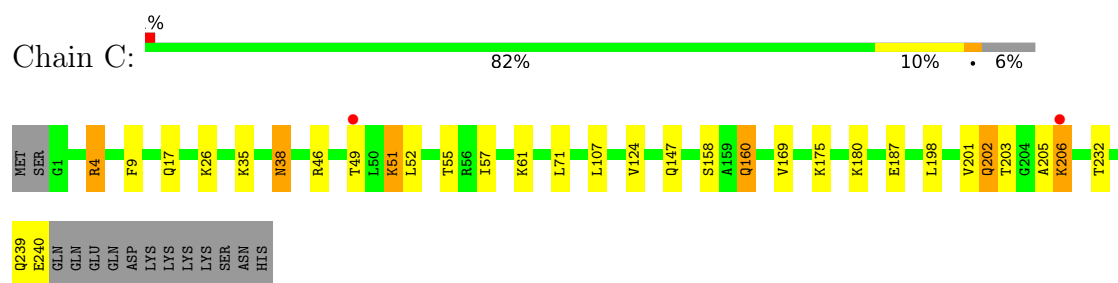
- Molecule 2: Proteasome subunit alpha type-3



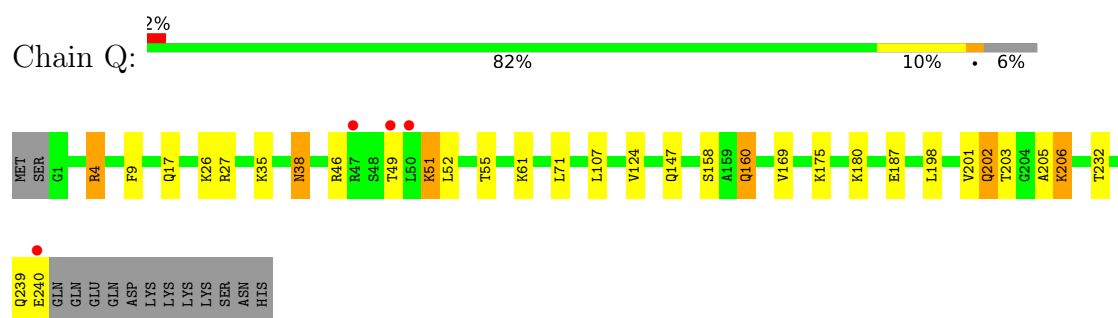
- Molecule 2: Proteasome subunit alpha type-3



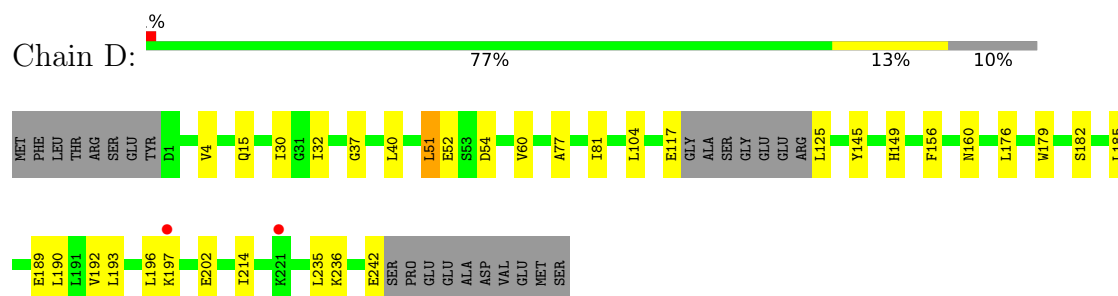
- Molecule 3: Proteasome subunit alpha type-4



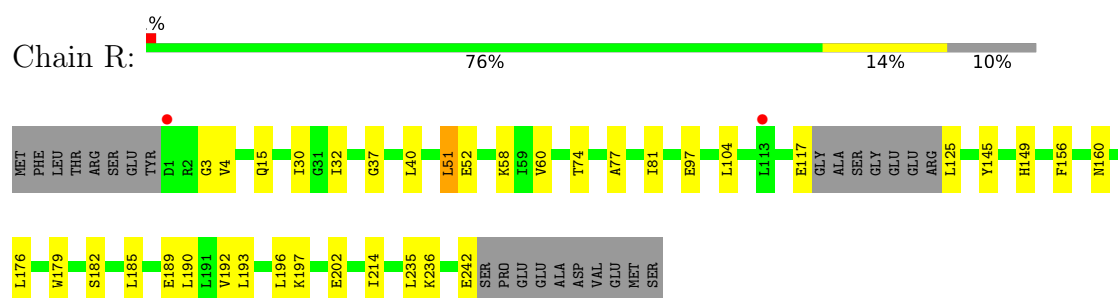
• Molecule 3: Proteasome subunit alpha type-4



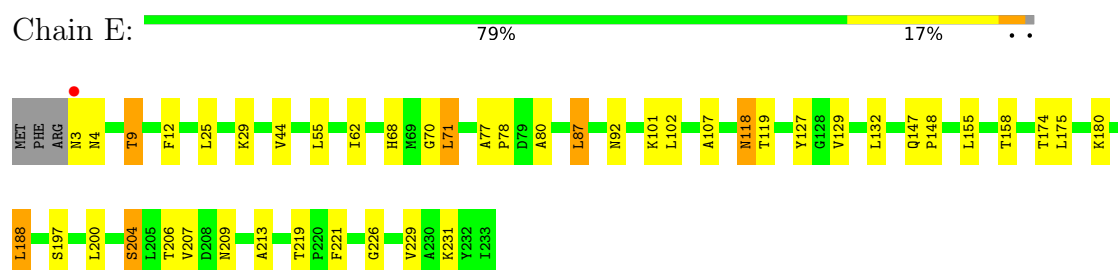
• Molecule 4: Proteasome subunit alpha type-5



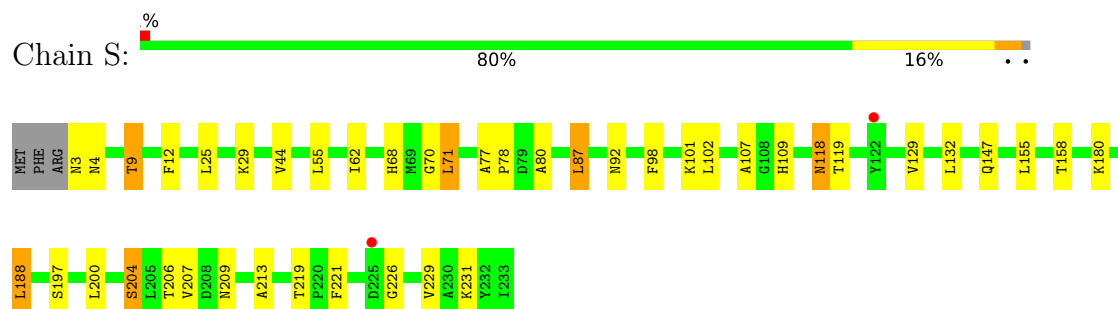
• Molecule 4: Proteasome subunit alpha type-5



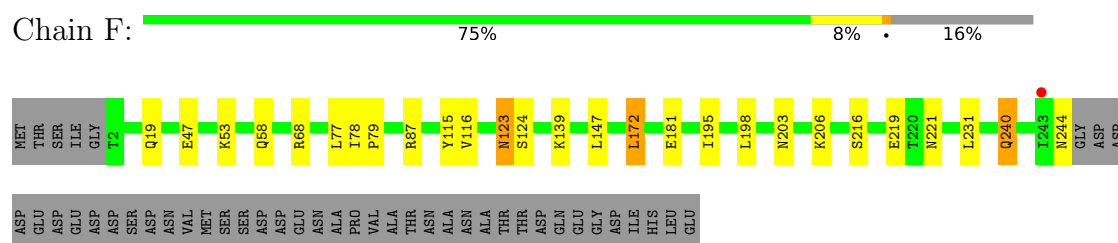
• Molecule 5: Proteasome subunit alpha type-6



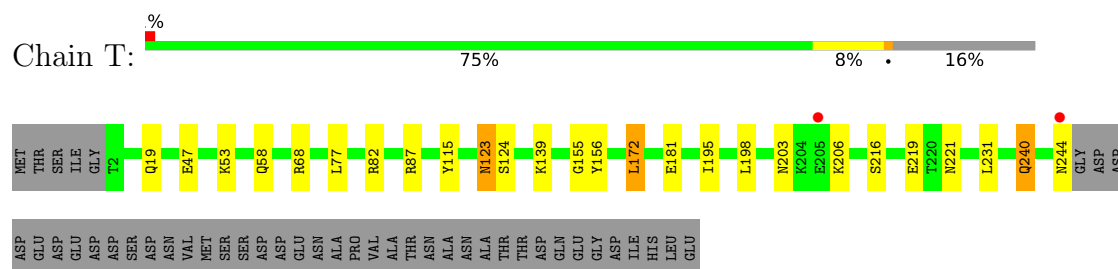
- Molecule 5: Proteasome subunit alpha type-6



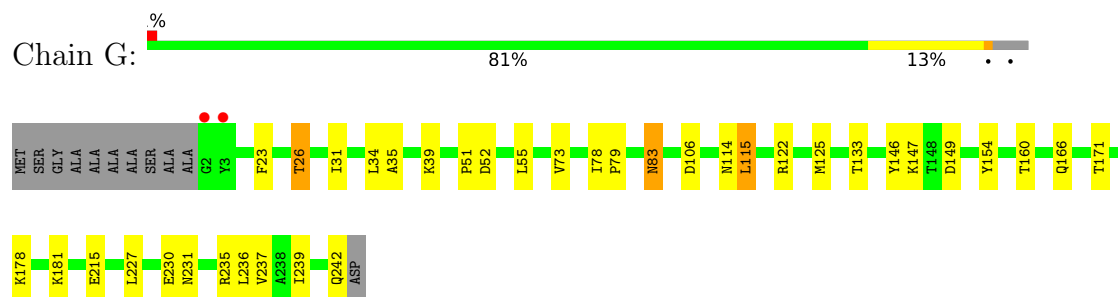
- Molecule 6: Probable proteasome subunit alpha type-7



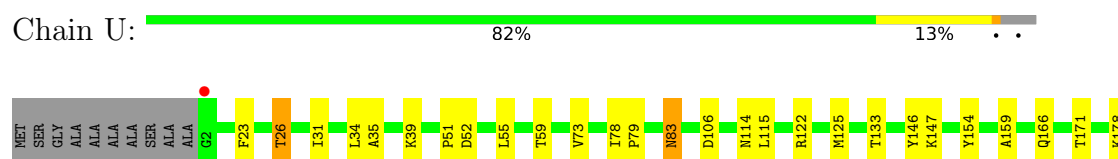
- Molecule 6: Probable proteasome subunit alpha type-7

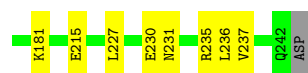


- Molecule 7: Proteasome subunit alpha type-1



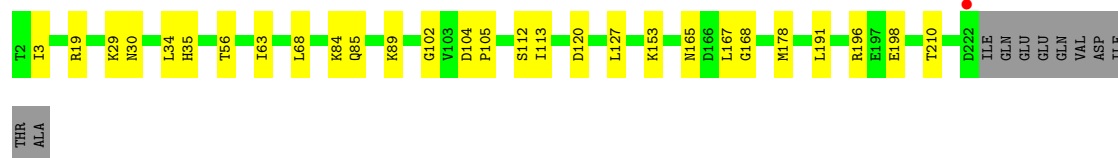
- Molecule 7: Proteasome subunit alpha type-1





- Molecule 8: Proteasome subunit beta type-2

Chain H: 84% 12%



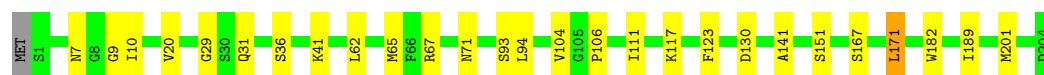
- Molecule 8: Proteasome subunit beta type-2

Chain V: 85% 11%



- Molecule 9: Proteasome subunit beta type-3

Chain I: 86% 13%



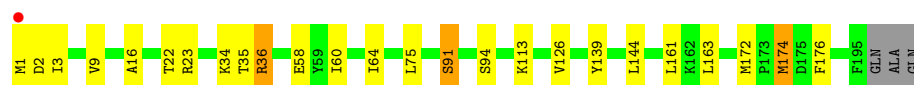
- Molecule 9: Proteasome subunit beta type-3

Chain W: 85% 14%



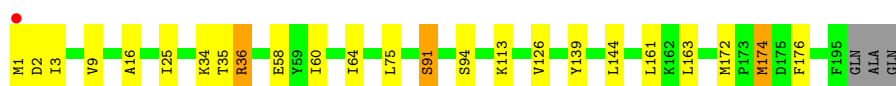
- Molecule 10: Proteasome subunit beta type-4

Chain J: 86% 11%



- Molecule 10: Proteasome subunit beta type-4

Chain X: 86% 11%



- Molecule 11: Proteasome subunit beta type-5

Chain K: 90% 8%



- Molecule 11: Proteasome subunit beta type-5

Chain Y: 90% 8%



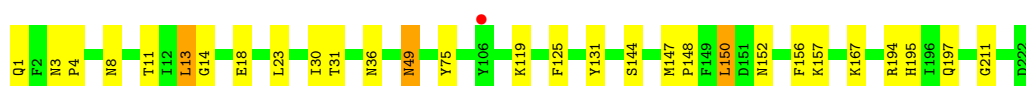
- Molecule 12: Proteasome subunit beta type-6

Chain L: 86% 12%



- Molecule 12: Proteasome subunit beta type-6

Chain Z: 87% 12%



- Molecule 13: Proteasome subunit beta type-7

Chain M: 83% 11% 5%



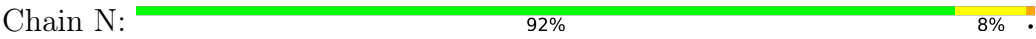
- Molecule 13: Proteasome subunit beta type-7

Chain a: 80% 14% 5%

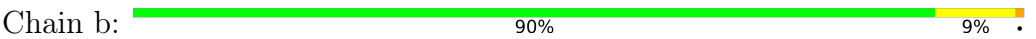




● Molecule 14: Proteasome subunit beta type-1



● Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.00Å 300.67Å 144.54Å 90.00° 113.09° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-2.60) 97.4 (30.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.182 , 0.222 0.176 , 0.224	Depositor DCC
R_{free} test set	15884 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	1.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	49970	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: MG, MES, A1IFK

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	1.02	0/1952	1.39	0/2642
1	O	1.03	0/1952	1.40	0/2642
2	B	1.02	0/1934	1.40	0/2618
2	P	1.02	0/1934	1.41	0/2618
3	C	1.03	0/1910	1.43	0/2586
3	Q	1.04	0/1910	1.44	0/2586
4	D	1.03	0/1837	1.44	0/2475
4	R	1.03	0/1837	1.43	0/2475
5	E	1.03	0/1800	1.40	0/2433
5	S	1.03	0/1800	1.40	0/2433
6	F	1.02	0/1932	1.40	2/2609 (0.1%)
6	T	1.03	0/1932	1.42	2/2609 (0.1%)
7	G	1.01	1/1945 (0.1%)	1.42	0/2634
7	U	1.02	0/1945	1.41	0/2634
8	H	1.02	0/1708	1.38	0/2316
8	V	1.03	0/1708	1.40	0/2316
9	I	1.01	0/1611	1.38	2/2174 (0.1%)
9	W	1.00	0/1611	1.38	2/2174 (0.1%)
10	J	0.99	0/1589	1.35	1/2142 (0.0%)
10	X	0.99	0/1589	1.36	0/2142
11	K	0.99	0/1674	1.36	0/2264
11	Y	0.99	0/1674	1.36	0/2264
12	L	1.01	0/1795	1.33	0/2420
12	Z	1.00	0/1795	1.34	0/2420
13	M	1.02	0/1855	1.32	0/2514
13	a	1.02	0/1855	1.33	1/2514 (0.0%)
14	N	1.01	0/1541	1.38	0/2087
14	b	1.02	0/1541	1.39	0/2087
All	All	1.02	1/50166 (0.0%)	1.39	10/67828 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	149	ASP	N-CA	5.25	1.49	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	77	LEU	CA-C-N	5.95	123.99	120.24
6	T	77	LEU	C-N-CA	5.95	123.99	120.24
13	a	188	ASP	CA-CB-CG	5.58	118.19	112.60
6	F	77	LEU	CA-C-N	5.36	123.61	120.24
6	F	77	LEU	C-N-CA	5.36	123.61	120.24
10	J	23	ARG	CB-CA-C	5.29	118.74	111.23
9	I	67	ARG	CA-C-N	5.25	127.26	120.44
9	I	67	ARG	C-N-CA	5.25	127.26	120.44
9	W	67	ARG	CA-C-N	5.17	127.17	120.44
9	W	67	ARG	C-N-CA	5.17	127.17	120.44

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	7	0
1	O	1915	0	1929	10	0
2	B	1904	0	1904	14	0
2	P	1904	0	1904	15	0
3	C	1881	0	1895	19	0
3	Q	1881	0	1895	22	0
4	D	1813	0	1797	11	0
4	R	1813	0	1797	14	0
5	E	1773	0	1775	23	0
5	S	1773	0	1775	23	0
6	F	1892	0	1883	10	0
6	T	1892	0	1883	10	0
7	G	1907	0	1901	16	0
7	U	1907	0	1901	18	0
8	H	1677	0	1678	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	V	1677	0	1678	10	0
9	I	1581	0	1574	19	0
9	W	1581	0	1574	22	0
10	J	1561	0	1569	10	0
10	X	1561	0	1569	11	0
11	K	1637	0	1585	17	0
11	Y	1637	0	1585	20	0
12	L	1757	0	1711	17	0
12	Z	1757	0	1711	16	0
13	M	1824	0	1832	10	0
13	a	1824	0	1832	16	0
14	N	1512	0	1481	9	0
14	b	1512	0	1481	22	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	K	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	H	12	0	13	0	0
16	J	12	0	13	0	0
16	V	12	0	13	0	0
16	X	12	0	13	1	0
16	b	12	0	13	12	0
17	H	64	0	0	6	0
17	K	64	0	0	2	0
17	V	64	0	0	5	0
17	Y	64	0	0	4	0
18	A	14	0	0	0	0
18	B	14	0	0	0	0
18	C	11	0	0	0	0
18	D	11	0	0	0	0
18	E	5	0	0	0	0
18	F	11	0	0	0	0
18	G	13	0	0	0	0
18	H	18	0	0	0	0
18	I	17	0	0	0	0
18	J	19	0	0	0	0
18	K	18	0	0	0	0
18	L	22	0	0	0	0
18	M	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	N	14	0	0	0	0
18	O	15	0	0	0	0
18	P	11	0	0	0	0
18	Q	8	0	0	1	0
18	R	7	0	0	0	0
18	S	5	0	0	0	0
18	T	7	0	0	0	0
18	U	20	0	0	0	0
18	V	10	0	0	0	0
18	W	16	0	0	0	0
18	X	15	0	0	0	0
18	Y	15	0	0	0	0
18	Z	14	0	0	0	0
18	a	15	0	0	0	0
18	b	18	0	0	1	0
All	All	49970	0	49093	375	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 4.

All (375) 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)
14:b:115:LEU:CD1	16:b:201:MES:H62	1.54	1.36
11:K:73:ARG:HH21	11:K:73:ARG:HG3	1.12	1.12
14:b:115:LEU:HD13	16:b:201:MES:H62	1.23	1.12
14:b:115:LEU:HD11	16:b:201:MES:H62	1.29	1.03
14:b:115:LEU:CD1	16:b:201:MES:C6	2.41	0.98
14:b:115:LEU:HD13	16:b:201:MES:C6	1.95	0.94
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.40	0.85
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.41	0.84
11:Y:4:LEU:HD23	11:Y:4:LEU:C	2.06	0.80
6:F:123:ASN:C	6:F:123:ASN:HD22	1.90	0.80
11:K:4:LEU:C	11:K:4:LEU:HD23	2.08	0.79
17:V:302:A1IFK:C5'	9:W:130:ASP:CB	2.62	0.77
14:b:152:VAL:HA	14:b:175:MET:HE1	1.68	0.76
14:b:115:LEU:HD11	16:b:201:MES:C6	2.13	0.75
7:G:23:PHE:O	7:G:26:THR:HB	1.85	0.75
14:N:152:VAL:HA	14:N:175:MET:HE1	1.69	0.74
7:U:23:PHE:O	7:U:26:THR:HB	1.87	0.74
6:T:123:ASN:C	6:T:123:ASN:HD22	1.95	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:115:LEU:HD21	16:b:201:MES:O1	1.89	0.73
17:H:303:A1IFK:C5'	9:I:130:ASP:HB3	2.19	0.73
17:V:302:A1IFK:C5'	9:W:130:ASP:HB2	2.19	0.72
17:V:302:A1IFK:C5'	9:W:130:ASP:HB3	2.20	0.72
17:H:303:A1IFK:C6'	9:I:130:ASP:HB2	2.20	0.71
11:K:73:ARG:HG3	11:K:73:ARG:NH2	1.91	0.69
17:V:302:A1IFK:C6'	9:W:130:ASP:HB2	2.22	0.69
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.76	0.68
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.59	0.67
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.75	0.67
1:O:12:PHE:H	2:P:20:GLN:HE22	1.44	0.66
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.61	0.66
3:C:51:LYS:O	3:C:52:LEU:HB2	1.96	0.65
11:Y:73:ARG:HH21	11:Y:73:ARG:CG	2.10	0.65
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.61	0.65
12:L:8:ASN:HA	12:L:30:ILE:O	1.98	0.64
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.62	0.64
11:K:27:ALA:O	12:L:137:ARG:NH2	2.30	0.64
12:Z:8:ASN:HA	12:Z:30:ILE:O	1.97	0.64
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.72	0.63
11:Y:69:ARG:CG	11:Y:69:ARG:HH11	2.11	0.63
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.81	0.63
17:H:303:A1IFK:C5'	9:I:130:ASP:CB	2.76	0.62
3:C:35:LYS:HG2	3:C:158:SER:O	1.99	0.62
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.81	0.62
3:Q:202:GLN:HG3	3:Q:203:THR:N	2.15	0.61
11:K:4:LEU:C	11:K:4:LEU:CD2	2.73	0.61
5:E:71:LEU:C	5:E:71:LEU:HD23	2.25	0.61
3:C:202:GLN:HG3	3:C:203:THR:N	2.15	0.61
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.00	0.61
5:S:71:LEU:C	5:S:71:LEU:HD23	2.25	0.61
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.48	0.60
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.02	0.60
3:C:202:GLN:HG3	3:C:203:THR:H	1.67	0.60
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.83	0.60
11:K:53:GLN:O	11:K:57:THR:HG23	2.02	0.59
5:E:12:PHE:H	6:F:19:GLN:HE22	1.51	0.59
14:b:115:LEU:CD2	16:b:201:MES:O1	2.51	0.59
6:F:123:ASN:HD22	6:F:124:SER:N	2.01	0.58
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.68	0.58
1:A:12:PHE:H	2:B:20:GLN:HE22	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:123:ASN:HD22	6:T:124:SER:N	2.02	0.58
2:B:12:PHE:H	3:C:17:GLN:HE22	1.52	0.58
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.51	0.57
12:Z:4:PRO:O	13:a:104:ARG:NH1	2.34	0.57
6:F:240:GLN:HE21	6:F:240:GLN:HA	1.68	0.57
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.52	0.57
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.41	0.56
11:K:4:LEU:HD22	11:K:15:ALA:HB3	1.88	0.56
5:S:12:PHE:H	6:T:19:GLN:HE22	1.54	0.56
8:H:35:HIS:CB	8:H:56:THR:HG21	2.36	0.56
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.87	0.55
5:E:9:THR:HG21	5:E:119:THR:HA	1.88	0.55
3:C:9:PHE:H	4:D:15:GLN:HE22	1.53	0.55
8:H:165:ASN:HD22	13:a:156:ARG:HH11	1.54	0.55
6:T:240:GLN:HE21	6:T:240:GLN:HA	1.70	0.55
8:V:35:HIS:CB	8:V:56:THR:HG21	2.36	0.55
7:G:34:LEU:C	7:G:34:LEU:HD23	2.32	0.55
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.88	0.55
5:E:68:HIS:HE1	5:E:102:LEU:O	1.90	0.54
3:C:198:LEU:HA	3:C:201:VAL:HG12	1.88	0.54
7:U:83:ASN:C	7:U:83:ASN:HD22	2.14	0.54
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.88	0.54
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.37	0.54
2:P:15:GLU:O	3:Q:27:ARG:NH1	2.40	0.54
10:J:174:MET:HA	10:X:174:MET:HA	1.89	0.54
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.42	0.54
5:S:68:HIS:HE1	5:S:102:LEU:O	1.91	0.54
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.89	0.54
3:C:38:ASN:H	3:C:38:ASN:HD22	1.56	0.53
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.91	0.53
8:V:210:THR:HG21	9:W:167:SER:HB3	1.90	0.53
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.43	0.53
10:X:1:MET:HA	10:X:34:LYS:CE	2.39	0.53
10:J:1:MET:HA	10:J:34:LYS:CE	2.38	0.53
7:U:34:LEU:C	7:U:34:LEU:HD23	2.34	0.53
5:S:9:THR:HG21	5:S:119:THR:HA	1.91	0.53
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.73	0.53
5:S:71:LEU:HD23	5:S:71:LEU:O	2.09	0.53
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.74	0.53
3:Q:46:ARG:NH1	3:Q:55:THR:HG21	2.24	0.52
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:170:TYR:O	17:Y:302:A1IFK:C56	2.57	0.52
11:K:170:TYR:O	17:K:302:A1IFK:C56	2.56	0.52
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.10	0.52
5:S:98:PHE:O	13:a:91:TYR:HA	2.09	0.52
10:X:1:MET:HA	10:X:34:LYS:HE3	1.92	0.52
3:C:46:ARG:NH1	3:C:55:THR:HG21	2.25	0.52
3:Q:38:ASN:HD22	3:Q:38:ASN:H	1.57	0.52
10:J:1:MET:HA	10:J:34:LYS:HE3	1.92	0.52
11:Y:4:LEU:HD22	11:Y:15:ALA:HB3	1.92	0.51
8:V:222:ASP:OD1	9:W:74:LYS:NZ	2.42	0.51
11:Y:73:ARG:CG	11:Y:73:ARG:NH2	2.71	0.51
5:E:71:LEU:HD23	5:E:71:LEU:O	2.11	0.51
6:F:123:ASN:C	6:F:123:ASN:ND2	2.63	0.51
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.46	0.51
7:G:73:VAL:HG12	7:G:133:THR:HB	1.91	0.51
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.92	0.51
14:b:128:GLY:HA2	16:b:201:MES:O2S	2.11	0.51
11:K:35:ILE:HB	11:K:45:MET:CE	2.41	0.51
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.93	0.50
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.93	0.50
7:G:83:ASN:C	7:G:83:ASN:HD22	2.20	0.50
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.92	0.50
11:Y:73:ARG:NH2	11:Y:73:ARG:HG3	2.26	0.50
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.75	0.50
11:K:67:GLU:CB	11:K:72:GLU:O	2.60	0.50
7:U:73:VAL:HG12	7:U:133:THR:HB	1.93	0.50
14:b:45:ARG:NH1	18:b:301:HOH:O	2.37	0.50
13:M:43:ILE:HG12	13:M:43:ILE:O	2.11	0.50
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.94	0.50
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.27	0.50
4:R:51:LEU:C	4:R:51:LEU:HD12	2.37	0.49
4:D:51:LEU:HD12	4:D:51:LEU:C	2.37	0.49
4:D:51:LEU:HD12	4:D:52:GLU:N	2.27	0.49
8:H:29:LYS:HE2	12:Z:194:ARG:NH2	2.27	0.49
13:a:43:ILE:HG12	13:a:43:ILE:O	2.11	0.49
3:C:202:GLN:CG	3:C:203:THR:H	2.25	0.49
13:a:30:TYR:OH	16:b:201:MES:H61	2.13	0.49
4:R:185:LEU:O	4:R:189:GLU:HG3	2.13	0.49
1:O:119:GLN:O	1:O:122:THR:HB	2.13	0.49
7:G:78:ILE:N	7:G:79:PRO:CD	2.76	0.49
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:201:VAL:HG13	3:C:202:GLN:N	2.27	0.48
3:Q:202:GLN:CG	3:Q:203:THR:H	2.26	0.48
11:K:67:GLU:HA	11:K:72:GLU:O	2.13	0.48
11:Y:35:ILE:HB	11:Y:45:MET:CE	2.44	0.48
3:Q:38:ASN:HD22	3:Q:38:ASN:N	2.12	0.48
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.79	0.48
5:E:68:HIS:CD2	5:E:101:LYS:HE2	2.49	0.48
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.95	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.96	0.48
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.95	0.48
1:A:83:ARG:HE	7:G:114:ASN:ND2	2.12	0.48
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.95	0.48
4:D:77:ALA:O	4:D:81:ILE:HG12	2.13	0.48
1:O:83:ARG:HE	7:U:114:ASN:ND2	2.12	0.48
7:U:78:ILE:N	7:U:79:PRO:CD	2.76	0.47
1:A:83:ARG:HE	7:G:114:ASN:HD21	1.62	0.47
4:R:51:LEU:HD12	4:R:52:GLU:N	2.29	0.47
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.80	0.47
17:H:303:A1IFK:C6'	9:I:130:ASP:CB	2.92	0.47
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.49	0.47
3:C:38:ASN:HD22	3:C:38:ASN:N	2.11	0.47
10:J:3:ILE:HD12	10:J:176:PHE:CG	2.50	0.47
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.16	0.47
11:Y:69:ARG:CG	11:Y:69:ARG:NH1	2.73	0.47
1:A:119:GLN:O	1:A:122:THR:HB	2.14	0.47
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.11	0.47
3:C:71:LEU:C	3:C:71:LEU:HD23	2.39	0.47
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.97	0.47
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.63	0.47
14:b:115:LEU:HD11	16:b:201:MES:H21	1.95	0.47
3:C:202:GLN:CG	3:C:203:THR:N	2.78	0.47
14:N:35:THR:HG21	13:a:228:TYR:HE2	1.80	0.47
8:V:84:LYS:HG3	8:V:85:GLN:N	2.29	0.47
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.96	0.47
1:A:149:GLN:O	1:A:156:TYR:HA	2.15	0.47
1:O:149:GLN:O	1:O:156:TYR:HA	2.15	0.47
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.30	0.47
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.97	0.46
8:H:210:THR:HG21	9:I:167:SER:HB3	1.96	0.46
4:R:77:ALA:O	4:R:81:ILE:HG12	2.15	0.46
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:147:MET:N	12:L:148:PRO:HD2	2.30	0.46
2:P:42:GLY:HA2	2:P:145:TYR:CE1	2.50	0.46
10:X:91:SER:HA	10:X:94:SER:OG	2.16	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.96	0.46
1:O:55:LEU:HB3	7:U:159:ALA:O	2.16	0.46
1:O:115:ALA:HB1	1:O:154:GLY:O	2.16	0.46
5:S:155:LEU:HD13	5:S:158:THR:HB	1.98	0.46
6:T:156:TYR:CE2	7:U:55:LEU:HD23	2.51	0.46
5:E:70:GLY:HA3	5:E:221:PHE:CE2	2.51	0.46
12:L:18:GLU:O	12:L:119:LYS:HA	2.16	0.46
3:Q:71:LEU:C	3:Q:71:LEU:HD23	2.41	0.46
4:D:185:LEU:O	4:D:189:GLU:HG3	2.15	0.46
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.62	0.46
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.97	0.46
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.63	0.46
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.46
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.50	0.46
10:X:25:ILE:HD11	11:Y:134:THR:HG21	1.97	0.46
2:B:42:GLY:HA2	2:B:145:TYR:CE1	2.51	0.46
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.98	0.46
11:Y:100:MET:HE2	11:Y:129:VAL:HG23	1.97	0.46
5:S:68:HIS:CD2	5:S:101:LYS:HE2	2.52	0.45
5:S:118:ASN:N	5:S:118:ASN:HD22	2.13	0.45
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.51	0.45
5:S:109:HIS:HB3	6:T:82:ARG:NH2	2.31	0.45
14:b:115:LEU:CD2	16:b:201:MES:C6	2.95	0.45
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.98	0.45
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.98	0.45
8:H:19:ARG:NH1	8:H:167:LEU:O	2.49	0.45
8:H:84:LYS:HG3	8:H:85:GLN:N	2.30	0.45
16:X:201:MES:H62	11:Y:98:GLY:HA3	1.98	0.45
12:Z:13:LEU:C	12:Z:13:LEU:HD12	2.42	0.45
5:E:155:LEU:HD13	5:E:158:THR:HB	1.99	0.45
8:H:168:GLY:O	17:H:303:A1IFK:C56	2.65	0.45
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.14	0.45
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.51	0.45
5:E:118:ASN:N	5:E:118:ASN:HD22	2.14	0.45
9:I:7:ASN:HA	9:I:29:GLY:O	2.17	0.45
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.98	0.45
12:L:13:LEU:HD12	12:L:14:GLY:N	2.32	0.45
4:R:149:HIS:O	4:R:156:PHE:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.99	0.45
5:S:206:THR:OG1	5:S:209:ASN:HB2	2.17	0.45
13:M:96:LEU:O	13:M:100:MET:HG2	2.18	0.44
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.99	0.44
3:Q:202:GLN:CG	3:Q:203:THR:N	2.79	0.44
9:W:65:MET:CE	9:W:93:SER:HB3	2.47	0.44
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.32	0.44
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.51	0.44
17:V:302:A1IFK:C57	17:V:302:A1IFK:C1	2.95	0.44
4:D:104:LEU:C	4:D:104:LEU:HD13	2.42	0.44
9:I:171:LEU:HD11	9:I:201:MET:HB3	1.99	0.44
13:M:27:LEU:HB2	13:M:192:SER:HB3	2.00	0.44
4:R:104:LEU:HD13	4:R:104:LEU:C	2.43	0.44
5:S:62:ILE:HG21	5:S:213:ALA:HB2	1.99	0.44
11:Y:25:TRP:CZ3	12:Z:144:SER:HA	2.53	0.44
1:A:44:VAL:HG23	1:A:211:LEU:HD21	1.99	0.44
5:E:226:GLY:O	5:E:229:VAL:HG22	2.18	0.44
1:O:44:VAL:HG23	1:O:211:LEU:HD21	1.98	0.44
9:W:7:ASN:HA	9:W:29:GLY:O	2.17	0.44
10:X:60:ILE:O	10:X:64:ILE:HG12	2.17	0.44
11:Y:73:ARG:HH21	11:Y:73:ARG:HG3	1.82	0.44
12:L:13:LEU:HD12	12:L:13:LEU:C	2.42	0.44
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.99	0.44
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.65	0.44
2:P:3:ARG:NH2	4:R:3:GLY:HA2	2.33	0.44
5:E:62:ILE:HG21	5:E:213:ALA:HB2	2.00	0.44
5:S:226:GLY:O	5:S:229:VAL:HG22	2.18	0.44
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.43	0.44
12:Z:13:LEU:HD12	12:Z:14:GLY:N	2.32	0.44
9:W:65:MET:HE1	9:W:93:SER:HB3	2.00	0.43
13:a:96:LEU:O	13:a:100:MET:HG2	2.17	0.43
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.54	0.43
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.98	0.43
10:X:139:TYR:CE2	10:X:172:MET:HE2	2.54	0.43
1:A:115:ALA:HB1	1:A:154:GLY:O	2.17	0.43
9:I:65:MET:CE	9:I:93:SER:HB3	2.49	0.43
11:K:86:LEU:C	11:K:86:LEU:HD13	2.43	0.43
5:S:44:VAL:HG23	5:S:188:LEU:HD13	1.99	0.43
5:E:127:TYR:O	5:E:148:PRO:CB	2.67	0.43
5:E:206:THR:OG1	5:E:209:ASN:HB2	2.19	0.43
17:H:303:A1IFK:C5'	9:I:130:ASP:HB2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:37:ILE:HG23	11:K:60:GLY:HA2	2.00	0.43
9:W:94:LEU:HD11	9:W:106:PRO:HG2	1.99	0.43
12:Z:18:GLU:O	12:Z:119:LYS:HA	2.19	0.43
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.53	0.43
5:S:71:LEU:C	5:S:71:LEU:CD2	2.92	0.43
8:V:112:SER:OG	8:V:120:ASP:HB2	2.19	0.43
13:a:27:LEU:HB2	13:a:192:SER:HB3	2.01	0.43
3:C:201:VAL:O	3:C:202:GLN:CB	2.66	0.43
11:K:25:TRP:CZ3	12:L:144:SER:HA	2.54	0.43
13:a:147:GLY:O	13:a:151:ALA:HB3	2.19	0.43
7:G:34:LEU:HD23	7:G:35:ALA:N	2.34	0.43
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.01	0.43
5:E:9:THR:CG2	5:E:119:THR:HA	2.48	0.43
13:M:43:ILE:HG21	13:M:64:GLU:HG2	2.01	0.42
8:V:214:LYS:O	9:W:197:ARG:HA	2.19	0.42
9:W:171:LEU:HD11	9:W:201:MET:HB3	2.01	0.42
13:a:43:ILE:HG21	13:a:64:GLU:HG2	2.01	0.42
14:b:14:LEU:HD11	14:b:100:ALA:HB3	2.00	0.42
5:E:44:VAL:HG23	5:E:188:LEU:HD13	2.00	0.42
11:K:100:MET:HE2	11:K:129:VAL:HG23	2.01	0.42
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.52	0.42
13:a:26:ASN:HA	13:a:39:VAL:O	2.18	0.42
9:I:62:LEU:CD1	9:I:104:VAL:HG21	2.49	0.42
2:B:180:LYS:O	2:B:183:MET:HB2	2.19	0.42
2:B:204:ALA:O	2:B:209:ARG:NH2	2.52	0.42
4:D:149:HIS:O	4:D:156:PHE:HA	2.19	0.42
10:J:139:TYR:CE2	10:J:172:MET:HE2	2.54	0.42
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.55	0.42
12:L:196:ILE:HG12	8:V:24:PRO:O	2.18	0.42
13:M:26:ASN:HA	13:M:39:VAL:O	2.19	0.42
14:N:133:PHE:HA	14:b:132:THR:O	2.20	0.42
7:U:34:LEU:HD23	7:U:35:ALA:N	2.35	0.42
2:B:213:ALA:HA	2:B:227:LYS:O	2.19	0.42
1:O:83:ARG:HE	7:U:114:ASN:HD21	1.67	0.42
2:P:95:GLN:HE21	9:W:68:TYR:HA	1.84	0.42
14:N:14:LEU:HD11	14:N:100:ALA:HB3	2.01	0.42
5:S:197:SER:HA	5:S:200:LEU:CD1	2.49	0.42
9:W:111:ILE:HD12	9:W:189:ILE:HG22	2.01	0.42
17:Y:302:A1IFK:N	17:Y:302:A1IFK:C'	2.83	0.42
3:C:46:ARG:NH1	3:C:206:LYS:HG2	2.35	0.42
12:L:195:HIS:HD2	12:L:197:GLN:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:62:LEU:CD1	9:W:104:VAL:HG21	2.49	0.42
13:a:127:LEU:HG	13:a:142:LEU:HD12	2.00	0.42
9:I:65:MET:HE1	9:I:93:SER:HB3	2.00	0.42
5:S:200:LEU:HD13	5:S:204:SER:HA	2.01	0.42
7:U:227:LEU:HB3	7:U:231:ASN:HB2	2.01	0.42
11:Y:73:ARG:HH21	11:Y:73:ARG:HG2	1.84	0.42
7:G:147:LYS:O	7:G:154:TYR:HA	2.20	0.42
2:P:134:PHE:O	2:P:149:THR:HA	2.20	0.42
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.55	0.42
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.02	0.42
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	2.01	0.42
5:E:71:LEU:C	5:E:71:LEU:CD2	2.91	0.42
10:J:60:ILE:O	10:J:64:ILE:HG12	2.19	0.42
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.55	0.41
5:E:197:SER:HA	5:E:200:LEU:CD1	2.49	0.41
8:H:112:SER:OG	8:H:120:ASP:HB2	2.20	0.41
13:M:159:VAL:HG23	13:M:159:VAL:O	2.20	0.41
7:U:83:ASN:C	7:U:83:ASN:ND2	2.77	0.41
5:E:200:LEU:HD13	5:E:204:SER:HA	2.01	0.41
7:G:52:ASP:HB3	7:G:55:LEU:HG	2.02	0.41
7:G:73:VAL:CG1	7:G:133:THR:HB	2.50	0.41
3:Q:46:ARG:NH1	3:Q:206:LYS:HG2	2.35	0.41
5:S:9:THR:CG2	5:S:119:THR:HA	2.50	0.41
5:S:71:LEU:HA	5:S:132:LEU:O	2.19	0.41
11:Y:41:LEU:HD23	11:Y:41:LEU:HA	1.87	0.41
7:G:83:ASN:C	7:G:83:ASN:ND2	2.79	0.41
7:U:147:LYS:O	7:U:154:TYR:HA	2.20	0.41
13:a:159:VAL:HG23	13:a:159:VAL:O	2.20	0.41
3:Q:51:LYS:HB3	18:Q:305:HOH:O	2.20	0.41
7:G:239:ILE:O	7:G:242:GLN:HB3	2.21	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.83	0.41
9:I:111:ILE:HD12	9:I:189:ILE:HG22	2.02	0.41
11:K:25:TRP:CH2	12:L:144:SER:HA	2.55	0.41
11:K:41:LEU:HD23	11:K:41:LEU:HA	1.87	0.41
12:Z:152:ASN:O	12:Z:156:PHE:HA	2.20	0.41
5:E:71:LEU:HA	5:E:132:LEU:O	2.21	0.41
7:U:73:VAL:CG1	7:U:133:THR:HB	2.51	0.41
2:B:134:PHE:O	2:B:149:THR:HA	2.20	0.41
5:E:80:ALA:HB2	5:E:129:VAL:HG21	2.03	0.41
6:F:116:VAL:HG21	6:F:147:LEU:HD21	2.02	0.41
7:G:115:LEU:HD12	7:G:115:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:91:SER:HA	10:J:94:SER:OG	2.20	0.41
4:R:97:GLU:OE1	12:Z:75:TYR:OH	2.26	0.41
7:U:52:ASP:HB3	7:U:55:LEU:HG	2.02	0.41
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.56	0.41
8:H:102:GLY:HA2	8:H:178:MET:SD	2.61	0.41
3:Q:160:GLN:HA	3:Q:160:GLN:NE2	2.22	0.41
5:S:80:ALA:HB2	5:S:129:VAL:HG21	2.03	0.41
6:F:87:ARG:HG2	6:F:115:TYR:CD2	2.56	0.41
12:L:152:ASN:O	12:L:156:PHE:HA	2.21	0.41
9:W:167:SER:O	9:W:171:LEU:HB2	2.21	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.40
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.02	0.40
7:U:78:ILE:HG22	7:U:79:PRO:HD3	2.03	0.40
14:b:83:LYS:HG3	14:b:119:VAL:HG22	2.03	0.40
7:G:227:LEU:HB3	7:G:231:ASN:HB2	2.03	0.40
17:K:302:A1IFK:O19	17:K:302:A1IFK:C22	2.69	0.40
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.56	0.40
4:R:58:LYS:HE2	4:R:74:THR:HG21	2.03	0.40
6:T:87:ARG:HG2	6:T:115:TYR:CD2	2.56	0.40
17:Y:302:A1IFK:O19	17:Y:302:A1IFK:C22	2.69	0.40
14:b:45:ARG:HG2	14:b:52:THR:HB	2.04	0.40
6:F:78:ILE:N	6:F:79:PRO:CD	2.85	0.40
1:O:37:ILE:HD12	1:O:192:ALA:HB2	2.03	0.40
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.34	0.40
2:P:8:ARG:HD2	3:Q:4:ARG:NH2	2.36	0.40
13:a:139:SER:HB3	13:a:141:THR:O	2.21	0.40
5:E:174:THR:O	5:E:175:LEU:C	2.64	0.40
2:P:55:LEU:HD12	2:P:55:LEU:HA	1.98	0.40
17:Y:302:A1IFK:O27	17:Y:302:A1IFK:C15	2.70	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%)	240 (97%)	5 (2%)	3 (1%)	10	23
1	O	248/250 (99%)	240 (97%)	5 (2%)	3 (1%)	10	23
2	B	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	16	34
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	16	34
3	C	238/254 (94%)	225 (94%)	10 (4%)	3 (1%)	9	21
3	Q	238/254 (94%)	225 (94%)	10 (4%)	3 (1%)	9	21
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	217 (95%)	12 (5%)	0	100	100
5	S	229/234 (98%)	216 (94%)	13 (6%)	0	100	100
6	F	241/288 (84%)	232 (96%)	8 (3%)	1 (0%)	30	51
6	T	241/288 (84%)	232 (96%)	8 (3%)	1 (0%)	30	51
7	G	239/252 (95%)	231 (97%)	7 (3%)	1 (0%)	30	51
7	U	239/252 (95%)	229 (96%)	9 (4%)	1 (0%)	30	51
8	H	219/231 (95%)	215 (98%)	4 (2%)	0	100	100
8	V	219/231 (95%)	215 (98%)	4 (2%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
10	J	193/198 (98%)	190 (98%)	1 (0%)	2 (1%)	12	28
10	X	193/198 (98%)	190 (98%)	1 (0%)	2 (1%)	12	28
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%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6272/6610 (95%)	6061 (97%)	187 (3%)	24 (0%)	30	51

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	202	GLN
6	F	203	ASN
3	Q	202	GLN
6	T	203	ASN
3	C	239	GLN
1	O	2	THR
3	Q	239	GLN
1	A	2	THR
1	A	50	LYS
1	A	166	LYS
3	C	205	ALA
1	O	166	LYS
3	Q	205	ALA
2	B	221	ASP
1	O	50	LYS
2	B	51	VAL
10	J	2	ASP
2	P	51	VAL
2	P	221	ASP
10	X	2	ASP
7	G	51	PRO
10	J	9	VAL
7	U	51	PRO
10	X	9	VAL

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%)	201 (96%)	8 (4%)	29	56
1	O	209/209 (100%)	201 (96%)	8 (4%)	29	56
2	B	203/216 (94%)	185 (91%)	18 (9%)	9	20
2	P	203/216 (94%)	187 (92%)	16 (8%)	11	26
3	C	212/226 (94%)	195 (92%)	17 (8%)	11	25
3	Q	212/226 (94%)	195 (92%)	17 (8%)	11	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	194/215 (90%)	177 (91%)	17 (9%)	9	21
4	R	194/215 (90%)	178 (92%)	16 (8%)	10	24
5	E	190/193 (98%)	173 (91%)	17 (9%)	9	20
5	S	190/193 (98%)	173 (91%)	17 (9%)	9	20
6	F	201/239 (84%)	187 (93%)	14 (7%)	14	31
6	T	201/239 (84%)	187 (93%)	14 (7%)	14	31
7	G	206/210 (98%)	189 (92%)	17 (8%)	10	23
7	U	206/210 (98%)	190 (92%)	16 (8%)	11	26
8	H	180/189 (95%)	168 (93%)	12 (7%)	15	33
8	V	180/189 (95%)	168 (93%)	12 (7%)	15	33
9	I	172/173 (99%)	166 (96%)	6 (4%)	32	59
9	W	172/173 (99%)	166 (96%)	6 (4%)	32	59
10	J	173/175 (99%)	164 (95%)	9 (5%)	21	44
10	X	173/175 (99%)	165 (95%)	8 (5%)	24	49
11	K	168/168 (100%)	161 (96%)	7 (4%)	26	52
11	Y	168/168 (100%)	160 (95%)	8 (5%)	23	47
12	L	185/185 (100%)	176 (95%)	9 (5%)	22	47
12	Z	185/185 (100%)	177 (96%)	8 (4%)	26	51
13	M	199/208 (96%)	183 (92%)	16 (8%)	11	25
13	a	199/208 (96%)	183 (92%)	16 (8%)	11	25
14	N	162/162 (100%)	157 (97%)	5 (3%)	35	63
14	b	162/162 (100%)	157 (97%)	5 (3%)	35	63
All	All	5308/5536 (96%)	4969 (94%)	339 (6%)	16	35

All (339) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	29	LYS
1	A	59	GLU
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	177	LYS

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Mol	Chain	Res	Type
1	A	231	LYS
2	B	3	ARG
2	B	8	ARG
2	B	17	ARG
2	B	50	LYS
2	B	56	LEU
2	B	58	GLN
2	B	62	THR
2	B	65	LEU
2	B	79	LEU
2	B	102	ASN
2	B	180	LYS
2	B	184	LYS
2	B	185	VAL
2	B	191	LEU
2	B	194	LYS
2	B	197	SER
2	B	237	ILE
2	B	239	VAL
3	C	4	ARG
3	C	26	LYS
3	C	38	ASN
3	C	49	THR
3	C	51	LYS
3	C	61	LYS
3	C	107	LEU
3	C	124	VAL
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	187	GLU
3	C	206	LYS
3	C	232	THR
3	C	240	GLU
4	D	4	VAL
4	D	40	LEU
4	D	51	LEU
4	D	54	ASP
4	D	60	VAL
4	D	117	GLU

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Mol	Chain	Res	Type
4	D	125	LEU
4	D	176	LEU
4	D	182	SER
4	D	190	LEU
4	D	193	LEU
4	D	197	LYS
4	D	202	GLU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	3	ASN
5	E	4	ASN
5	E	9	THR
5	E	25	LEU
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	87	LEU
5	E	92	ASN
5	E	118	ASN
5	E	147	GLN
5	E	180	LYS
5	E	188	LEU
5	E	204	SER
5	E	207	VAL
5	E	219	THR
5	E	231	LYS
6	F	47	GLU
6	F	53	LYS
6	F	58	GLN
6	F	68	ARG
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	198	LEU
6	F	206	LYS
6	F	221	ASN
6	F	231	LEU
6	F	240	GLN
6	F	244	ASN

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Mol	Chain	Res	Type
7	G	26	THR
7	G	31	ILE
7	G	39	LYS
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	160	THR
7	G	166	GLN
7	G	171	THR
7	G	178	LYS
7	G	181	LYS
7	G	215	GLU
7	G	230	GLU
7	G	235	ARG
7	G	236	LEU
7	G	237	VAL
8	H	3	ILE
8	H	30	ASN
8	H	34	LEU
8	H	63	ILE
8	H	68	LEU
8	H	89	LYS
8	H	113	ILE
8	H	127	LEU
8	H	153	LYS
8	H	191	LEU
8	H	196	ARG
8	H	198	GLU
9	I	31	GLN
9	I	117	LYS
9	I	123	PHE
9	I	151	SER
9	I	171	LEU
9	I	182	TRP
10	J	22	THR
10	J	35	THR
10	J	36	ARG
10	J	75	LEU
10	J	91	SER
10	J	113	LYS
10	J	144	LEU

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Mol	Chain	Res	Type
10	J	163	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	31	VAL
11	K	35	ILE
11	K	41	LEU
11	K	73	ARG
11	K	148	LEU
12	L	1	GLN
12	L	11	THR
12	L	13	LEU
12	L	23	LEU
12	L	49	ASN
12	L	137	ARG
12	L	150	LEU
12	L	157	LYS
12	L	167	LYS
13	M	2	GLN
13	M	10	SER
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	106	LYS
13	M	135	VAL
13	M	161	ARG
13	M	187	ARG
13	M	192	SER
13	M	212	LEU
13	M	215	GLU
13	M	225	ILE
13	M	226	LYS
13	M	233	ILE
14	N	9	LYS
14	N	36	ARG
14	N	119	VAL
14	N	144	GLU
14	N	178	LEU
1	O	2	THR
1	O	29	LYS
1	O	59	GLU

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Mol	Chain	Res	Type
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
1	O	177	LYS
1	O	231	LYS
2	P	3	ARG
2	P	17	ARG
2	P	50	LYS
2	P	56	LEU
2	P	58	GLN
2	P	62	THR
2	P	65	LEU
2	P	79	LEU
2	P	180	LYS
2	P	184	LYS
2	P	185	VAL
2	P	191	LEU
2	P	194	LYS
2	P	197	SER
2	P	237	ILE
2	P	239	VAL
3	Q	4	ARG
3	Q	26	LYS
3	Q	38	ASN
3	Q	49	THR
3	Q	51	LYS
3	Q	61	LYS
3	Q	107	LEU
3	Q	124	VAL
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	187	GLU
3	Q	206	LYS
3	Q	232	THR
3	Q	240	GLU
4	R	4	VAL
4	R	40	LEU
4	R	51	LEU
4	R	60	VAL

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Mol	Chain	Res	Type
4	R	117	GLU
4	R	125	LEU
4	R	176	LEU
4	R	182	SER
4	R	190	LEU
4	R	193	LEU
4	R	197	LYS
4	R	202	GLU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	3	ASN
5	S	4	ASN
5	S	9	THR
5	S	25	LEU
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	87	LEU
5	S	92	ASN
5	S	118	ASN
5	S	147	GLN
5	S	180	LYS
5	S	188	LEU
5	S	204	SER
5	S	207	VAL
5	S	219	THR
5	S	231	LYS
6	T	47	GLU
6	T	53	LYS
6	T	58	GLN
6	T	68	ARG
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	198	LEU
6	T	206	LYS
6	T	221	ASN
6	T	231	LEU
6	T	240	GLN

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Mol	Chain	Res	Type
6	T	244	ASN
7	U	26	THR
7	U	31	ILE
7	U	39	LYS
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	166	GLN
7	U	171	THR
7	U	178	LYS
7	U	181	LYS
7	U	215	GLU
7	U	230	GLU
7	U	235	ARG
7	U	236	LEU
7	U	237	VAL
8	V	3	ILE
8	V	30	ASN
8	V	34	LEU
8	V	63	ILE
8	V	68	LEU
8	V	89	LYS
8	V	113	ILE
8	V	127	LEU
8	V	153	LYS
8	V	191	LEU
8	V	196	ARG
8	V	198	GLU
9	W	31	GLN
9	W	117	LYS
9	W	123	PHE
9	W	151	SER
9	W	171	LEU
9	W	182	TRP
10	X	35	THR
10	X	36	ARG
10	X	75	LEU
10	X	91	SER
10	X	113	LYS
10	X	144	LEU
10	X	163	LEU

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Mol	Chain	Res	Type
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	31	VAL
11	Y	35	ILE
11	Y	41	LEU
11	Y	69	ARG
11	Y	73	ARG
11	Y	148	LEU
12	Z	1	GLN
12	Z	11	THR
12	Z	13	LEU
12	Z	23	LEU
12	Z	49	ASN
12	Z	150	LEU
12	Z	157	LYS
12	Z	167	LYS
13	a	2	GLN
13	a	10	SER
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	106	LYS
13	a	135	VAL
13	a	161	ARG
13	a	187	ARG
13	a	192	SER
13	a	212	LEU
13	a	215	GLU
13	a	225	ILE
13	a	226	LYS
13	a	233	ILE
14	b	9	LYS
14	b	36	ARG
14	b	119	VAL
14	b	144	GLU
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (186) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
1	A	149	GLN
2	B	20	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	155	ASN
2	B	167	ASN
2	B	176	GLN
2	B	232	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	165	ASN
3	C	233	GLN
4	D	15	GLN
4	D	100	ASN
4	D	106	GLN
4	D	146	GLN
4	D	160	ASN
4	D	198	GLN
4	D	217	GLN
4	D	225	ASN
5	E	68	HIS
5	E	90	GLN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	143	HIS
6	F	191	GLN
6	F	203	ASN
6	F	240	GLN

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Mol	Chain	Res	Type
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	175	ASN
8	H	22	GLN
8	H	30	ASN
8	H	57	GLN
8	H	66	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
9	I	63	ASN
9	I	88	GLN
9	I	172	ASN
10	J	37	GLN
10	J	55	GLN
10	J	63	ASN
10	J	146	HIS
10	J	147	HIS
10	J	191	GLN
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	143	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	29	ASN
12	L	36	ASN
12	L	49	ASN
12	L	79	HIS
12	L	80	ASN
13	M	2	GLN
13	M	18	ASN
13	M	48	ASN
13	M	62	HIS
13	M	102	GLN
13	M	108	ASN

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Mol	Chain	Res	Type
13	M	179	ASN
13	M	194	ASN
14	N	38	HIS
14	N	69	GLN
14	N	161	GLN
1	O	30	GLN
1	O	149	GLN
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	146	GLN
2	P	155	ASN
2	P	167	ASN
2	P	176	GLN
2	P	232	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	165	ASN
3	Q	233	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	106	GLN
4	R	146	GLN
4	R	160	ASN
4	R	198	GLN
4	R	207	ASN
4	R	217	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	147	GLN
5	S	151	ASN
5	S	184	ASN

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Mol	Chain	Res	Type
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	143	HIS
6	T	191	GLN
6	T	203	ASN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	175	ASN
7	U	186	ASN
8	V	30	ASN
8	V	57	GLN
8	V	66	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	31	GLN
9	W	37	ASN
9	W	44	HIS
9	W	63	ASN
9	W	88	GLN
10	X	37	GLN
10	X	55	GLN
10	X	63	ASN
10	X	118	GLN
10	X	146	HIS
10	X	147	HIS
10	X	191	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	29	ASN

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Mol	Chain	Res	Type
12	Z	36	ASN
12	Z	49	ASN
12	Z	76	HIS
12	Z	80	ASN
12	Z	135	GLN
12	Z	159	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	69	GLN
14	b	141	ASN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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	A1IFK	K	302	11	63,68,68	2.00	14 (22%)	79,96,96	1.36	8 (10%)
16	MES	V	301	-	12,12,12	0.72	0	15,16,16	0.35	0
16	MES	H	301	-	12,12,12	0.71	0	15,16,16	0.32	0
17	A1IFK	H	303	8	63,68,68	1.79	8 (12%)	79,96,96	1.55	11 (13%)
16	MES	J	201	-	12,12,12	0.77	0	15,16,16	0.45	0
17	A1IFK	V	302	8	63,68,68	1.80	8 (12%)	79,96,96	1.58	14 (17%)
16	MES	X	201	-	12,12,12	0.73	0	15,16,16	0.32	0
16	MES	b	201	-	12,12,12	0.81	0	15,16,16	0.70	1 (6%)
17	A1IFK	Y	302	11	63,68,68	2.12	11 (17%)	79,96,96	1.40	10 (12%)

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	A1IFK	K	302	11	-	10/49/99/99	0/4/5/5
16	MES	V	301	-	-	1/6/14/14	0/1/1/1
16	MES	H	301	-	-	2/6/14/14	0/1/1/1
17	A1IFK	H	303	8	-	2/49/99/99	0/4/5/5
16	MES	J	201	-	-	5/6/14/14	0/1/1/1
17	A1IFK	V	302	8	-	3/49/99/99	0/4/5/5
16	MES	X	201	-	-	1/6/14/14	0/1/1/1
16	MES	b	201	-	-	0/6/14/14	0/1/1/1
17	A1IFK	Y	302	11	-	9/49/99/99	0/4/5/5

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	302	A1IFK	CB2-CA2	7.68	1.65	1.53
17	H	303	A1IFK	CB1-CG	-6.93	1.35	1.51
17	K	302	A1IFK	CB1-CG	-6.90	1.35	1.51
17	Y	302	A1IFK	CB1-CG	-6.80	1.35	1.51
17	K	302	A1IFK	O58-C11	-6.20	1.36	1.44
17	Y	302	A1IFK	C'-C1'	-5.89	1.36	1.50
17	V	302	A1IFK	CB1-CG	-5.84	1.37	1.51
17	V	302	A1IFK	C'-C1'	-5.73	1.37	1.50
17	Y	302	A1IFK	O58-C11	-5.51	1.37	1.44
17	H	303	A1IFK	C'-C1'	-5.32	1.38	1.50
17	K	302	A1IFK	C'-C1'	-4.94	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	V	302	A1IFK	O58-C11	-4.85	1.37	1.44
17	K	302	A1IFK	OG1-CB2	-4.62	1.37	1.43
17	V	302	A1IFK	O20-C21	-4.44	1.40	1.48
17	H	303	A1IFK	OG1-CB2	-4.37	1.38	1.43
17	V	302	A1IFK	OG1-CB2	-4.19	1.38	1.43
17	H	303	A1IFK	O58-C11	-4.15	1.38	1.44
17	H	303	A1IFK	O20-C21	-3.73	1.41	1.48
17	Y	302	A1IFK	O20-C21	-3.63	1.42	1.48
17	H	303	A1IFK	CB2-CA2	3.43	1.58	1.53
17	Y	302	A1IFK	OG1-CB2	-3.41	1.39	1.43
17	K	302	A1IFK	C57-C11	-3.36	1.48	1.52
17	K	302	A1IFK	CB2-CA2	3.26	1.58	1.53
17	K	302	A1IFK	O20-C21	-2.86	1.43	1.48
17	K	302	A1IFK	O55-C2	-2.59	1.34	1.39
17	Y	302	A1IFK	OH-CZ	-2.46	1.32	1.37
17	K	302	A1IFK	C50-C49	-2.44	1.45	1.52
17	Y	302	A1IFK	C57-C11	-2.41	1.49	1.52
17	K	302	A1IFK	CD1-CG	-2.38	1.34	1.38
17	V	302	A1IFK	C18-N17	-2.32	1.31	1.35
17	V	302	A1IFK	O55-C2	-2.27	1.35	1.39
17	Y	302	A1IFK	CD1-CG	-2.23	1.34	1.38
17	V	302	A1IFK	C2-C3	-2.22	1.50	1.54
17	K	302	A1IFK	OH-CZ	-2.18	1.33	1.37
17	Y	302	A1IFK	C53-C54	-2.12	1.47	1.53
17	K	302	A1IFK	C12-N	-2.12	1.29	1.34
17	Y	302	A1IFK	CE1-CZ	-2.12	1.34	1.38
17	K	302	A1IFK	CE1-CZ	-2.07	1.34	1.38
17	H	303	A1IFK	C12-N	-2.04	1.29	1.34
17	K	302	A1IFK	CE1-CD1	-2.04	1.35	1.38
17	H	303	A1IFK	C18-N17	-2.01	1.31	1.35

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	303	A1IFK	O20-C18-N17	5.62	119.30	110.78
17	Y	302	A1IFK	O20-C18-N17	5.06	118.45	110.78
17	V	302	A1IFK	O20-C18-N17	5.03	118.41	110.78
17	K	302	A1IFK	O20-C18-N17	4.94	118.28	110.78
17	Y	302	A1IFK	C25-N17-C16	4.57	122.00	112.68
17	K	302	A1IFK	C25-N17-C16	4.50	121.86	112.68
17	H	303	A1IFK	C21-O20-C18	-4.33	116.15	120.92
17	V	302	A1IFK	C25-N17-C16	4.30	121.45	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	303	A1IFK	C25-N17-C16	4.13	121.11	112.68
17	V	302	A1IFK	C13-N14-C26	-4.12	104.74	111.14
17	V	302	A1IFK	O55-C2-C11	3.33	114.09	106.08
17	V	302	A1IFK	C13-N14-C15	-3.27	106.07	111.14
17	V	302	A1IFK	C21-O20-C18	-3.24	117.34	120.92
17	H	303	A1IFK	C3-N4-C1	-3.15	118.39	123.37
17	Y	302	A1IFK	C48-C49-C54	-3.08	104.55	111.71
17	H	303	A1IFK	C13-N14-C26	-3.07	106.38	111.14
17	H	303	A1IFK	O20-C18-O19	-2.95	121.69	126.43
17	V	302	A1IFK	O20-C18-O19	-2.87	121.82	126.43
17	H	303	A1IFK	O19-C18-N17	-2.86	119.00	124.30
17	K	302	A1IFK	O20-C18-O19	-2.86	121.83	126.43
17	Y	302	A1IFK	C13-N14-C26	-2.74	106.88	111.14
17	K	302	A1IFK	C48-C49-C54	-2.74	105.33	111.71
17	Y	302	A1IFK	O19-C18-N17	-2.72	119.26	124.30
17	V	302	A1IFK	CB2-CA2-N2	-2.69	105.71	111.75
17	V	302	A1IFK	C'-OG-CB	-2.64	106.73	112.66
17	Y	302	A1IFK	O20-C18-O19	-2.58	122.28	126.43
17	Y	302	A1IFK	OG1-CB2-CA2	2.53	113.16	108.85
17	V	302	A1IFK	O19-C18-N17	-2.51	119.65	124.30
17	H	303	A1IFK	O55-C2-C11	2.50	112.08	106.08
17	Y	302	A1IFK	CM-OH-CZ	-2.49	112.16	117.50
17	K	302	A1IFK	O19-C18-N17	-2.38	119.89	124.30
17	H	303	A1IFK	C48-C49-C54	-2.34	106.26	111.71
16	b	201	MES	O1S-S-C8	-2.26	103.31	106.73
17	Y	302	A1IFK	O55-C2-C11	2.22	111.42	106.08
17	V	302	A1IFK	OG1-CB2-CA2	2.19	112.57	108.85
17	V	302	A1IFK	C12-C13-N14	-2.18	108.34	113.41
17	K	302	A1IFK	OG1-CB2-CA2	2.16	112.53	108.85
17	K	302	A1IFK	CM-OH-CZ	-2.16	112.87	117.50
17	H	303	A1IFK	C12-C13-N14	-2.13	108.45	113.41
17	H	303	A1IFK	C26-N14-C15	2.07	113.31	108.84
17	K	302	A1IFK	O55-C2-C11	2.06	111.03	106.08
17	V	302	A1IFK	C26-C25-N17	2.05	114.50	110.42
17	V	302	A1IFK	C51-C50-C49	-2.01	107.84	112.08
17	Y	302	A1IFK	C15-C16-N17	2.01	114.42	110.42

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	J	201	MES	C8-C7-N4-C3

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Mol	Chain	Res	Type	Atoms
16	J	201	MES	C7-C8-S-O2S
16	J	201	MES	C7-C8-S-O3S
17	Y	302	A1IFK	CA-CB-OG-C'
17	K	302	A1IFK	C24-C21-O20-C18
17	K	302	A1IFK	C22-C21-O20-C18
17	K	302	A1IFK	C23-C21-O20-C18
17	Y	302	A1IFK	C22-C21-O20-C18
17	Y	302	A1IFK	C23-C21-O20-C18
17	Y	302	A1IFK	C24-C21-O20-C18
16	H	301	MES	C8-C7-N4-C3
16	H	301	MES	C8-C7-N4-C5
17	K	302	A1IFK	N1-CA1-CB1-CG
17	K	302	A1IFK	O-C-CA-N
17	H	303	A1IFK	N1-CA1-CB1-CG
16	J	201	MES	C7-C8-S-O1S
17	Y	302	A1IFK	N1-CA1-CB1-CG
17	Y	302	A1IFK	O-C-CA-N
17	Y	302	A1IFK	N4-C3-C48-C49
17	V	302	A1IFK	CA-CB-OG-C'
17	V	302	A1IFK	O19-C18-O20-C21
16	J	201	MES	C8-C7-N4-C5
16	V	301	MES	N4-C7-C8-S
17	K	302	A1IFK	N-CA-CB-OG
17	K	302	A1IFK	N1-C-CA-N
17	K	302	A1IFK	O1-C1-CA1-N1
17	Y	302	A1IFK	O1-C1-CA1-N1
16	X	201	MES	C8-C7-N4-C5
17	V	302	A1IFK	O-C-CA-N
17	K	302	A1IFK	O-C-CA-CB
17	Y	302	A1IFK	N4-C1-CA1-N1
17	H	303	A1IFK	O-C-CA-N
17	K	302	A1IFK	N4-C1-CA1-N1

There are no ring outliers.

6 monomers are involved in 30 short contacts:

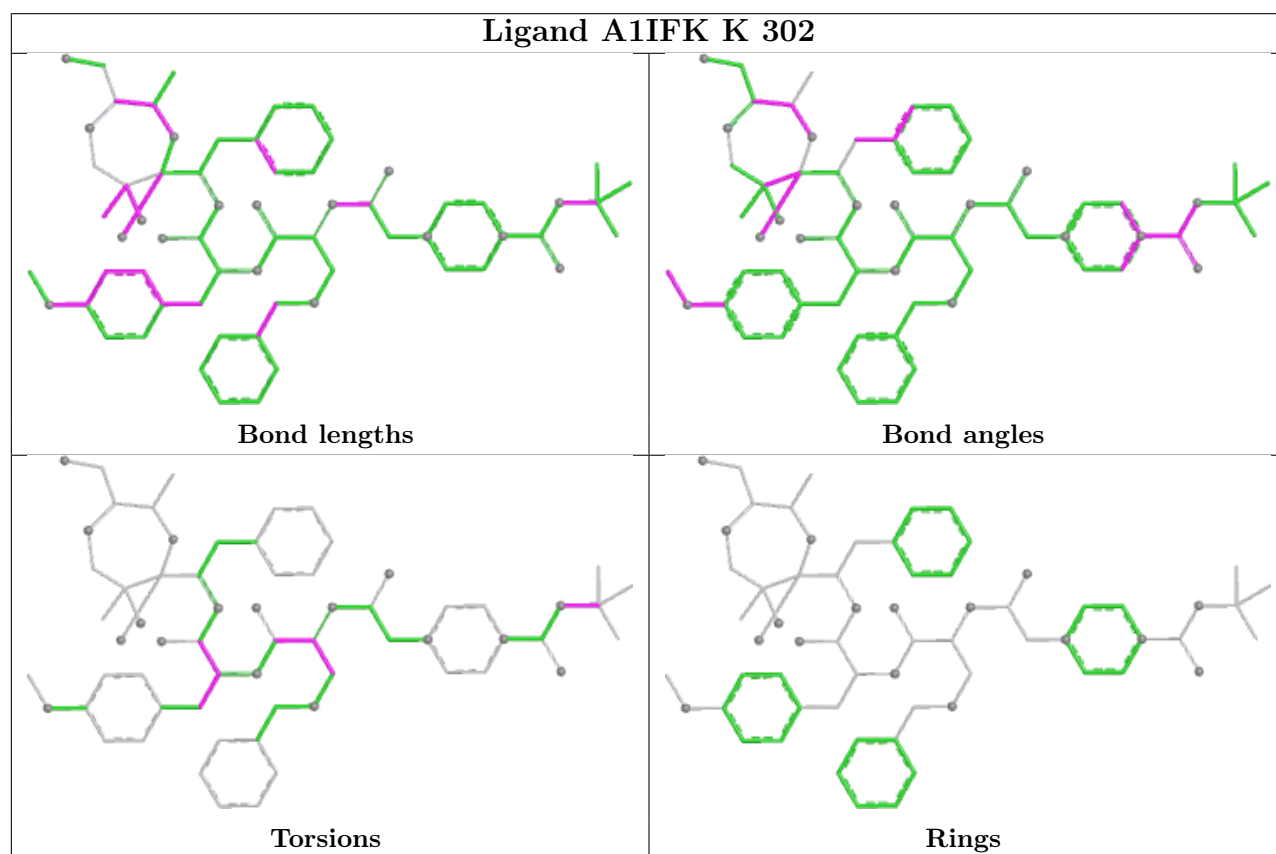
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	302	A1IFK	2	0
17	H	303	A1IFK	6	0
17	V	302	A1IFK	5	0
16	X	201	MES	1	0
16	b	201	MES	12	0

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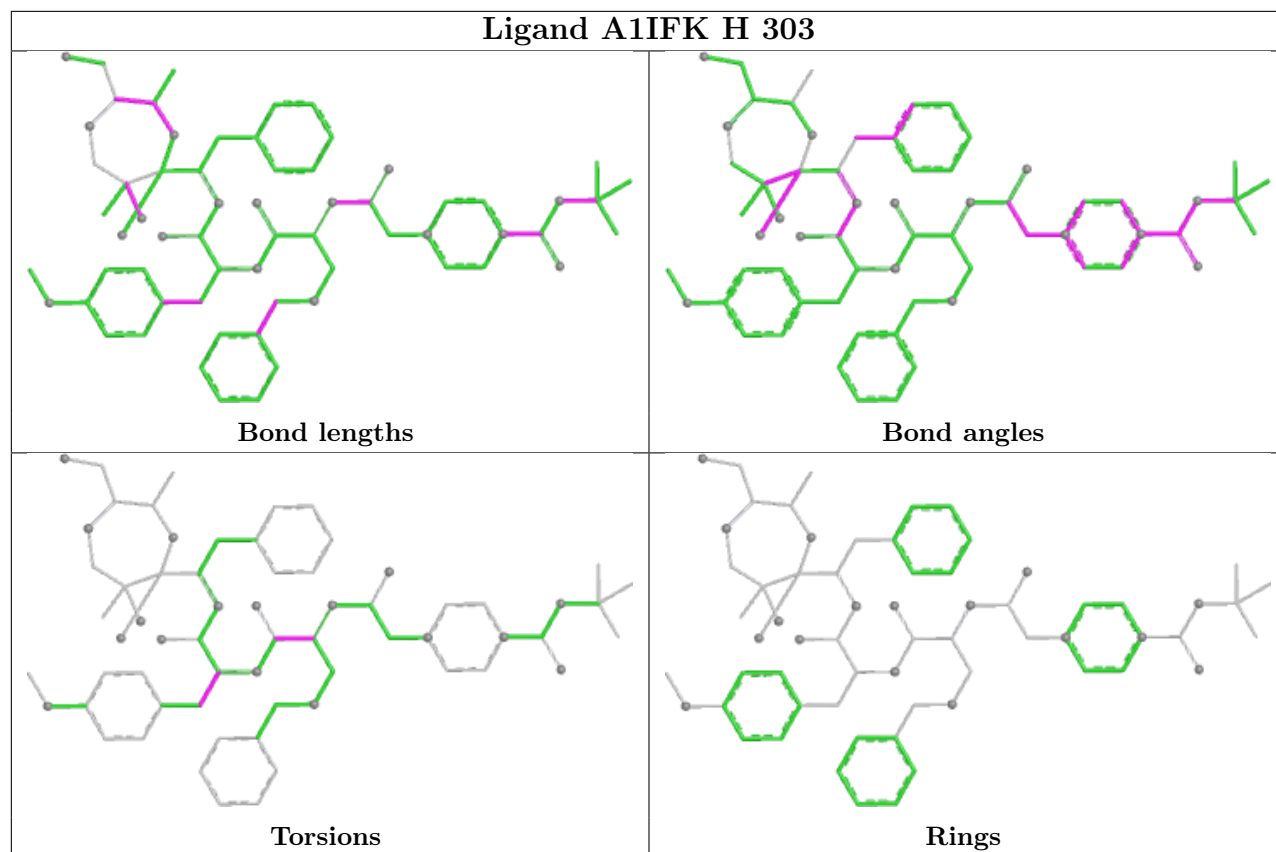
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	302	A1IFK	4	0

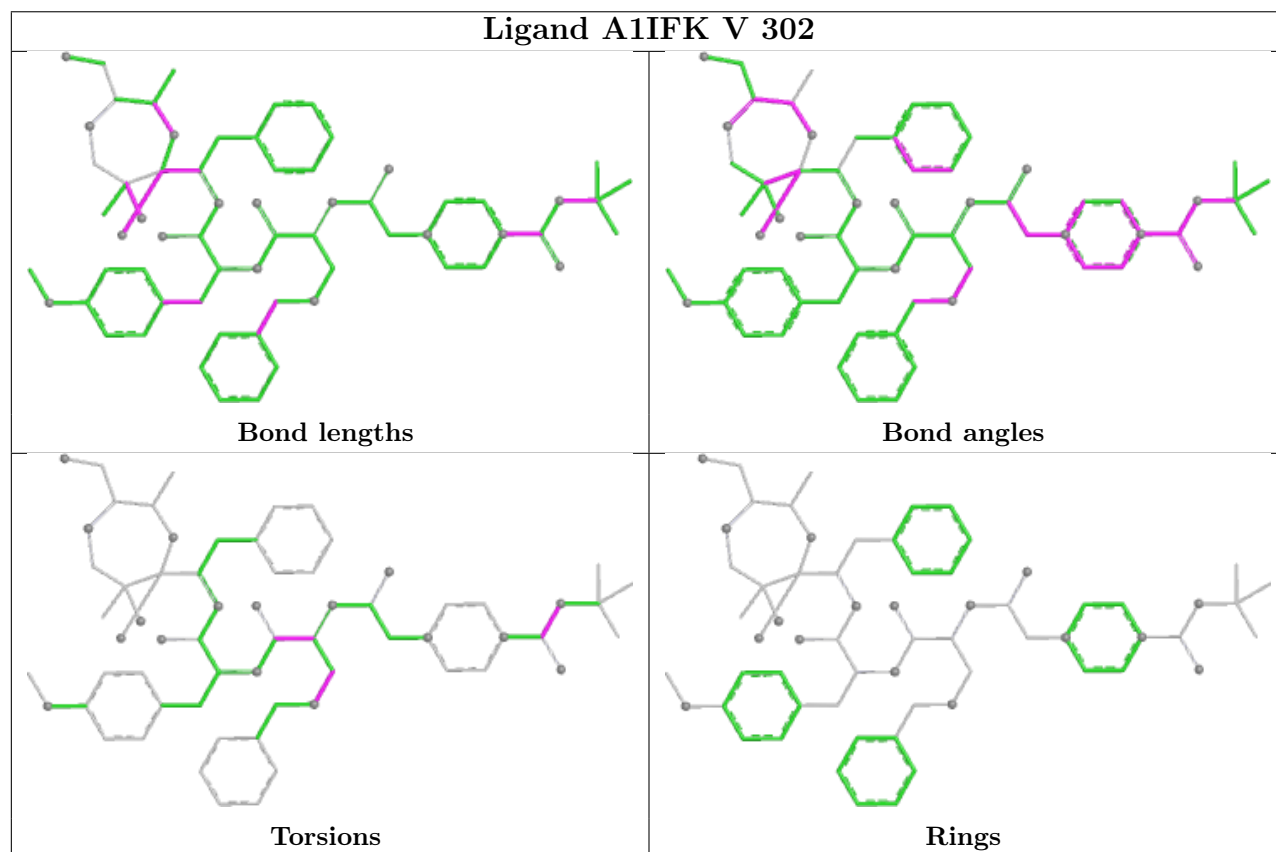
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

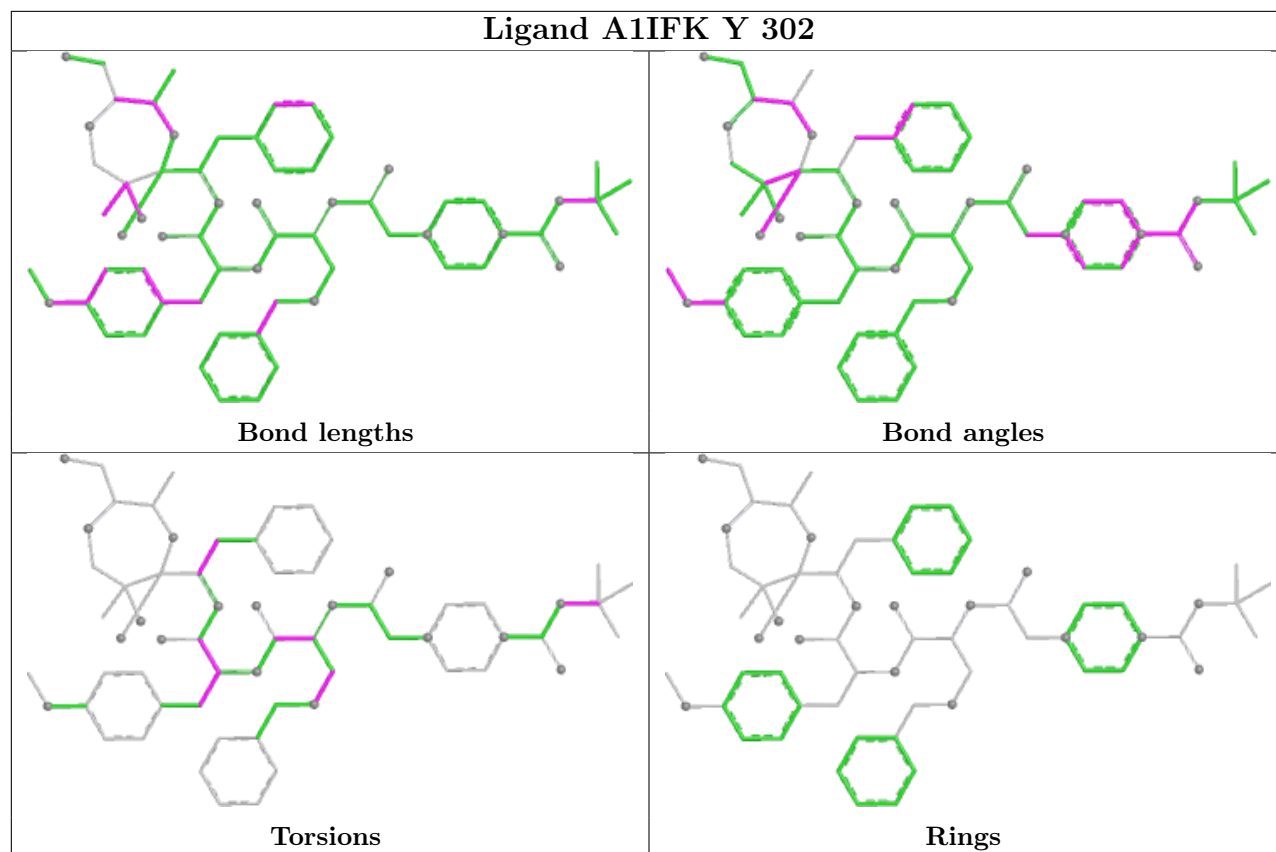


Ligand A1IFK H 303



Ligand A1IFK V 302





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%)	-0.47	2 (0%) 82 80	45, 60, 95, 136	0
1	O	250/250 (100%)	-0.46	1 (0%) 88 86	49, 67, 104, 131	0
2	B	244/258 (94%)	-0.24	5 (2%) 65 60	43, 64, 121, 166	0
2	P	244/258 (94%)	-0.16	7 (2%) 53 48	48, 67, 122, 153	0
3	C	240/254 (94%)	-0.29	2 (0%) 82 80	44, 66, 126, 155	0
3	Q	240/254 (94%)	-0.17	4 (1%) 69 64	53, 80, 142, 171	0
4	D	235/260 (90%)	-0.41	2 (0%) 81 78	47, 69, 101, 134	0
4	R	235/260 (90%)	-0.30	2 (0%) 81 78	51, 72, 109, 134	0
5	E	231/234 (98%)	-0.34	1 (0%) 88 86	50, 71, 103, 129	0
5	S	231/234 (98%)	-0.27	2 (0%) 81 78	49, 77, 113, 132	0
6	F	243/288 (84%)	-0.41	1 (0%) 88 86	42, 65, 106, 135	0
6	T	243/288 (84%)	-0.32	2 (0%) 82 80	47, 71, 113, 136	0
7	G	241/252 (95%)	-0.41	2 (0%) 82 80	43, 62, 98, 133	0
7	U	241/252 (95%)	-0.45	1 (0%) 88 86	46, 63, 97, 118	0
8	H	221/231 (95%)	-0.46	1 (0%) 87 85	44, 58, 84, 135	0
8	V	221/231 (95%)	-0.44	0 100 100	44, 63, 84, 130	0
9	I	204/205 (99%)	-0.60	0 100 100	41, 55, 82, 111	0
9	W	204/205 (99%)	-0.62	0 100 100	40, 57, 82, 112	0
10	J	195/198 (98%)	-0.55	1 (0%) 87 85	38, 55, 82, 118	0
10	X	195/198 (98%)	-0.59	1 (0%) 87 85	43, 58, 80, 130	0
11	K	211/211 (100%)	-0.60	1 (0%) 87 85	42, 55, 76, 101	0
11	Y	211/211 (100%)	-0.55	0 100 100	45, 57, 81, 102	0
12	L	222/222 (100%)	-0.62	0 100 100	39, 58, 81, 91	0
12	Z	222/222 (100%)	-0.50	1 (0%) 87 85	41, 59, 87, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.54	2 (0%) 81 78	41, 58, 84, 121	0
13	a	233/246 (94%)	-0.55	3 (1%) 75 71	43, 58, 80, 127	0
14	N	196/196 (100%)	-0.65	0 100 100	40, 54, 80, 111	0
14	b	196/196 (100%)	-0.57	0 100 100	41, 54, 84, 104	0
All	All	6332/6610 (95%)	-0.44	44 (0%) 84 82	38, 62, 104, 171	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	51	VAL	4.3
3	Q	50	LEU	4.0
2	B	51	VAL	4.0
13	a	233	ILE	4.0
2	B	50	LYS	3.3
1	A	1	MET	3.2
12	Z	106	TYR	3.2
4	R	1	ASP	3.1
2	P	219	ALA	3.1
13	a	232	LYS	3.0
13	M	1	THR	2.9
13	M	233	ILE	2.9
8	H	222	ASP	2.8
10	X	1	MET	2.8
5	S	122	TYR	2.7
7	U	2	GLY	2.7
2	P	218	GLY	2.6
1	A	2	THR	2.6
10	J	1	MET	2.5
3	Q	240	GLU	2.5
11	K	73	ARG	2.4
13	a	1	THR	2.4
7	G	2	GLY	2.3
2	B	219	ALA	2.3
3	C	206	LYS	2.3
6	F	243	ILE	2.2
4	D	221	LYS	2.2
2	P	52	THR	2.2
6	T	244	ASN	2.2
1	O	2	THR	2.2
2	P	1	GLY	2.2
5	E	3	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
5	S	225	ASP	2.2
2	B	62	THR	2.1
6	T	205	GLU	2.1
4	D	197	LYS	2.1
3	Q	47	ARG	2.1
2	P	60	THR	2.1
2	B	205	LEU	2.1
2	P	241	THR	2.0
3	C	49	THR	2.0
4	R	113	LEU	2.0
7	G	3	TYR	2.0
3	Q	49	THR	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.

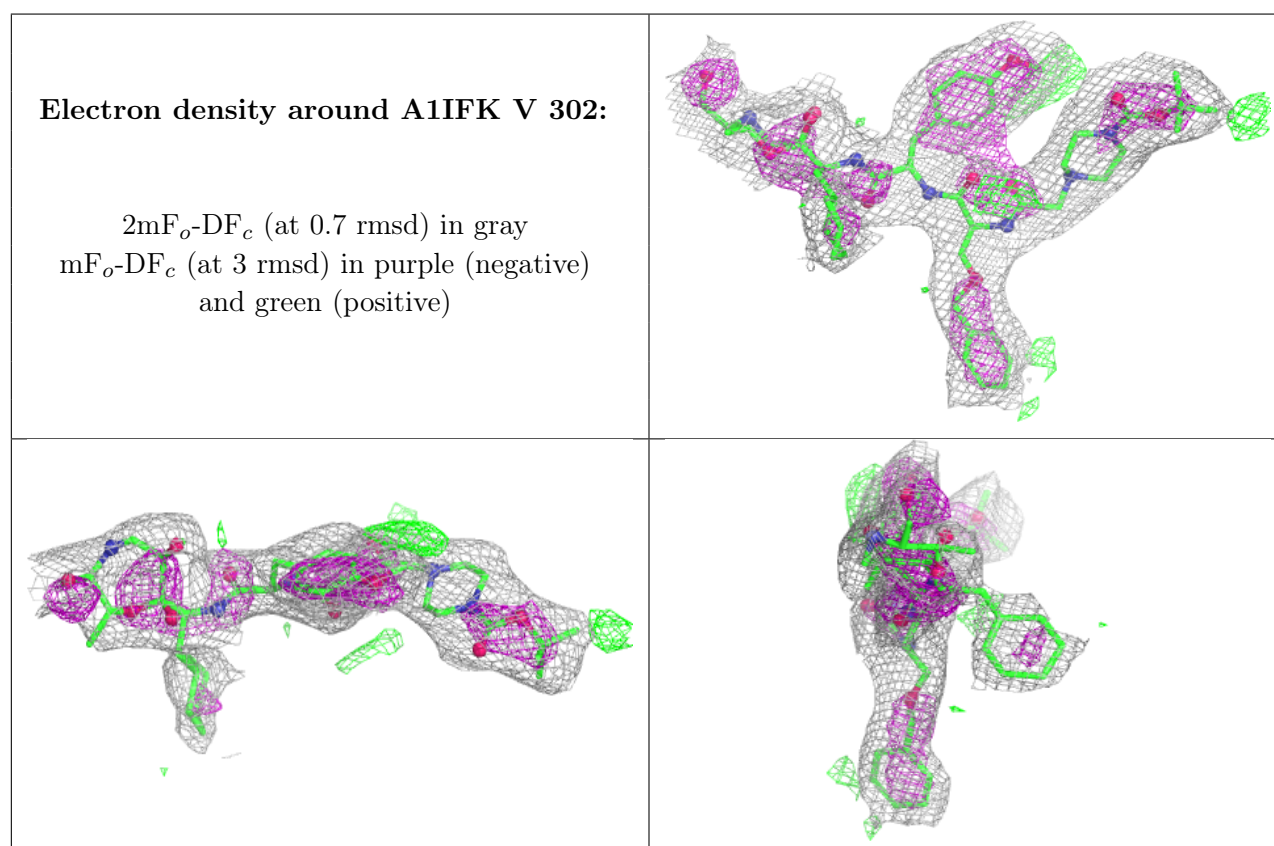
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	MES	b	201	12/12	0.75	0.48	20,20,20,20	0
15	MG	H	302	1/1	0.87	0.15	101,101,101,101	0
17	A1IFK	V	302	64/64	0.92	0.11	36,52,67,98	0
17	A1IFK	K	302	64/64	0.93	0.11	30,44,54,70	0
17	A1IFK	Y	302	64/64	0.93	0.11	29,46,55,68	0
16	MES	V	301	12/12	0.94	0.15	94,101,107,108	0
16	MES	H	301	12/12	0.94	0.13	79,95,98,99	0
17	A1IFK	H	303	64/64	0.94	0.11	34,51,66,148	0
15	MG	I	301	1/1	0.95	0.18	149,149,149,149	0
15	MG	Z	301	1/1	0.96	0.14	127,127,127,127	0
16	MES	X	201	12/12	0.97	0.09	79,81,88,88	0

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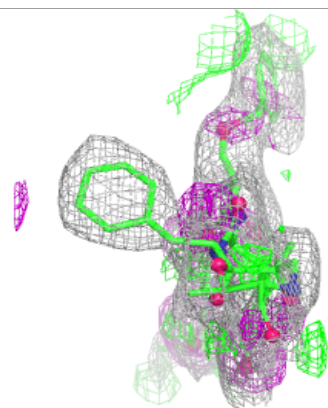
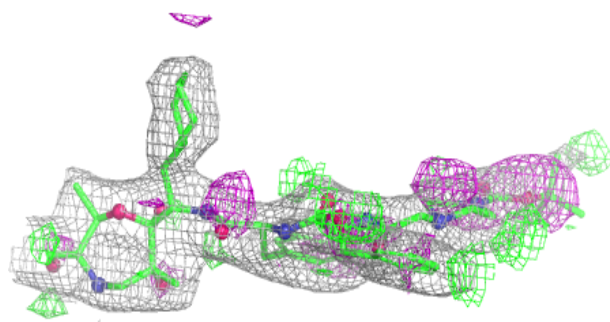
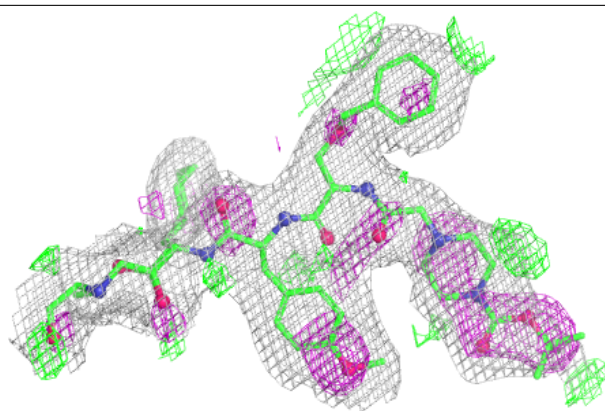
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	MES	J	201	12/12	0.97	0.10	66,82,89,89	0
15	MG	G	301	1/1	0.98	0.06	81,81,81,81	0
15	MG	Y	301	1/1	0.98	0.09	93,93,93,93	0
15	MG	N	201	1/1	0.99	0.07	74,74,74,74	0
15	MG	K	301	1/1	0.99	0.06	85,85,85,85	0

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.

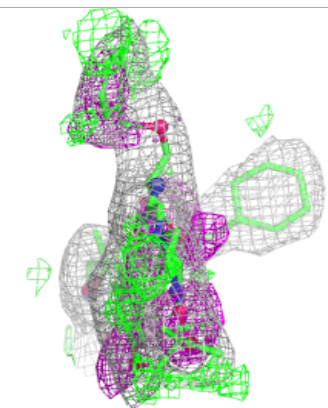
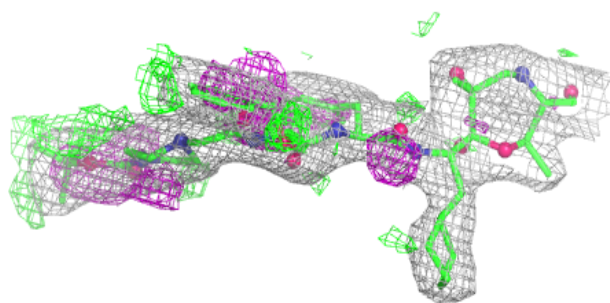
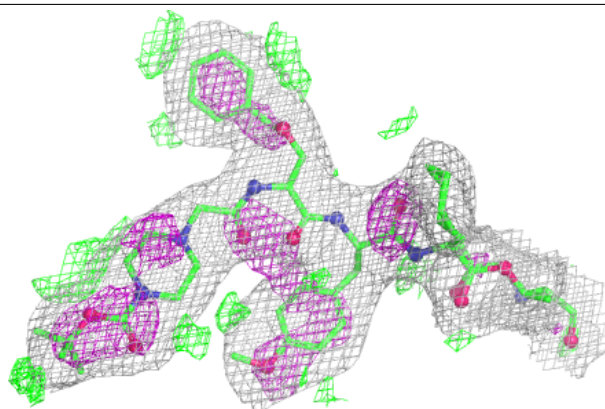


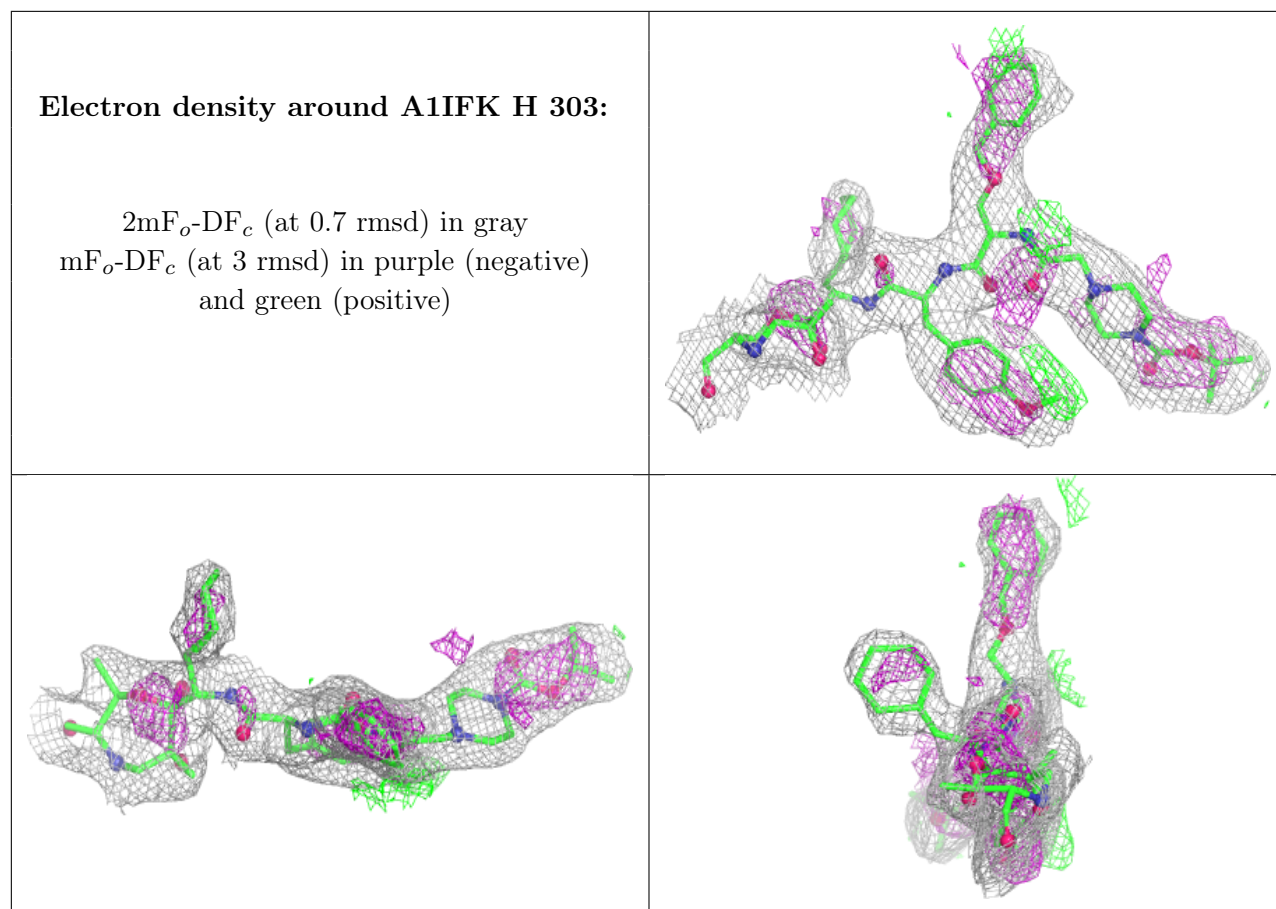
Electron density around A1IFK K 302:

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

**Electron density around A1IFK 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.