



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 08:54 PM UTC

PDB ID : 9FSV / pdb_00009fsv
Title : Yeast 20S proteasome with human beta2i (1-53) in complex with epoxyketone inhibitor 16
Authors : Maurits, E.; Huber, E.M.; Dekker, P.M.; Wang, X.; Heinemeyer, W.; Florea, B.I.; Groll, M.; Overkleeft, H.S.
Deposited on : 2024-06-22
Resolution : 2.75 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

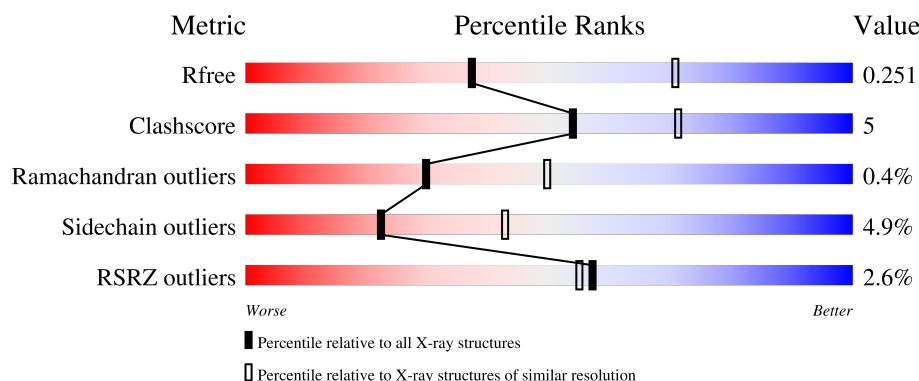
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	
1	O	250	
2	B	258	
2	P	258	

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Mol	Chain	Length	Quality of chain
3	C	254	
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	225	
8	V	225	
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 20 unique types of molecules in this entry. The entry contains 49917 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-10, Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	225	Total	C	N	O	S	0	0	0
			1709	1077	290	334	8			
8	V	222	Total	C	N	O	S	0	0	0
			1681	1062	286	325	8			

- 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	1	0
			1835	1160	316	352	7			
13	a	233	Total	C	N	O	S	0	1	0
			1835	1160	316	352	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	I	1	Total	Mg	0	0
			1	1		

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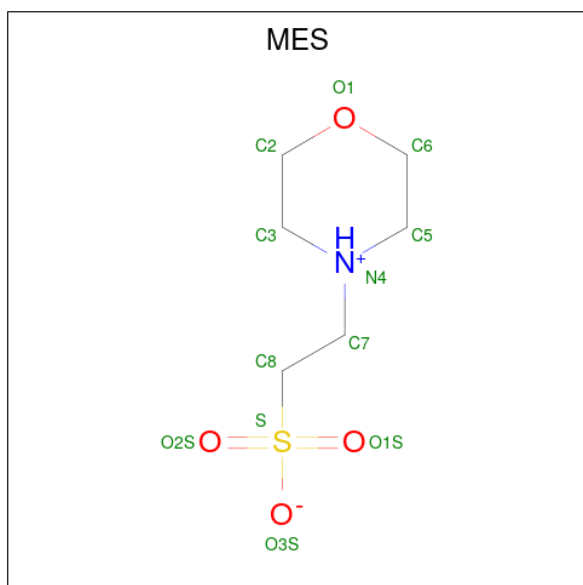
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	K	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		
15	V	1	Total	Mg	0	0
			1	1		
15	W	1	Total	Mg	0	0
			1	1		
15	Y	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		

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

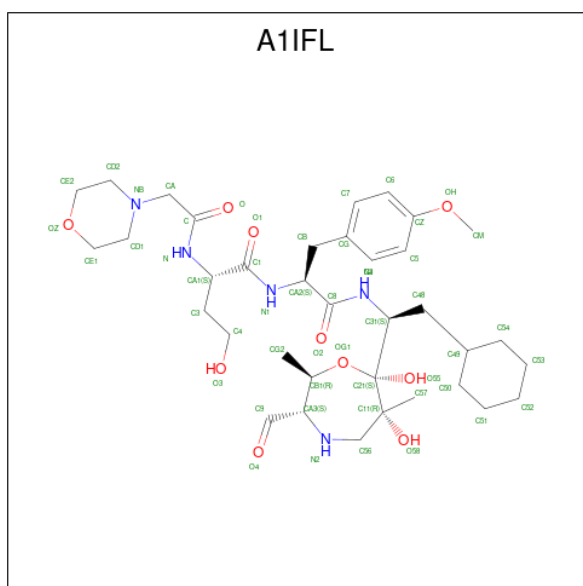
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Cl	0	0
			1	1		
16	N	1	Total	Cl	0	0
			1	1		
16	U	1	Total	Cl	0	0
			1	1		

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 18 is (2S)-N-[(2S)-1-[(1S)-2-cyclohexyl-1-[(2R,3S,6R,7S)-3-methanoyl-2,6-dimethyl-6,7-bis(oxidanyl)-1,4-oxazepan-7-yl]ethyl]amino]-3-(4-methoxyphenyl)-1-oxidanylidene-propan-2-yl]-2-(2-morpholin-4-ylethanoylamino)-4-oxidanyl-butanamide (CCD ID: A1IFL) (formula: C₃₆H₅₇N₅O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	H	1	Total	C	N	O	0	0
			51	36	5	10		
18	K	1	Total	C	N	O	0	0
			51	36	5	10		
18	V	1	Total	C	N	O	0	0
			51	36	5	10		
18	Y	1	Total	C	N	O	0	0
			51	36	5	10		

- Molecule 19 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	K	1	Total	O	S	0	0
			5	4	1		
19	N	1	Total	O	S	0	0
			5	4	1		
19	Y	1	Total	O	S	0	0
			5	4	1		
19	b	1	Total	O	S	0	0
			5	4	1		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	7	Total	O	0	0
			7	7		
20	B	14	Total	O	0	0
			14	14		
20	C	6	Total	O	0	0
			6	6		
20	D	9	Total	O	0	0
			9	9		
20	E	3	Total	O	0	0
			3	3		
20	F	13	Total	O	0	0
			13	13		
20	G	12	Total	O	0	0
			12	12		
20	H	14	Total	O	0	0
			14	14		

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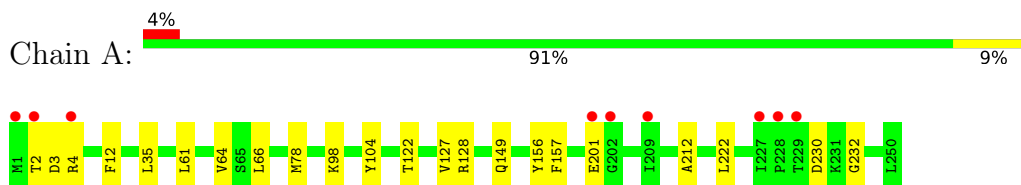
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	I	12	Total 12	O 12	0	0
20	J	10	Total 10	O 10	0	0
20	K	19	Total 19	O 19	0	0
20	L	25	Total 25	O 25	0	0
20	M	18	Total 18	O 18	0	0
20	N	10	Total 10	O 10	0	0
20	O	6	Total 6	O 6	0	0
20	P	3	Total 3	O 3	0	0
20	Q	7	Total 7	O 7	0	0
20	R	5	Total 5	O 5	0	0
20	S	3	Total 3	O 3	0	0
20	T	8	Total 8	O 8	0	0
20	U	16	Total 16	O 16	0	0
20	V	10	Total 10	O 10	0	0
20	W	10	Total 10	O 10	0	0
20	X	15	Total 15	O 15	0	0
20	Y	11	Total 11	O 11	0	0
20	Z	12	Total 12	O 12	0	0
20	a	17	Total 17	O 17	0	0
20	b	13	Total 13	O 13	0	0

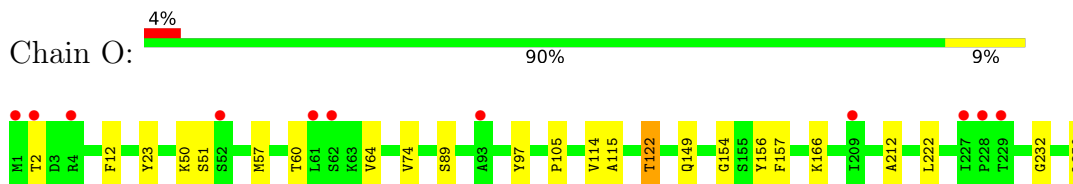
3 Residue-property plots [i](#)

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

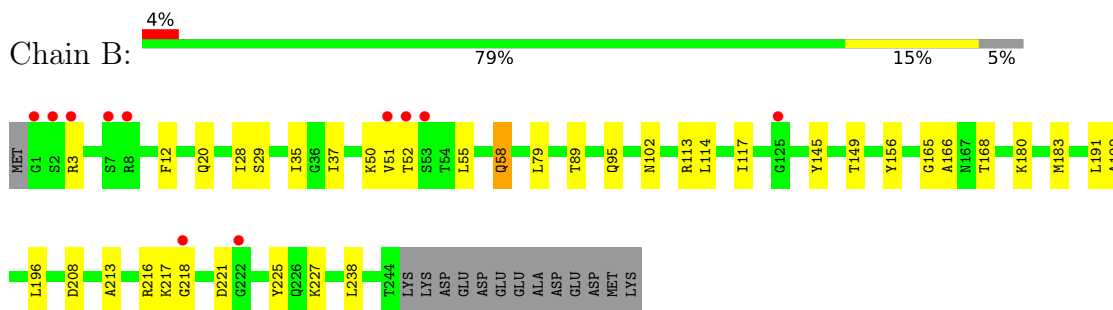
- Molecule 1: Proteasome subunit alpha type-2



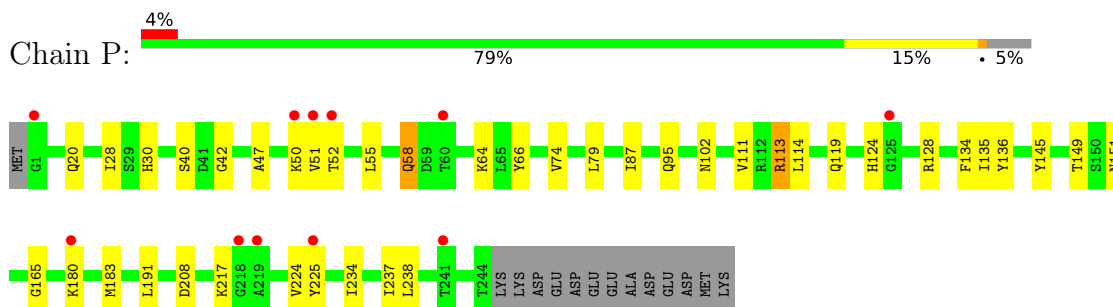
- Molecule 1: Proteasome subunit alpha type-2



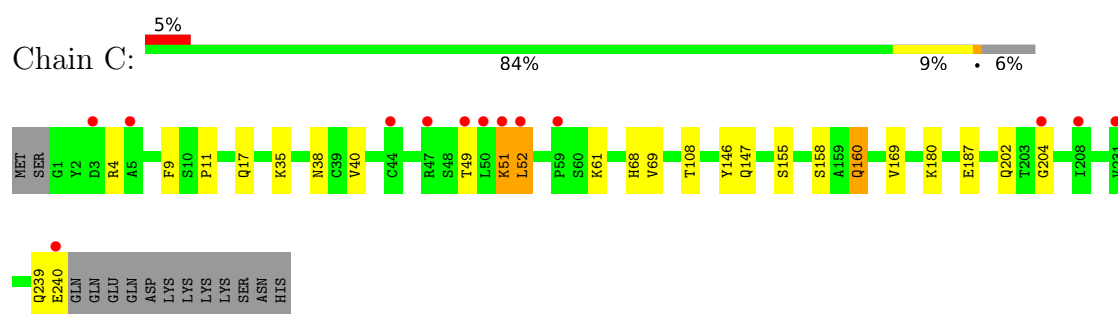
- Molecule 2: Proteasome subunit alpha type-3



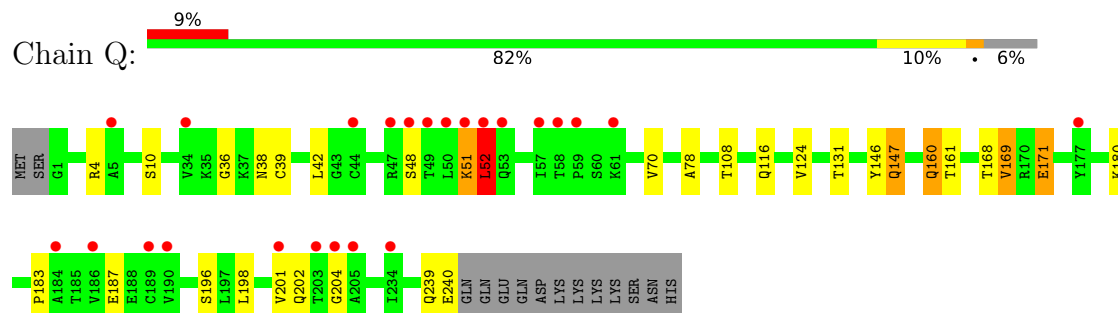
- Molecule 2: Proteasome subunit alpha type-3



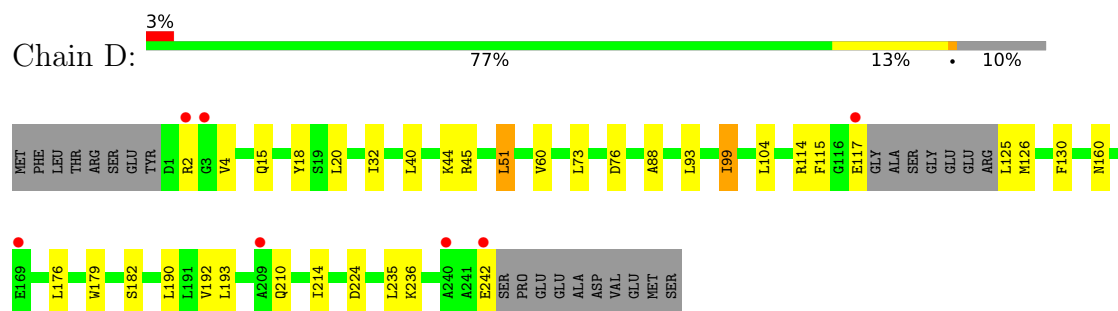
- Molecule 3: Proteasome subunit alpha type-4



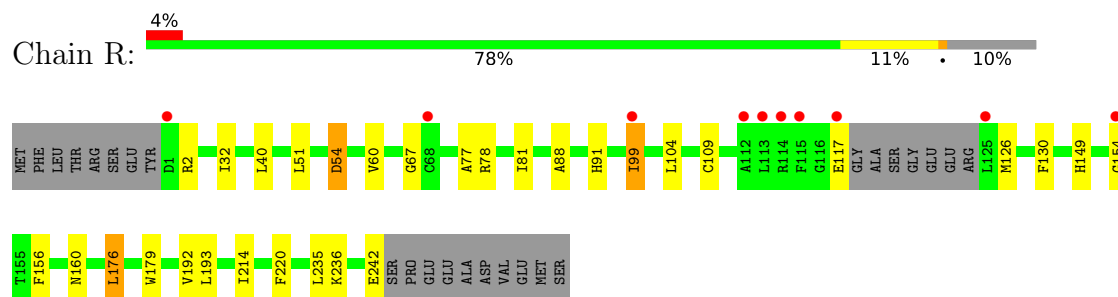
- Molecule 3: Proteasome subunit alpha type-4



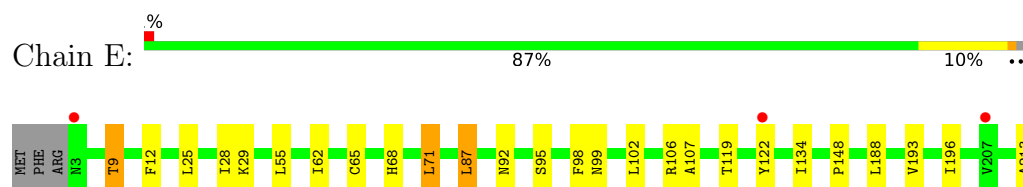
- Molecule 4: Proteasome subunit alpha type-5



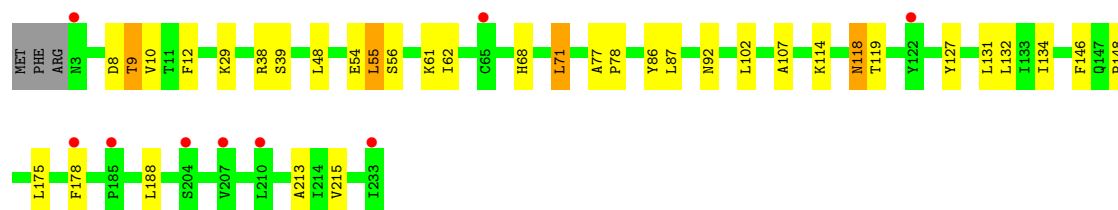
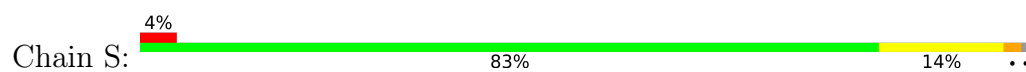
- Molecule 4: Proteasome subunit alpha type-5



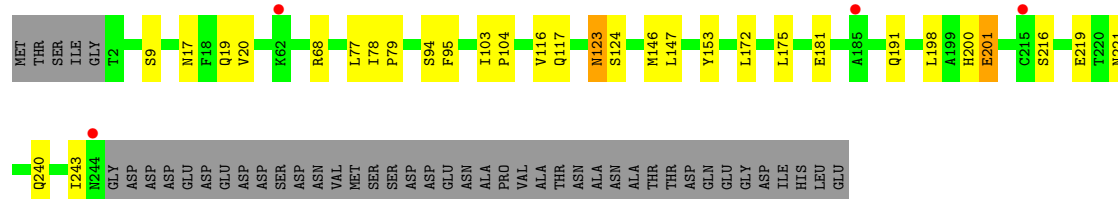
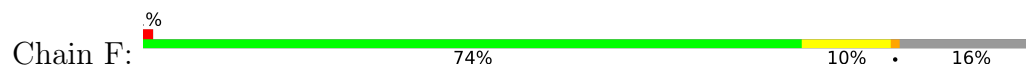
- Molecule 5: Proteasome subunit alpha type-6



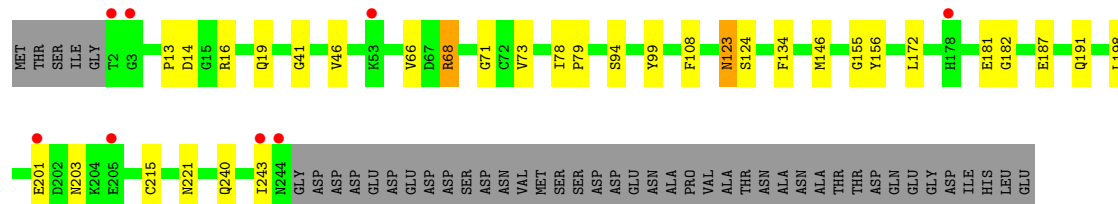
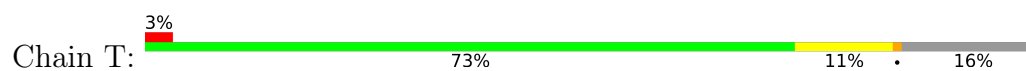
- Molecule 5: Proteasome subunit alpha type-6



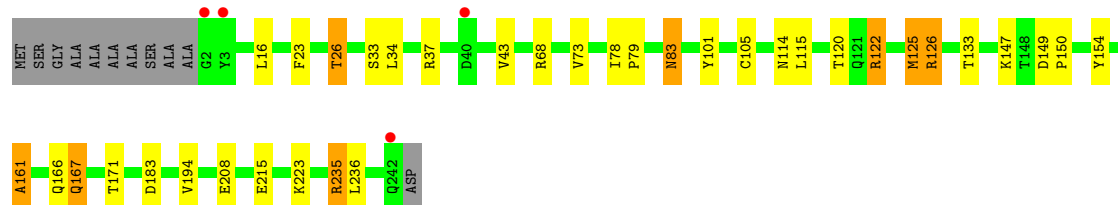
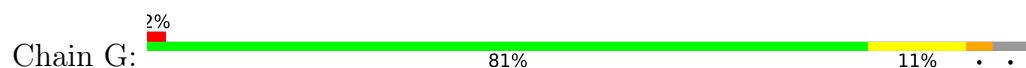
- Molecule 6: Probable proteasome subunit alpha type-7



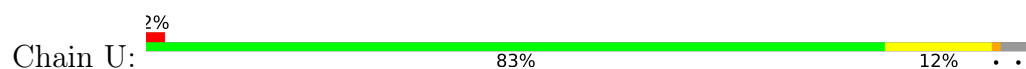
- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 7: Proteasome subunit alpha type-1

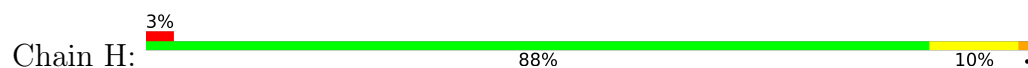


- Molecule 7: Proteasome subunit alpha type-1

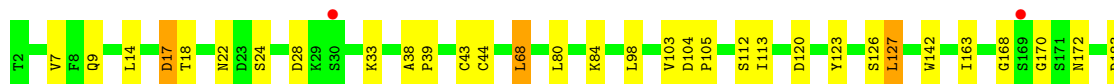
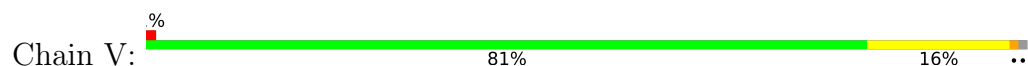




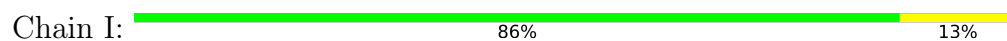
- Molecule 8: Proteasome subunit beta type-10, Proteasome subunit beta type-2



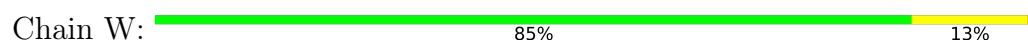
- Molecule 8: Proteasome subunit beta type-10, Proteasome subunit beta type-2



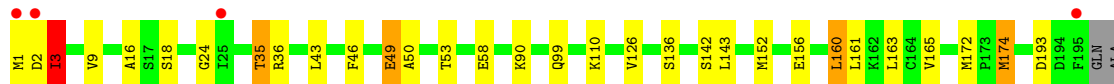
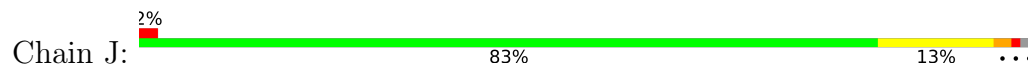
- Molecule 9: Proteasome subunit beta type-3



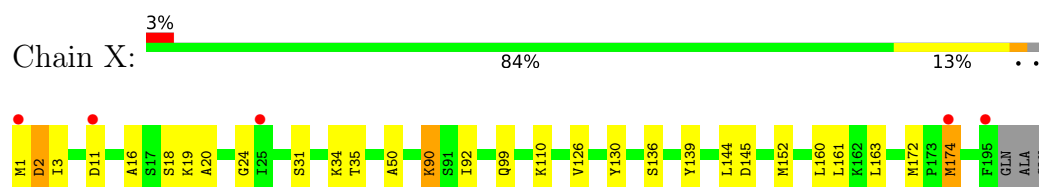
- Molecule 9: Proteasome subunit beta type-3



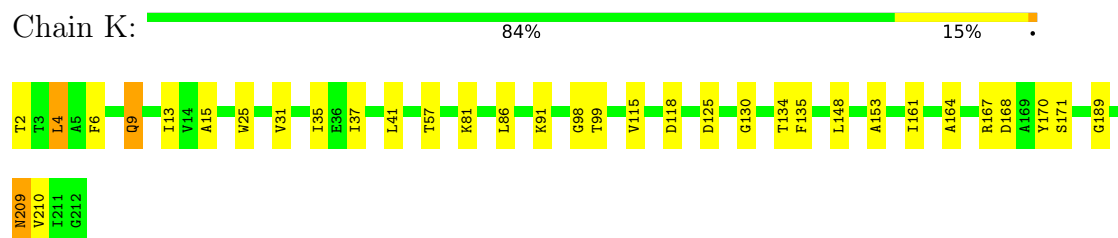
- Molecule 10: Proteasome subunit beta type-4



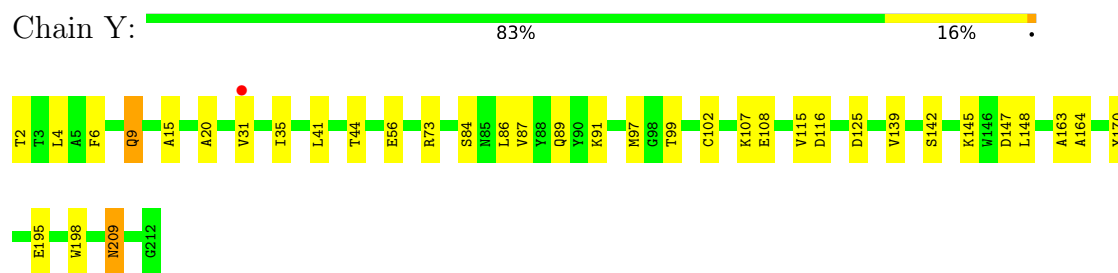
- Molecule 10: Proteasome subunit beta type-4



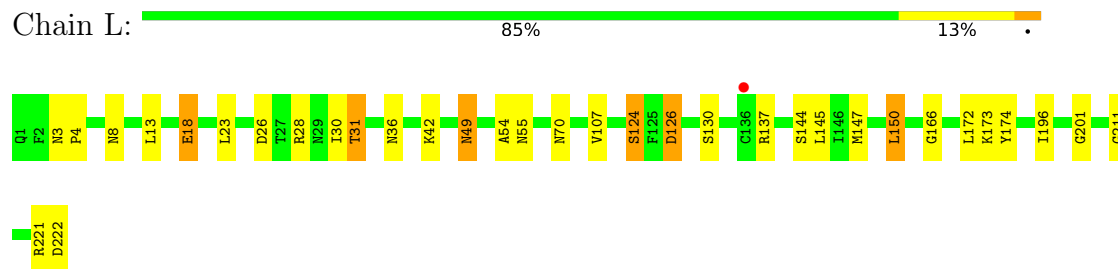
• Molecule 11: Proteasome subunit beta type-5



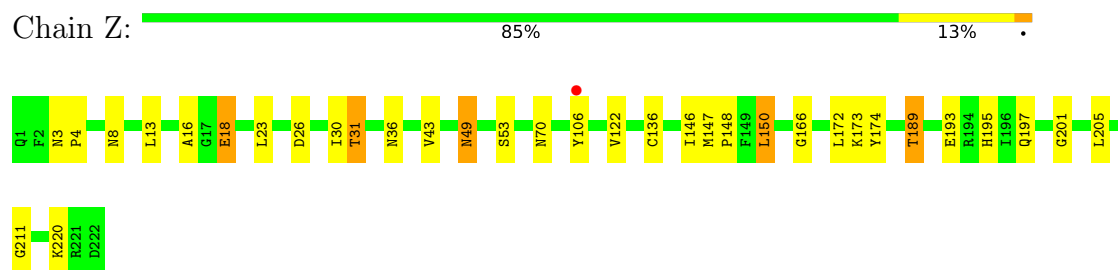
• Molecule 11: Proteasome subunit beta type-5



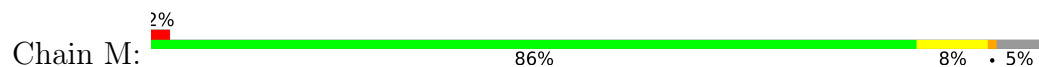
• Molecule 12: Proteasome subunit beta type-6



• Molecule 12: Proteasome subunit beta type-6

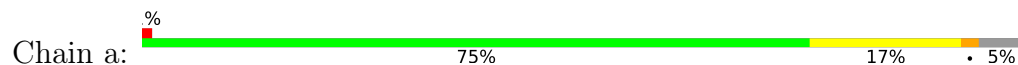


• Molecule 13: Proteasome subunit beta type-7

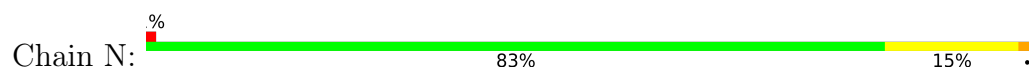




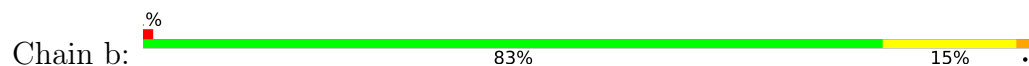
• Molecule 13: Proteasome subunit beta type-7



• 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	134.70Å 300.60Å 144.48Å 90.00° 112.83° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 30.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	94.9 (30.00-2.75) 94.9 (30.00-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.213 , 0.247 0.220 , 0.251	Depositor DCC
R_{free} test set	12976 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.9	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	0.94	EDS
Total number of atoms	49917	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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, CL, SO4, A1IFL, MES

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	1.03	0/1952	1.40	0/2642
1	O	1.05	0/1952	1.45	1/2642 (0.0%)
2	B	1.00	0/1934	1.45	0/2618
2	P	1.03	0/1934	1.44	0/2618
3	C	1.04	0/1910	1.48	0/2586
3	Q	1.05	0/1910	1.47	0/2586
4	D	1.03	0/1837	1.48	2/2475 (0.1%)
4	R	1.04	0/1837	1.49	0/2475
5	E	1.02	0/1800	1.43	0/2433
5	S	1.04	0/1800	1.43	0/2433
6	F	1.03	0/1932	1.49	4/2609 (0.2%)
6	T	1.03	0/1932	1.46	1/2609 (0.0%)
7	G	1.04	2/1945 (0.1%)	1.44	0/2634
7	U	1.05	1/1945 (0.1%)	1.45	2/2634 (0.1%)
8	H	1.03	0/1739	1.46	0/2355
8	V	1.04	0/1711	1.45	2/2319 (0.1%)
9	I	1.04	0/1611	1.45	6/2174 (0.3%)
9	W	1.03	0/1611	1.44	2/2174 (0.1%)
10	J	0.99	0/1589	1.39	1/2142 (0.0%)
10	X	1.02	0/1589	1.39	3/2142 (0.1%)
11	K	1.02	0/1674	1.46	4/2264 (0.2%)
11	Y	1.03	0/1674	1.42	0/2264
12	L	1.02	0/1795	1.40	1/2420 (0.0%)
12	Z	1.00	0/1795	1.42	0/2420
13	M	1.01	0/1866	1.40	2/2528 (0.1%)
13	a	1.03	0/1866	1.44	1/2528 (0.0%)
14	N	1.02	0/1541	1.43	4/2087 (0.2%)
14	b	1.02	0/1541	1.41	2/2087 (0.1%)
All	All	1.03	3/50222 (0.0%)	1.44	38/67898 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	167	GLN	C-O	6.24	1.31	1.24
7	U	105	CYS	C-O	5.08	1.29	1.24
7	G	161	ALA	C-O	5.01	1.29	1.23

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	118	ASP	CA-CB-CG	7.44	120.04	112.60
9	W	9	GLY	CA-C-O	-6.80	117.41	122.37
6	F	104	PRO	CA-C-N	6.17	124.13	120.24
6	F	104	PRO	C-N-CA	6.17	124.13	120.24
10	X	145	ASP	CA-CB-CG	6.13	118.73	112.60
4	D	40	LEU	CA-C-N	5.96	125.70	121.65
4	D	40	LEU	C-N-CA	5.96	125.70	121.65
9	I	124	ASP	CA-CB-CG	5.96	118.56	112.60
12	L	222	ASP	CA-CB-CG	5.95	118.55	112.60
10	X	90	LYS	CA-C-N	5.69	128.18	120.38
10	X	90	LYS	C-N-CA	5.69	128.18	120.38
11	K	130	GLY	CA-C-O	-5.68	118.22	122.37
10	J	193	ASP	CA-CB-CG	5.54	118.14	112.60
14	b	85	LEU	CA-C-N	5.44	127.58	120.28
14	b	85	LEU	C-N-CA	5.44	127.58	120.28
9	I	34	GLY	CA-C-O	-5.37	116.70	121.64
9	I	67	ARG	CA-C-N	5.36	127.73	120.65
9	I	67	ARG	C-N-CA	5.36	127.73	120.65
11	K	168	ASP	CA-CB-CG	5.28	117.88	112.60
14	N	128	GLY	CA-C-N	5.22	127.53	120.38
14	N	128	GLY	C-N-CA	5.22	127.53	120.38
1	O	74	VAL	CA-C-O	-5.22	116.34	121.67
6	T	182	GLY	CA-C-O	-5.21	118.70	122.45
14	N	159	LEU	CA-C-N	5.20	127.19	120.44
14	N	159	LEU	C-N-CA	5.20	127.19	120.44
13	a	188	ASP	CA-CB-CG	5.20	117.80	112.60
13	M	25	ASP	CA-CB-CG	5.17	117.77	112.60
9	I	183	GLY	CA-C-O	-5.12	118.89	122.22
6	F	77	LEU	CA-C-N	5.10	125.33	120.43
6	F	77	LEU	C-N-CA	5.10	125.33	120.43
13	M	43	ILE	CB-CA-C	5.10	115.92	111.08
7	U	216	VAL	CA-C-N	5.09	126.04	122.33
7	U	216	VAL	C-N-CA	5.09	126.04	122.33
8	V	28	ASP	CA-CB-CG	5.07	117.67	112.60
11	K	189	GLY	CA-C-O	-5.06	118.74	122.23
9	W	124	ASP	CA-CB-CG	5.02	117.62	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	96	GLU	N-CA-C	-5.02	106.67	112.89
8	V	183	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

There are no planarity outliers.

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	13	0
1	O	1915	0	1929	11	0
2	B	1904	0	1904	21	0
2	P	1904	0	1904	24	0
3	C	1881	0	1895	13	0
3	Q	1881	0	1895	15	0
4	D	1813	0	1797	21	0
4	R	1813	0	1797	17	0
5	E	1773	0	1775	21	0
5	S	1773	0	1775	24	0
6	F	1892	0	1883	16	0
6	T	1892	0	1883	17	0
7	G	1907	0	1901	26	0
7	U	1907	0	1901	15	0
8	H	1709	0	1693	16	0
8	V	1681	0	1673	23	0
9	I	1581	0	1574	18	0
9	W	1581	0	1574	22	0
10	J	1561	0	1569	26	0
10	X	1561	0	1569	16	0
11	K	1637	0	1585	23	0
11	Y	1637	0	1585	28	0
12	L	1757	0	1711	29	0
12	Z	1757	0	1711	24	0
13	M	1835	0	1844	10	0
13	a	1835	0	1844	29	0
14	N	1512	0	1481	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	b	1512	0	1481	22	0
15	G	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	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
17	H	12	0	13	0	0
17	K	12	0	13	1	0
17	V	12	0	13	0	0
17	Y	12	0	13	0	0
18	H	51	0	0	1	0
18	K	51	0	0	2	0
18	V	51	0	0	3	0
18	Y	51	0	0	2	0
19	K	5	0	0	0	0
19	N	5	0	0	0	0
19	Y	5	0	0	0	0
19	b	5	0	0	0	0
20	A	7	0	0	0	0
20	B	14	0	0	0	0
20	C	6	0	0	0	0
20	D	9	0	0	2	0
20	E	3	0	0	0	0
20	F	13	0	0	0	0
20	G	12	0	0	0	0
20	H	14	0	0	1	0
20	I	12	0	0	0	0
20	J	10	0	0	0	0
20	K	19	0	0	0	0
20	L	25	0	0	0	0
20	M	18	0	0	0	0
20	N	10	0	0	0	0
20	O	6	0	0	0	0
20	P	3	0	0	0	0
20	Q	7	0	0	1	0
20	R	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	S	3	0	0	0	0
20	T	8	0	0	0	0
20	U	16	0	0	0	0
20	V	10	0	0	0	0
20	W	10	0	0	0	0
20	X	15	0	0	0	0
20	Y	11	0	0	0	0
20	Z	12	0	0	0	0
20	a	17	0	0	0	0
20	b	13	0	0	0	0
All	All	49917	0	49114	481	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 5.

All (481) 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)
10:X:1:MET:HA	10:X:34:LYS:HE2	1.21	1.14
10:J:3:ILE:CG2	10:J:18:SER:HB3	1.97	0.95
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.55	0.88
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.36	0.86
14:b:152:VAL:HA	14:b:175:MET:HE1	1.58	0.86
10:X:1:MET:CA	10:X:34:LYS:HE2	2.09	0.81
7:U:23:PHE:O	7:U:26:THR:HB	1.80	0.81
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.63	0.81
8:V:218:VAL:HB	9:W:194:VAL:CG1	2.12	0.80
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.31	0.79
14:N:152:VAL:HA	14:N:175:MET:HE1	1.65	0.78
13:a:93:PHE:CZ	13:a:128:ARG:HG2	2.20	0.76
10:J:143:LEU:HD21	11:Y:142:SER:OG	1.87	0.75
10:J:3:ILE:HG21	10:J:18:SER:HB3	1.69	0.74
8:V:218:VAL:HB	9:W:194:VAL:HG11	1.70	0.73
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.54	0.72
5:E:12:PHE:H	6:F:19:GLN:HE22	1.36	0.72
11:Y:31:VAL:HG11	18:Y:304:A1IFL:C53	2.20	0.72
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.71	0.71
5:S:68:HIS:HE1	5:S:102:LEU:O	1.73	0.71
10:J:3:ILE:CG2	10:J:18:SER:CB	2.69	0.70
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.56	0.70
11:Y:87:VAL:HG11	11:Y:97:MET:CE	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.04	0.70
11:K:209:ASN:O	9:W:37:ASN:ND2	2.25	0.69
13:a:119:VAL:HG23	13:a:200:ILE:HG22	1.73	0.69
11:K:4:LEU:HD23	11:K:161:ILE:HD11	1.75	0.69
10:J:2:ASP:O	10:J:3:ILE:HB	1.92	0.68
10:J:172:MET:SD	10:J:174:MET:HE1	2.33	0.68
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.59	0.67
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.95	0.67
9:W:192:ASP:N	9:W:192:ASP:OD1	2.26	0.66
7:G:23:PHE:O	7:G:26:THR:HB	1.95	0.66
14:N:14:LEU:HD11	14:N:100:ALA:HB3	1.77	0.66
10:X:1:MET:SD	10:X:2:ASP:N	2.62	0.66
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.78	0.66
14:N:6:VAL:HG23	14:N:155:ILE:HD11	1.78	0.65
4:D:114:ARG:HD3	20:D:309:HOH:O	1.97	0.65
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.80	0.64
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.31	0.63
3:Q:52:LEU:N	20:Q:301:HOH:O	2.30	0.63
11:Y:209:ASN:HD22	11:Y:209:ASN:H	1.45	0.63
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.29	0.63
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	1.79	0.63
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.47	0.63
3:C:51:LYS:O	3:C:52:LEU:HB2	1.97	0.63
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.80	0.63
2:B:58:GLN:NE2	2:B:208:ASP:HA	2.15	0.62
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.64	0.62
6:F:123:ASN:C	6:F:123:ASN:HD22	2.07	0.62
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.46	0.62
8:V:218:VAL:HB	9:W:194:VAL:HG12	1.80	0.62
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.34	0.62
10:J:16:ALA:CB	10:J:161:LEU:HD21	2.31	0.61
9:I:9:GLY:HA2	9:I:25:ASP:OD2	2.01	0.61
9:W:194:VAL:HG12	9:W:194:VAL:O	2.02	0.60
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.84	0.60
8:H:218:VAL:CG2	9:I:194:VAL:HG12	2.32	0.59
11:K:31:VAL:HG11	18:K:304:A1IFL:C53	2.32	0.59
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.32	0.59
4:R:77:ALA:O	4:R:81:ILE:HG12	2.02	0.59
3:C:9:PHE:H	4:D:15:GLN:HE22	1.48	0.59
11:Y:2:THR:HG21	11:Y:164:ALA:CB	2.33	0.59
1:A:149:GLN:O	1:A:156:TYR:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.84	0.59
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.84	0.58
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.84	0.58
10:J:143:LEU:HD21	11:Y:142:SER:HG	1.69	0.58
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.52	0.58
8:H:103:VAL:HG11	8:H:180:ILE:HA	1.85	0.58
14:N:34:LEU:HD13	14:N:176:VAL:HG23	1.86	0.58
5:S:86:TYR:CD1	5:S:114:LYS:HE2	2.39	0.58
6:T:123:ASN:HD22	6:T:124:SER:N	2.02	0.58
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.34	0.58
4:D:45:ARG:NH1	20:D:301:HOH:O	2.37	0.57
10:J:3:ILE:O	10:J:3:ILE:HG23	2.04	0.57
4:R:176:LEU:HD22	5:S:55:LEU:HD22	1.85	0.57
2:B:29:SER:O	2:B:166:ALA:HA	2.04	0.57
12:L:126:ASP:OD1	12:L:126:ASP:C	2.46	0.57
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.87	0.57
12:Z:18:GLU:HG3	12:Z:174:TYR:CD2	2.39	0.57
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.00	0.56
5:S:12:PHE:H	6:T:19:GLN:HE22	1.53	0.56
1:O:12:PHE:H	2:P:20:GLN:HE22	1.54	0.56
3:C:11:PRO:HA	4:D:18:TYR:CD1	2.41	0.56
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.88	0.56
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.70	0.56
14:b:6:VAL:HG12	14:b:124:TYR:HB3	1.87	0.55
4:D:125:LEU:HD12	4:D:125:LEU:O	2.05	0.55
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.41	0.55
6:F:123:ASN:HD22	6:F:124:SER:N	2.04	0.55
13:a:127:LEU:HG	13:a:142:LEU:HD12	1.88	0.55
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.88	0.55
2:P:225:TYR:CD1	8:V:223:ILE:HG21	2.42	0.55
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.54	0.55
18:V:303:A1IFL:C8	18:V:303:A1IFL:C57	2.85	0.55
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.88	0.55
12:L:31:THR:HG23	12:L:36:ASN:ND2	2.16	0.55
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.89	0.55
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.88	0.54
14:N:55:ILE:HD11	14:N:93:LEU:HD13	1.89	0.54
7:G:126:ARG:HG3	7:G:126:ARG:HH11	1.72	0.54
10:J:3:ILE:HG22	10:J:18:SER:OG	2.08	0.54
6:T:41:GLY:HA3	6:T:215:CYS:O	2.08	0.54
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.90	0.54
10:X:1:MET:N	10:X:20:ALA:O	2.36	0.53
7:G:34:LEU:C	7:G:34:LEU:HD23	2.33	0.53
3:C:35:LYS:HG2	3:C:158:SER:O	2.08	0.53
4:R:126:MET:HE1	4:R:130:PHE:CE2	2.43	0.53
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.44	0.53
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.89	0.53
14:b:6:VAL:HG12	14:b:124:TYR:CB	2.38	0.53
6:T:123:ASN:HD22	6:T:123:ASN:C	2.17	0.53
13:a:7:THR:HA	13:a:55:GLY:O	2.08	0.53
8:V:172:ASN:HD22	8:V:192:THR:HA	1.73	0.53
7:G:78:ILE:HG22	7:G:79:PRO:HD3	1.89	0.53
13:a:51:VAL:HG22	13:a:116:VAL:HG22	1.90	0.53
14:b:6:VAL:CG2	14:b:155:ILE:HD11	2.38	0.53
4:D:93:LEU:CD1	11:K:57:THR:HG22	2.38	0.53
8:H:218:VAL:HB	9:I:194:VAL:CG1	2.38	0.53
11:K:98:GLY:HA3	17:K:302:MES:H32	1.90	0.53
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.90	0.52
4:R:67:GLY:HA3	4:R:220:PHE:CE1	2.43	0.52
5:S:71:LEU:C	5:S:71:LEU:CD2	2.82	0.52
2:P:113:ARG:CG	2:P:113:ARG:HH21	2.22	0.52
2:P:113:ARG:HH21	2:P:113:ARG:HG3	1.73	0.52
2:B:145:TYR:OH	2:B:217:LYS:HB2	2.09	0.52
11:K:134:THR:HG22	10:X:139:TYR:CZ	2.45	0.52
7:G:73:VAL:HG12	7:G:133:THR:HB	1.90	0.52
11:Y:87:VAL:HG11	11:Y:97:MET:HE2	1.91	0.52
7:G:83:ASN:C	7:G:83:ASN:HD22	2.18	0.52
14:b:134:ILE:HG21	14:b:158:SER:O	2.10	0.52
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.39	0.52
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.07	0.51
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.88	0.51
8:V:126:SER:O	8:V:127:LEU:HD13	2.10	0.51
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.09	0.51
4:D:88:ALA:HA	4:D:99:ILE:HD12	1.91	0.51
13:a:6:VAL:O	13:a:56:ASP:HA	2.09	0.51
7:G:37:ARG:NH2	7:G:183:ASP:HB3	2.26	0.51
14:N:35:THR:HG21	13:a:228:TYR:HE2	1.76	0.51
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.75	0.51
4:R:149:HIS:O	4:R:156:PHE:HA	2.11	0.51
14:b:77:THR:O	14:b:81:VAL:HG23	2.10	0.51
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:71:LEU:C	5:S:71:LEU:HD22	2.36	0.51
12:L:145:LEU:O	9:W:147:GLY:HA3	2.10	0.51
2:P:74:VAL:HA	2:P:135:ILE:O	2.10	0.51
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.11	0.51
7:G:37:ARG:HH21	7:G:183:ASP:HB3	1.77	0.50
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.76	0.50
6:F:201:GLU:N	6:F:201:GLU:OE1	2.44	0.50
7:G:166:GLN:HG3	7:G:167:GLN:N	2.25	0.50
11:K:99:THR:HG22	11:K:115:VAL:O	2.11	0.50
5:S:38:ARG:NH1	5:S:39:SER:O	2.44	0.50
13:a:93:PHE:CE1	13:a:128:ARG:HG2	2.46	0.50
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.93	0.50
11:Y:87:VAL:CG1	11:Y:97:MET:CE	2.88	0.50
13:a:43:ILE:HD11	13:a:53:ILE:HD11	1.93	0.50
6:F:146:MET:O	6:F:153:TYR:HA	2.12	0.50
14:N:155:ILE:HD12	14:N:175:MET:HE3	1.92	0.50
2:P:145:TYR:OH	2:P:217:LYS:N	2.45	0.50
1:A:78:MET:HE1	7:G:16:LEU:HD11	1.93	0.50
2:B:225:TYR:CD1	8:H:223:ILE:HG21	2.46	0.50
10:J:160:LEU:HD12	10:J:160:LEU:O	2.11	0.50
13:a:53:ILE:HG21	13:a:60:MET:HG3	1.93	0.50
2:P:58:GLN:NE2	2:P:208:ASP:HA	2.27	0.50
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.93	0.49
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.41	0.49
14:b:55:ILE:O	14:b:59:VAL:HG23	2.12	0.49
9:I:42:ILE:HG21	9:I:187:TYR:CD1	2.48	0.49
1:O:149:GLN:O	1:O:156:TYR:HA	2.12	0.49
2:P:145:TYR:OH	2:P:217:LYS:HB2	2.12	0.49
1:O:97:TYR:CE1	1:O:105:PRO:HA	2.48	0.49
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.45	0.49
1:A:128:ARG:NE	7:G:120:THR:O	2.39	0.49
13:a:26:ASN:HA	13:a:39:VAL:O	2.12	0.49
7:G:147:LYS:O	7:G:154:TYR:HA	2.12	0.49
6:T:198:LEU:HD12	6:T:243:ILE:HG22	1.94	0.49
5:E:12:PHE:HB2	6:F:19:GLN:HE22	1.78	0.49
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.95	0.49
18:H:302:A1IFL:C8	18:H:302:A1IFL:C57	2.91	0.49
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.95	0.49
1:A:4:ARG:CZ	5:E:122:TYR:HE2	2.26	0.49
6:F:198:LEU:HD12	6:F:243:ILE:HG22	1.95	0.49
11:Y:44:THR:O	11:Y:99:THR:OG1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:49:GLU:O	10:J:53:THR:HG23	2.14	0.48
6:T:14:ASP:OD2	6:T:16:ARG:NH1	2.46	0.48
9:W:62:LEU:CD1	9:W:104:VAL:HG21	2.44	0.48
13:a:129:TYR:CD1	13:a:137:TYR:CZ	3.02	0.48
11:K:13:ILE:HG13	11:K:153:ALA:HB1	1.95	0.48
12:L:26:ASP:HA	12:L:201:GLY:O	2.13	0.48
7:U:78:ILE:N	7:U:79:PRO:CD	2.76	0.48
5:E:65:CYS:SG	5:E:71:LEU:HD13	2.54	0.48
4:R:91:HIS:HB3	4:R:99:ILE:HG21	1.95	0.48
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.43	0.48
5:E:62:ILE:HG21	5:E:213:ALA:HB2	1.94	0.48
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.95	0.48
8:H:218:VAL:HB	9:I:194:VAL:HG12	1.94	0.48
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.96	0.48
11:K:2:THR:OG1	11:K:171:SER:OG	2.32	0.48
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.49	0.48
2:P:134:PHE:O	2:P:149:THR:HA	2.14	0.48
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.96	0.48
1:A:64:VAL:HG11	1:A:212:ALA:HB3	1.96	0.47
11:Y:170:TYR:O	18:Y:304:A1IFL:C56	2.62	0.47
13:a:48:ASN:H	13:a:48:ASN:HD22	1.61	0.47
3:Q:202:GLN:CG	3:Q:202:GLN:O	2.61	0.47
1:A:127:VAL:HG12	7:G:122:ARG:HD2	1.96	0.47
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.96	0.47
14:b:14:LEU:HD23	14:b:44:CYS:SG	2.54	0.47
3:C:202:GLN:O	3:C:202:GLN:HG2	2.14	0.47
8:H:165:ASN:HD22	13:a:156:ARG:HH11	1.61	0.47
5:S:71:LEU:HA	5:S:132:LEU:O	2.14	0.47
2:B:149:THR:O	2:B:156:TYR:HA	2.13	0.47
8:V:112:SER:OG	8:V:120:ASP:HB2	2.13	0.47
11:K:9:GLN:NE2	11:K:148:LEU:O	2.48	0.47
14:b:14:LEU:HD11	14:b:100:ALA:HB3	1.97	0.47
2:B:180:LYS:O	2:B:183:MET:HB2	2.15	0.47
4:D:4:VAL:HG13	4:D:15:GLN:HG3	1.96	0.47
5:E:12:PHE:H	6:F:19:GLN:NE2	2.10	0.47
11:K:4:LEU:HD21	11:K:15:ALA:HB3	1.97	0.47
2:P:42:GLY:HA2	2:P:145:TYR:CE1	2.50	0.47
6:T:13:PRO:O	7:U:24:LYS:HD2	2.15	0.47
7:U:166:GLN:HG3	7:U:167:GLN:N	2.29	0.47
9:W:27:ARG:HD3	9:W:179:LEU:O	2.15	0.47
9:W:65:MET:O	9:W:68:TYR:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.97	0.47
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.45	0.47
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.13	0.47
8:V:126:SER:O	8:V:127:LEU:CD1	2.63	0.47
7:G:78:ILE:CG2	7:G:79:PRO:HD3	2.45	0.47
12:L:8:ASN:HA	12:L:30:ILE:O	2.15	0.47
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	1.97	0.47
4:D:104:LEU:C	4:D:104:LEU:HD13	2.41	0.46
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.96	0.46
13:a:56:ASP:OD2	13:a:58:SER:N	2.48	0.46
5:S:131:LEU:HB2	5:S:146:PHE:HB3	1.97	0.46
12:Z:4:PRO:O	13:a:104:ARG:NH1	2.46	0.46
4:D:73:LEU:O	4:D:76:ASP:HB2	2.15	0.46
5:E:28:ILE:HD11	5:E:148:PRO:HD3	1.97	0.46
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.97	0.46
14:N:6:VAL:HG13	14:N:124:TYR:HB2	1.97	0.46
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.96	0.46
7:U:73:VAL:HG12	7:U:133:THR:HB	1.98	0.46
3:C:68:HIS:CE1	3:C:69:VAL:HG23	2.50	0.46
3:C:202:GLN:O	3:C:202:GLN:CG	2.63	0.46
2:B:216:ARG:C	2:B:218:GLY:H	2.24	0.46
4:R:54:ASP:OD1	4:R:54:ASP:N	2.39	0.46
4:R:176:LEU:HA	5:S:55:LEU:HD21	1.98	0.46
5:S:118:ASN:N	5:S:118:ASN:HD22	2.14	0.46
13:a:150:MET:HE2	13:a:183:VAL:CG1	2.46	0.46
4:D:126:MET:HE1	4:D:130:PHE:CE2	2.51	0.46
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.25	0.46
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.51	0.46
2:P:30:HIS:O	2:P:50:LYS:NZ	2.41	0.45
1:A:66:LEU:C	1:A:66:LEU:HD23	2.41	0.45
2:B:12:PHE:H	3:C:17:GLN:HE22	1.63	0.45
3:C:108:THR:HG21	3:C:146:TYR:HB3	1.99	0.45
5:E:99:ASN:HB2	13:M:94:GLU:HG2	1.98	0.45
10:J:46:PHE:HD1	10:J:53:THR:HB	1.80	0.45
11:K:170:TYR:O	18:K:304:A1IFL:C56	2.65	0.45
11:Y:145:LYS:HB2	11:Y:148:LEU:CD1	2.47	0.45
13:a:129:TYR:O	13:a:136:THR:HA	2.15	0.45
7:G:125:MET:HE2	7:G:125:MET:HB3	1.69	0.45
7:G:235:ARG:HA	7:G:235:ARG:NE	2.32	0.45
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.52	0.45
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:95:PHE:CE1	6:F:103:ILE:HA	2.52	0.45
11:K:86:LEU:C	11:K:86:LEU:HD13	2.42	0.45
6:F:200:HIS:CG	6:F:200:HIS:O	2.70	0.45
7:G:78:ILE:N	7:G:79:PRO:CD	2.79	0.45
11:K:209:ASN:ND2	11:K:210:VAL:HG23	2.32	0.45
1:O:89:SER:OG	1:O:114:VAL:HG22	2.16	0.45
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.99	0.45
2:P:234:ILE:O	2:P:237:ILE:HG22	2.17	0.45
13:a:154:LEU:HD11	13:a:183:VAL:HG21	1.99	0.45
8:H:196:ARG:NH1	12:Z:189:THR:HB	2.32	0.44
14:N:14:LEU:O	14:N:175:MET:HA	2.17	0.44
2:P:151:ASN:OD1	2:P:151:ASN:C	2.61	0.44
10:X:11:ASP:OD1	10:X:11:ASP:N	2.50	0.44
2:B:28:ILE:O	2:B:165:GLY:HA2	2.17	0.44
2:B:114:LEU:HD23	2:B:114:LEU:HA	1.84	0.44
3:C:35:LYS:HA	3:C:40:VAL:HA	1.99	0.44
4:D:126:MET:HE1	4:D:130:PHE:CZ	2.51	0.44
10:J:46:PHE:CD1	10:J:53:THR:HB	2.52	0.44
12:L:28:ARG:HG2	12:L:30:ILE:HG23	1.99	0.44
8:V:192:THR:HG22	8:V:192:THR:O	2.17	0.44
8:V:210:THR:HG21	9:W:167:SER:HB3	1.99	0.44
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.82	0.44
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.52	0.44
6:T:68:ARG:HD2	13:a:72:THR:OG1	2.17	0.44
8:V:14:LEU:HB3	8:V:44:CYS:SG	2.57	0.44
10:X:19:LYS:HD2	10:X:31:SER:HA	1.99	0.44
12:L:30:ILE:HD12	12:L:30:ILE:C	2.42	0.44
11:K:2:THR:HG21	11:K:164:ALA:CB	2.48	0.44
3:Q:42:LEU:HD11	3:Q:70:VAL:HG23	1.99	0.44
5:S:71:LEU:HD22	5:S:71:LEU:O	2.17	0.44
8:V:218:VAL:CB	9:W:194:VAL:HG12	2.46	0.44
18:V:303:A1IFL:C57	18:V:303:A1IFL:N4	2.79	0.44
2:B:145:TYR:OH	2:B:217:LYS:N	2.48	0.44
8:H:18:THR:HG23	8:H:172:ASN:O	2.18	0.44
8:H:218:VAL:HG23	9:I:194:VAL:HG12	1.99	0.44
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.98	0.44
13:a:6:VAL:HA	13:a:29:SER:O	2.18	0.44
1:O:64:VAL:HG11	1:O:212:ALA:CB	2.48	0.44
14:b:89:ASN:HB2	14:b:93:LEU:CD1	2.48	0.44
5:E:95:SER:O	5:E:99:ASN:HA	2.18	0.44
8:H:24:SER:HB2	20:H:403:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:4:PRO:O	13:M:104:ARG:NH1	2.46	0.44
12:L:55:ASN:O	12:L:107:VAL:HA	2.18	0.44
10:J:58:GLU:OE1	11:K:81:LYS:NZ	2.51	0.44
12:L:42:LYS:HD2	12:L:55:ASN:ND2	2.30	0.44
6:T:14:ASP:CB	6:T:16:ARG:HD3	2.48	0.44
11:Y:56:GLU:OE2	11:Y:99:THR:OG1	2.36	0.44
12:Z:43:VAL:HG12	12:Z:205:LEU:HD22	2.00	0.44
4:D:93:LEU:HD12	11:K:57:THR:HG22	2.00	0.43
5:E:68:HIS:HE1	5:E:102:LEU:O	2.01	0.43
7:G:101:TYR:OH	8:H:66:HIS:HE1	2.01	0.43
7:G:126:ARG:HH11	7:G:126:ARG:CG	2.31	0.43
14:N:67:THR:HA	14:N:71:GLY:O	2.18	0.43
5:S:48:LEU:O	5:S:61:LYS:HE2	2.19	0.43
9:I:200:LYS:HE3	11:Y:198:TRP:CE2	2.52	0.43
11:K:135:PHE:CE1	11:K:167:ARG:HB3	2.53	0.43
12:Z:13:LEU:C	12:Z:13:LEU:HD12	2.43	0.43
13:a:43:ILE:HD11	13:a:53:ILE:CD1	2.49	0.43
4:D:115:PHE:HA	4:D:126:MET:O	2.18	0.43
6:F:17:ASN:ND2	6:F:20:VAL:HG23	2.34	0.43
6:F:78:ILE:HB	6:F:79:PRO:HD3	2.01	0.43
9:I:41:LYS:O	9:I:51:GLY:HA2	2.18	0.43
3:Q:131:THR:O	3:Q:147:GLN:HA	2.19	0.43
6:T:146:MET:HB3	6:T:156:TYR:CE1	2.54	0.43
12:Z:26:ASP:HA	12:Z:201:GLY:O	2.17	0.43
6:F:216:SER:HB3	6:F:219:GLU:HB2	2.01	0.43
9:I:104:VAL:HG23	9:I:106:PRO:HD3	1.99	0.43
12:Z:147:MET:N	12:Z:148:PRO:CD	2.81	0.43
1:A:64:VAL:HG11	1:A:212:ALA:CB	2.48	0.43
10:J:174:MET:HA	10:X:174:MET:HA	2.00	0.43
6:T:78:ILE:HB	6:T:79:PRO:HD3	2.01	0.43
7:U:115:LEU:HD12	7:U:115:LEU:HA	1.83	0.43
2:B:3:ARG:CZ	5:E:122:TYR:OH	2.66	0.43
13:a:4:PRO:HD3	13:a:111:TRP:CE2	2.53	0.43
7:G:68:ARG:O	7:G:223:LYS:HA	2.19	0.43
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.01	0.43
10:J:3:ILE:HD13	10:J:3:ILE:C	2.43	0.43
12:L:36:ASN:HB3	13:M:137:TYR:CD1	2.53	0.43
12:L:54:ALA:HB1	12:L:107:VAL:HG21	2.00	0.43
6:F:9:SER:HB2	7:G:126:ARG:HD3	2.01	0.43
12:L:18:GLU:HG3	12:L:174:TYR:CD2	2.54	0.43
2:B:89:THR:HG21	2:B:117:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:193:VAL:O	5:E:196:ILE:HG22	2.19	0.43
2:P:114:LEU:HD23	2:P:114:LEU:HA	1.91	0.43
11:Y:87:VAL:CG1	11:Y:97:MET:HE1	2.49	0.43
3:C:155:SER:HB2	4:D:51:LEU:HD11	2.00	0.42
5:E:65:CYS:SG	5:E:71:LEU:CD1	3.07	0.42
8:H:139:GLU:OE1	14:N:29:ARG:NE	2.51	0.42
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.52	0.42
8:H:206:PRO:O	8:H:209:THR:OG1	2.20	0.42
12:L:124:SER:HB2	12:L:137:ARG:HG2	2.00	0.42
11:Y:2:THR:HG21	11:Y:164:ALA:HB3	2.00	0.42
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	2.01	0.42
12:Z:193:GLU:OE1	12:Z:220:LYS:NZ	2.46	0.42
10:J:174:MET:HB3	10:X:174:MET:HE3	2.01	0.42
5:S:9:THR:HG21	5:S:119:THR:HA	2.01	0.42
1:A:35:LEU:C	1:A:35:LEU:HD12	2.44	0.42
14:N:13:ILE:HG21	14:N:175:MET:CE	2.49	0.42
14:N:133:PHE:HA	14:b:132:THR:O	2.19	0.42
10:X:1:MET:HG2	10:X:34:LYS:CE	2.49	0.42
10:X:92:ILE:HD12	10:X:92:ILE:HA	1.92	0.42
11:K:25:TRP:CZ3	12:L:144:SER:HA	2.55	0.42
12:L:49:ASN:HD22	12:L:49:ASN:HA	1.56	0.42
14:N:132:THR:O	14:b:133:PHE:HA	2.20	0.42
8:V:43:CYS:SG	8:V:98:LEU:HB3	2.59	0.42
12:L:196:ILE:HG12	8:V:24:SER:O	2.20	0.42
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.85	0.42
2:P:111:VAL:HG22	2:P:136:TYR:CG	2.55	0.42
9:W:52:ILE:HG22	9:W:59:VAL:HG22	2.00	0.42
11:Y:139:VAL:HG21	11:Y:163:ALA:HB2	2.01	0.42
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.32	0.42
11:Y:99:THR:HG22	11:Y:115:VAL:O	2.19	0.42
1:A:222:LEU:HD12	1:A:222:LEU:HA	1.92	0.42
2:B:213:ALA:HA	2:B:227:LYS:O	2.20	0.42
7:G:43:VAL:HG11	7:G:194:VAL:HA	2.01	0.42
9:I:82:GLU:OE2	9:I:113:SER:OG	2.37	0.42
13:M:159:VAL:HG23	13:M:159:VAL:O	2.20	0.42
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.84	0.42
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.45	0.42
13:a:206:LEU:C	13:a:206:LEU:HD23	2.45	0.42
9:I:65:MET:HE1	9:I:93:SER:HB3	2.01	0.41
2:P:119:GLN:HG3	3:Q:78:ALA:HB1	2.02	0.41
8:V:123:TYR:HB3	8:V:142:TRP:CZ2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:155:SER:HB2	4:D:51:LEU:CD1	2.50	0.41
8:H:123:TYR:HB3	8:H:142:TRP:CZ2	2.55	0.41
14:N:32:ASP:OD2	14:N:185:ARG:NH2	2.54	0.41
11:K:37:ILE:HB	11:K:41:LEU:HB3	2.01	0.41
14:N:6:VAL:HG13	14:N:124:TYR:CB	2.50	0.41
3:Q:160:GLN:HG3	3:Q:161:THR:N	2.36	0.41
5:S:8:ASP:OD1	5:S:10:VAL:HG12	2.20	0.41
5:S:62:ILE:HG21	5:S:213:ALA:HB2	2.01	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.03	0.41
7:U:37:ARG:NH2	7:U:183:ASP:HB3	2.35	0.41
7:U:227:LEU:HB3	7:U:231:ASN:HB2	2.02	0.41
13:a:2:GLN:OE1	13:a:2:GLN:N	2.52	0.41
6:F:116:VAL:HG21	6:F:147:LEU:HD21	2.02	0.41
11:K:6:PHE:HA	11:K:125:ASP:O	2.20	0.41
1:O:57:MET:HE3	1:O:60:THR:HG21	2.03	0.41
2:P:28:ILE:O	2:P:165:GLY:HA2	2.20	0.41
7:U:196:PHE:CD1	7:U:196:PHE:C	2.98	0.41
11:Y:4:LEU:C	11:Y:4:LEU:HD12	2.46	0.41
12:Z:43:VAL:HG22	12:Z:53:SER:HB2	2.02	0.41
2:B:165:GLY:O	2:B:168:THR:HG23	2.20	0.41
7:G:73:VAL:CG1	7:G:133:THR:HB	2.50	0.41
10:J:50:ALA:O	11:K:91:LYS:NZ	2.53	0.41
6:T:66:VAL:HG11	6:T:108:PHE:CE1	2.56	0.41
6:T:187:GLU:O	6:T:191:GLN:HG2	2.19	0.41
11:Y:116:ASP:C	11:Y:116:ASP:OD2	2.64	0.41
5:E:98:PHE:O	13:M:91:TYR:HA	2.21	0.41
11:Y:86:LEU:O	11:Y:89:GLN:HB2	2.19	0.41
8:H:68:LEU:HD12	8:H:68:LEU:HA	1.90	0.41
12:Z:36:ASN:HB3	13:a:137:TYR:CE1	2.56	0.41
4:R:67:GLY:HA3	4:R:220:PHE:CD1	2.56	0.41
6:T:99:TYR:O	14:b:77:THR:OG1	2.32	0.41
8:V:18:THR:HG21	8:V:172:ASN:HB2	2.02	0.41
10:X:130:TYR:CB	10:X:144:LEU:HD13	2.51	0.41
1:A:12:PHE:H	2:B:20:GLN:HE22	1.69	0.41
2:B:216:ARG:HB3	2:B:218:GLY:H	1.86	0.41
4:D:44:LYS:HE3	4:D:210:GLN:HB2	2.03	0.41
6:F:175:LEU:HD21	6:F:191:GLN:NE2	2.35	0.41
10:J:35:THR:HG23	10:J:43:LEU:HD11	2.02	0.41
12:L:221:ARG:NH2	13:M:160:ASP:O	2.54	0.41
13:M:187:ARG:HG3	14:b:25:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:36:GLY:N	3:Q:39:CYS:O	2.51	0.41
3:Q:168:THR:O	3:Q:171:GLU:HB3	2.20	0.41
4:R:109:CYS:HB3	4:R:154:GLY:O	2.21	0.41
5:S:127:TYR:O	5:S:148:PRO:CB	2.69	0.41
6:T:71:GLY:O	6:T:134:PHE:HA	2.20	0.41
6:T:155:GLY:HA3	7:U:59:THR:HG21	2.02	0.41
9:W:62:LEU:HD23	9:W:62:LEU:HA	1.95	0.41
9:W:73:TYR:CZ	9:W:77:GLU:HG3	2.56	0.41
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.01	0.41
11:Y:87:VAL:CG1	11:Y:97:MET:HE2	2.50	0.41
5:E:71:LEU:C	5:E:71:LEU:CD2	2.94	0.41
14:N:83:LYS:HG3	14:N:119:VAL:HG22	2.03	0.41
2:P:180:LYS:O	2:P:183:MET:HB2	2.21	0.41
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.16	0.41
5:S:134:ILE:HD12	5:S:215:VAL:HG12	2.03	0.41
7:U:43:VAL:HG11	7:U:194:VAL:HA	2.02	0.41
1:A:98:LYS:HE3	1:A:104:TYR:CZ	2.56	0.40
13:M:34:LEU:HD12	14:b:164:LYS:O	2.21	0.40
13:M:96:LEU:O	13:M:100:MET:HG2	2.22	0.40
2:B:35:ILE:HD12	2:B:196:LEU:HG	2.02	0.40
10:J:2:ASP:O	10:J:3:ILE:CB	2.67	0.40
10:J:152:MET:HE2	10:J:156:GLU:HB3	2.03	0.40
4:R:78:ARG:HA	4:R:78:ARG:HD3	1.92	0.40
6:T:46:VAL:HB	6:T:73:VAL:HG21	2.02	0.40
9:W:62:LEU:HD11	9:W:104:VAL:HG21	2.02	0.40
9:W:130:ASP:OD1	9:W:130:ASP:C	2.64	0.40
11:K:161:ILE:HD13	11:K:161:ILE:HA	1.93	0.40
8:V:168:GLY:O	18:V:303:A1IFL:C56	2.69	0.40
12:Z:4:PRO:HB2	13:a:104:ARG:NH1	2.35	0.40
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.04	0.40
14:b:175:MET:HB2	14:b:186:LEU:HB2	2.03	0.40
5:E:134:ILE:HD12	5:E:215:VAL:HG12	2.02	0.40
7:G:33:SER:O	7:G:161:ALA:HA	2.22	0.40
8:H:32:GLU:OE1	8:H:188:ARG:HD2	2.22	0.40
12:L:147:MET:CE	9:W:176:ARG:NH2	2.85	0.40
1:O:115:ALA:HB1	1:O:154:GLY:O	2.21	0.40
3:Q:116:GLN:CD	3:Q:116:GLN:C	2.89	0.40
8:V:17:ASP:CG	8:V:33:LYS:HZ2	2.29	0.40
8:V:38:ALA:HB1	8:V:39:PRO:CD	2.51	0.40
8:V:68:LEU:HD12	8:V:68:LEU:HA	1.86	0.40
9:W:125:LEU:HD23	9:W:125:LEU:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:ILE:HD12	2:B:192:ALA:HB2	2.03	0.40
5:E:9:THR:HG21	5:E:119:THR:HA	2.02	0.40
2:P:66:TYR:CG	2:P:87:ILE:HD13	2.56	0.40
7:U:63:ILE:HG12	7:U:73:VAL:HG23	2.03	0.40
10:X:152:MET:HE1	10:X:160:LEU:HD22	2.03	0.40
14:b:83:LYS:HG3	14:b:119:VAL:HG22	2.03	0.40
14:b:176:VAL:HG12	14:b:178:LEU:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	234 (94%)	13 (5%)	1 (0%)	30	50
1	O	248/250 (99%)	238 (96%)	8 (3%)	2 (1%)	16	30
2	B	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	30	50
2	P	242/258 (94%)	235 (97%)	7 (3%)	0	100	100
3	C	238/254 (94%)	227 (95%)	9 (4%)	2 (1%)	16	30
3	Q	238/254 (94%)	230 (97%)	4 (2%)	4 (2%)	7	14
4	D	231/260 (89%)	223 (96%)	7 (3%)	1 (0%)	30	50
4	R	231/260 (89%)	222 (96%)	8 (4%)	1 (0%)	30	50
5	E	229/234 (98%)	219 (96%)	10 (4%)	0	100	100
5	S	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	235 (98%)	3 (1%)	1 (0%)	30	50
7	U	239/252 (95%)	232 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	223/225 (99%)	215 (96%)	7 (3%)	1 (0%)	30	50
8	V	220/225 (98%)	211 (96%)	9 (4%)	0	100	100
9	I	202/205 (98%)	188 (93%)	14 (7%)	0	100	100
9	W	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
10	J	193/198 (98%)	184 (95%)	6 (3%)	3 (2%)	7	14
10	X	193/198 (98%)	181 (94%)	11 (6%)	1 (0%)	24	43
11	K	209/211 (99%)	197 (94%)	12 (6%)	0	100	100
11	Y	209/211 (99%)	200 (96%)	8 (4%)	1 (0%)	24	43
12	L	220/222 (99%)	211 (96%)	8 (4%)	1 (0%)	24	43
12	Z	220/222 (99%)	212 (96%)	7 (3%)	1 (0%)	24	43
13	M	232/246 (94%)	224 (97%)	8 (3%)	0	100	100
13	a	232/246 (94%)	219 (94%)	11 (5%)	2 (1%)	14	28
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
All	All	6279/6598 (95%)	6025 (96%)	231 (4%)	23 (0%)	30	50

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	3	ILE
1	A	3	ASP
3	C	204	GLY
3	C	239	GLN
1	O	50	LYS
1	O	166	LYS
3	Q	52	LEU
3	Q	204	GLY
3	Q	239	GLN
12	L	166	GLY
12	Z	166	GLY
4	D	2	ARG
3	Q	183	PRO
4	R	2	ARG
11	Y	9	GLN
13	a	83	ALA
2	B	221	ASP
8	H	223	ILE

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Mol	Chain	Res	Type
7	G	105	CYS
10	J	24	GLY
10	X	24	GLY
13	a	229	GLY
10	J	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%)	203 (97%)	6 (3%)	37	61
1	O	209/209 (100%)	204 (98%)	5 (2%)	43	65
2	B	203/216 (94%)	193 (95%)	10 (5%)	22	43
2	P	203/216 (94%)	192 (95%)	11 (5%)	20	38
3	C	212/226 (94%)	200 (94%)	12 (6%)	18	35
3	Q	212/226 (94%)	199 (94%)	13 (6%)	17	31
4	D	194/215 (90%)	180 (93%)	14 (7%)	13	25
4	R	194/215 (90%)	182 (94%)	12 (6%)	16	31
5	E	190/193 (98%)	182 (96%)	8 (4%)	26	49
5	S	190/193 (98%)	182 (96%)	8 (4%)	26	49
6	F	201/239 (84%)	192 (96%)	9 (4%)	24	46
6	T	201/239 (84%)	192 (96%)	9 (4%)	24	46
7	G	206/210 (98%)	195 (95%)	11 (5%)	20	39
7	U	206/210 (98%)	197 (96%)	9 (4%)	25	47
8	H	183/183 (100%)	172 (94%)	11 (6%)	17	32
8	V	180/183 (98%)	169 (94%)	11 (6%)	17	31
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	71
9	W	172/173 (99%)	163 (95%)	9 (5%)	21	39
10	J	173/175 (99%)	160 (92%)	13 (8%)	12	24
10	X	173/175 (99%)	162 (94%)	11 (6%)	16	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	168/168 (100%)	164 (98%)	4 (2%)	43	65
11	Y	168/168 (100%)	159 (95%)	9 (5%)	20	38
12	L	185/185 (100%)	175 (95%)	10 (5%)	20	38
12	Z	185/185 (100%)	175 (95%)	10 (5%)	20	38
13	M	200/208 (96%)	191 (96%)	9 (4%)	24	46
13	a	200/208 (96%)	188 (94%)	12 (6%)	17	32
14	N	162/162 (100%)	156 (96%)	6 (4%)	30	54
14	b	162/162 (100%)	155 (96%)	7 (4%)	26	47
All	All	5313/5524 (96%)	5051 (95%)	262 (5%)	22	43

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	201	GLU
1	A	230	ASP
2	B	50	LYS
2	B	51	VAL
2	B	52	THR
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	102	ASN
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	49	THR
3	C	51	LYS
3	C	52	LEU
3	C	61	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS

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Mol	Chain	Res	Type
3	C	187	GLU
3	C	240	GLU
4	D	20	LEU
4	D	51	LEU
4	D	60	VAL
4	D	99	ILE
4	D	117	GLU
4	D	176	LEU
4	D	182	SER
4	D	190	LEU
4	D	193	LEU
4	D	214	ILE
4	D	224	ASP
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
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	106	ARG
5	E	188	LEU
6	F	68	ARG
6	F	94	SER
6	F	117	GLN
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	221	ASN
6	F	240	GLN
7	G	26	THR
7	G	83	ASN
7	G	114	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	126	ARG
7	G	208	GLU
7	G	215	GLU

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Mol	Chain	Res	Type
7	G	235	ARG
7	G	236	LEU
8	H	7	VAL
8	H	9	GLN
8	H	53	GLU
8	H	68	LEU
8	H	84	LYS
8	H	100	VAL
8	H	103	VAL
8	H	118	SER
8	H	127	LEU
8	H	144	GLN
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	1	MET
10	J	3	ILE
10	J	35	THR
10	J	49	GLU
10	J	90	LYS
10	J	99	GLN
10	J	110	LYS
10	J	136	SER
10	J	142	SER
10	J	160	LEU
10	J	163	LEU
10	J	165	VAL
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	209	ASN
12	L	18	GLU
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	124	SER
12	L	126	ASP
12	L	130	SER
12	L	150	LEU
12	L	172	LEU

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Mol	Chain	Res	Type
12	L	173	LYS
13	M	2	GLN
13	M	10	SER
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	192	SER
13	M	225	ILE
14	N	6	VAL
14	N	9	LYS
14	N	107	LYS
14	N	115	LEU
14	N	119	VAL
14	N	178	LEU
1	O	2	THR
1	O	51	SER
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	40	SER
2	P	51	VAL
2	P	52	THR
2	P	55	LEU
2	P	58	GLN
2	P	79	LEU
2	P	102	ASN
2	P	113	ARG
2	P	191	LEU
2	P	224	VAL
2	P	238	LEU
3	Q	4	ARG
3	Q	10	SER
3	Q	38	ASN
3	Q	48	SER
3	Q	51	LYS
3	Q	52	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	171	GLU

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Mol	Chain	Res	Type
3	Q	180	LYS
3	Q	187	GLU
3	Q	240	GLU
4	R	40	LEU
4	R	51	LEU
4	R	54	ASP
4	R	60	VAL
4	R	99	ILE
4	R	117	GLU
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	54	GLU
5	S	55	LEU
5	S	56	SER
5	S	71	LEU
5	S	118	ASN
5	S	188	LEU
6	T	68	ARG
6	T	94	SER
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	203	ASN
6	T	221	ASN
6	T	240	GLN
7	U	13	GLU
7	U	26	THR
7	U	83	ASN
7	U	115	LEU
7	U	125	MET
7	U	208	GLU
7	U	221	LYS
7	U	235	ARG
7	U	236	LEU
8	V	7	VAL

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Mol	Chain	Res	Type
8	V	9	GLN
8	V	17	ASP
8	V	22	ASN
8	V	68	LEU
8	V	84	LYS
8	V	103	VAL
8	V	127	LEU
8	V	188	ARG
8	V	196	ARG
8	V	222	ASP
9	W	12	VAL
9	W	31	GLN
9	W	37	ASN
9	W	134	ASP
9	W	171	LEU
9	W	182	TRP
9	W	190	LYS
9	W	192	ASP
9	W	194	VAL
10	X	2	ASP
10	X	3	ILE
10	X	18	SER
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
10	X	110	LYS
10	X	136	SER
10	X	163	LEU
10	X	172	MET
10	X	174	MET
11	Y	9	GLN
11	Y	35	ILE
11	Y	41	LEU
11	Y	73	ARG
11	Y	84	SER
11	Y	102	CYS
11	Y	147	ASP
11	Y	195	GLU
11	Y	209	ASN
12	Z	18	GLU
12	Z	23	LEU
12	Z	31	THR

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Mol	Chain	Res	Type
12	Z	49	ASN
12	Z	106	TYR
12	Z	136	CYS
12	Z	150	LEU
12	Z	172	LEU
12	Z	173	LYS
12	Z	189	THR
13	a	2	GLN
13	a	10	SER
13	a	48	ASN
13	a	69	ASP
13	a	70	LEU
13	a	104	ARG
13	a	106	LYS
13	a	116	VAL
13	a	119	VAL
13	a	161	ARG
13	a	187	ARG
13	a	192	SER
14	b	6	VAL
14	b	9	LYS
14	b	77	THR
14	b	107	LYS
14	b	115	LEU
14	b	119	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (171) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	93	HIS
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
2	B	232	GLN
3	C	14	HIS

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Mol	Chain	Res	Type
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	106	GLN
4	D	160	ASN
4	D	198	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	147	GLN
5	E	165	GLN
5	E	184	ASN
6	F	19	GLN
6	F	83	HIS
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	27	ASN
7	G	28	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	167	GLN
7	G	172	ASN
7	G	175	ASN
7	G	176	HIS
7	G	212	ASN
7	G	231	ASN
8	H	66	HIS
8	H	165	ASN

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Mol	Chain	Res	Type
9	I	44	HIS
9	I	63	ASN
9	I	88	GLN
10	J	55	GLN
10	J	191	GLN
11	K	85	ASN
11	K	143	ASN
11	K	190	ASN
11	K	209	ASN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	55	ASN
12	L	79	HIS
12	L	87	ASN
12	L	152	ASN
12	L	153	GLN
12	L	155	ASN
12	L	158	ASN
12	L	197	GLN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	211	ASN
13	M	213	GLN
14	N	38	HIS
14	N	69	GLN
14	N	92	ASN
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
1	O	119	GLN
1	O	123	GLN
1	O	149	GLN
1	O	190	HIS
1	O	241	GLN
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN

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Mol	Chain	Res	Type
2	P	124	HIS
2	P	155	ASN
2	P	232	GLN
3	Q	14	HIS
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	146	GLN
4	R	160	ASN
4	R	225	ASN
5	S	68	HIS
5	S	89	GLN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	147	GLN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	172	ASN
7	U	175	ASN
7	U	186	ASN
7	U	231	ASN
8	V	66	HIS
8	V	172	ASN
8	V	189	ASN
8	V	194	ASN

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Mol	Chain	Res	Type
9	W	44	HIS
9	W	63	ASN
9	W	88	GLN
9	W	168	GLN
9	W	203	GLN
10	X	55	GLN
10	X	78	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	143	ASN
11	Y	190	ASN
11	Y	209	ASN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	76	HIS
12	Z	80	ASN
12	Z	152	ASN
12	Z	153	GLN
12	Z	159	GLN
12	Z	195	HIS
12	Z	197	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	141	ASN
14	b	157	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 23 ligands modelled in this entry, 11 are monoatomic - leaving 12 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
19	SO4	K	303	-	4,4,4	0.33	0	6,6,6	0.08	0
19	SO4	N	202	-	4,4,4	0.33	0	6,6,6	0.07	0
17	MES	K	302	-	12,12,12	0.67	0	15,16,16	0.40	0
17	MES	V	302	-	12,12,12	0.70	0	15,16,16	0.51	0
18	A1IFL	Y	304	11	49,54,54	1.74	7 (14%)	58,75,75	1.23	6 (10%)
18	A1IFL	H	302	8	49,54,54	1.33	2 (4%)	58,75,75	1.27	7 (12%)
19	SO4	b	201	-	4,4,4	0.33	0	6,6,6	0.11	0
17	MES	H	301	-	12,12,12	0.72	0	15,16,16	0.42	0
18	A1IFL	K	304	11	49,54,54	1.62	6 (12%)	58,75,75	1.34	4 (6%)
19	SO4	Y	303	-	4,4,4	0.33	0	6,6,6	0.07	0
17	MES	Y	302	-	12,12,12	0.66	0	15,16,16	0.39	0
18	A1IFL	V	303	8	49,54,54	1.73	7 (14%)	58,75,75	1.33	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	MES	K	302	-	-	2/6/14/14	0/1/1/1
17	MES	V	302	-	-	2/6/14/14	0/1/1/1
18	A1IFL	Y	304	11	-	7/37/85/85	0/3/4/4
18	A1IFL	H	302	8	-	9/37/85/85	0/3/4/4
17	MES	H	301	-	-	1/6/14/14	0/1/1/1
18	A1IFL	K	304	11	-	8/37/85/85	0/3/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MES	Y	302	-	-	3/6/14/14	0/1/1/1
18	A1IFL	V	303	8	-	8/37/85/85	0/3/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	303	A1IFL	OG1-CB1	-6.65	1.34	1.43
18	K	304	A1IFL	CB-CG	-6.52	1.35	1.51
18	Y	304	A1IFL	CB-CG	-6.15	1.36	1.51
18	Y	304	A1IFL	O58-C11	-5.95	1.36	1.44
18	H	302	A1IFL	CB-CG	-5.94	1.37	1.51
18	V	303	A1IFL	CB-CG	-5.01	1.39	1.51
18	K	304	A1IFL	O58-C11	-4.97	1.37	1.44
18	Y	304	A1IFL	OG1-CB1	-4.19	1.38	1.43
18	V	303	A1IFL	O58-C11	-4.12	1.38	1.44
18	V	303	A1IFL	CB1-CA3	-3.66	1.47	1.53
18	K	304	A1IFL	OG1-CB1	-3.44	1.39	1.43
18	K	304	A1IFL	OG1-C21	-2.95	1.37	1.43
18	H	302	A1IFL	OG1-CB1	-2.83	1.40	1.43
18	V	303	A1IFL	OG1-C21	-2.79	1.38	1.43
18	Y	304	A1IFL	OG1-C21	-2.41	1.38	1.43
18	K	304	A1IFL	C54-C49	-2.40	1.45	1.52
18	Y	304	A1IFL	C57-C11	-2.18	1.49	1.52
18	V	303	A1IFL	C48-C31	-2.14	1.50	1.52
18	Y	304	A1IFL	C-N	-2.12	1.29	1.34
18	Y	304	A1IFL	C54-C49	-2.07	1.46	1.52
18	K	304	A1IFL	CA1-C1	-2.04	1.47	1.52
18	V	303	A1IFL	C21-C31	-2.01	1.50	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	304	A1IFL	C4-C3-CA1	-6.46	103.78	113.53
18	H	302	A1IFL	C4-C3-CA1	-4.60	106.59	113.53
18	V	303	A1IFL	CB1-CA3-N2	-4.08	102.57	111.75
18	Y	304	A1IFL	C4-C3-CA1	-3.96	107.56	113.53
18	V	303	A1IFL	O58-C11-C57	-3.71	102.99	108.87
18	K	304	A1IFL	CB1-CA3-N2	-3.32	104.29	111.75
18	H	302	A1IFL	CB-CA2-N1	-3.15	104.31	110.83
18	H	302	A1IFL	CM-OH-CZ	-2.99	111.08	117.50
18	Y	304	A1IFL	CB1-CA3-N2	-2.93	105.17	111.75
18	K	304	A1IFL	CM-OH-CZ	-2.88	111.33	117.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	304	A1IFL	O55-C21-C11	2.67	112.50	106.08
18	H	302	A1IFL	C21-C31-N4	2.67	114.11	110.53
18	H	302	A1IFL	O55-C21-C11	2.63	112.40	106.08
18	V	303	A1IFL	C-CA-NB	-2.51	107.57	113.41
18	Y	304	A1IFL	CM-OH-CZ	-2.51	112.12	117.50
18	K	304	A1IFL	O55-C21-C11	2.47	112.01	106.08
18	V	303	A1IFL	O55-C21-C11	2.38	111.81	106.08
18	V	303	A1IFL	CA-NB-CD1	-2.35	107.49	111.14
18	V	303	A1IFL	C48-C49-C50	-2.32	106.32	111.71
18	H	302	A1IFL	CB1-CA3-N2	-2.29	106.61	111.75
18	Y	304	A1IFL	C48-C49-C50	-2.21	106.56	111.71
18	H	302	A1IFL	C-CA-NB	-2.15	108.41	113.41
18	V	303	A1IFL	CM-OH-CZ	-2.11	112.97	117.50
18	Y	304	A1IFL	CA2-N1-C1	2.10	126.15	121.65
18	V	303	A1IFL	O4-C9-CA3	-2.08	119.36	124.86

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	MES	N4-C7-C8-S
17	Y	302	MES	C7-C8-S-O2S
18	H	302	A1IFL	CA1-C3-C4-O3
18	H	302	A1IFL	C31-C48-C49-C54
18	K	304	A1IFL	C21-C31-C48-C49
18	V	303	A1IFL	CA1-C3-C4-O3
18	V	303	A1IFL	C4-C3-CA1-C1
18	V	303	A1IFL	C21-C31-C48-C49
18	V	303	A1IFL	C31-C48-C49-C54
18	Y	304	A1IFL	C21-C31-C48-C49
18	H	302	A1IFL	N1-CA2-CB-CG
18	H	302	A1IFL	N4-C31-C48-C49
18	V	303	A1IFL	N4-C31-C48-C49
18	Y	304	A1IFL	N4-C31-C48-C49
18	H	302	A1IFL	C8-CA2-CB-CG
18	K	304	A1IFL	N4-C31-C48-C49
18	V	303	A1IFL	C4-C3-CA1-N
17	Y	302	MES	C7-C8-S-O3S
18	H	302	A1IFL	C6-CZ-OH-CM
17	K	302	MES	C8-C7-N4-C3
17	K	302	MES	C8-C7-N4-C5
18	H	302	A1IFL	C21-C31-C48-C49

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Mol	Chain	Res	Type	Atoms
18	H	302	A1IFL	C5-CZ-OH-CM
18	H	302	A1IFL	C31-C48-C49-C50
18	Y	304	A1IFL	N1-CA2-CB-CG
18	K	304	A1IFL	O2-C8-CA2-N1
17	Y	302	MES	C7-C8-S-O1S
18	Y	304	A1IFL	O1-C1-CA1-N
18	K	304	A1IFL	N4-C8-CA2-N1
17	V	302	MES	C8-C7-N4-C3
17	V	302	MES	C8-C7-N4-C5
18	K	304	A1IFL	C31-C48-C49-C54
18	V	303	A1IFL	C31-C48-C49-C50
18	V	303	A1IFL	N1-CA2-CB-CG
18	K	304	A1IFL	N1-CA2-CB-CG
18	Y	304	A1IFL	O2-C8-CA2-N1
18	Y	304	A1IFL	N4-C8-CA2-N1
18	Y	304	A1IFL	N1-C1-CA1-N
18	K	304	A1IFL	O2-C8-CA2-CB
18	K	304	A1IFL	C6-CZ-OH-CM

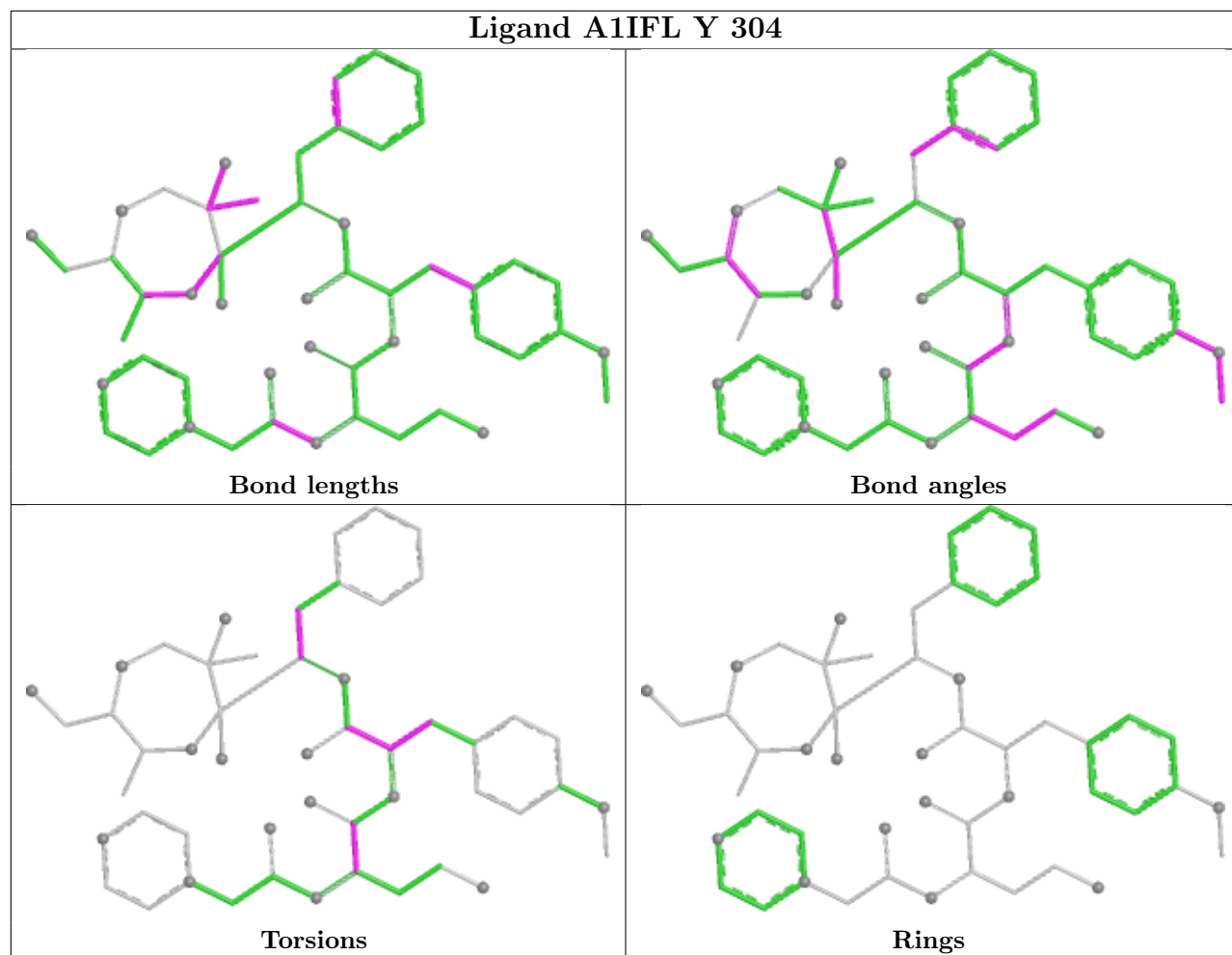
There are no ring outliers.

5 monomers are involved in 9 short contacts:

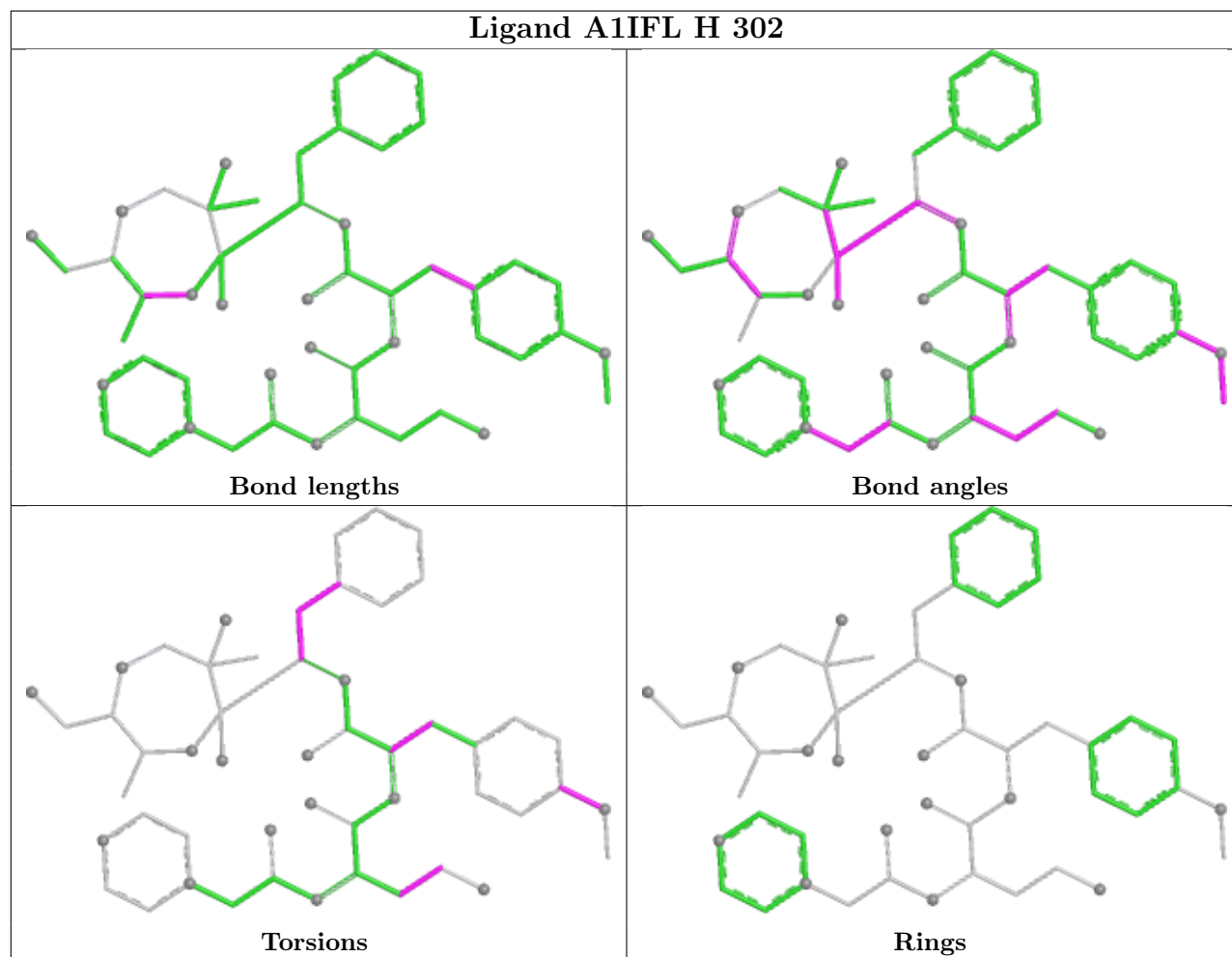
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	302	MES	1	0
18	Y	304	A1IFL	2	0
18	H	302	A1IFL	1	0
18	K	304	A1IFL	2	0
18	V	303	A1IFL	3	0

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.

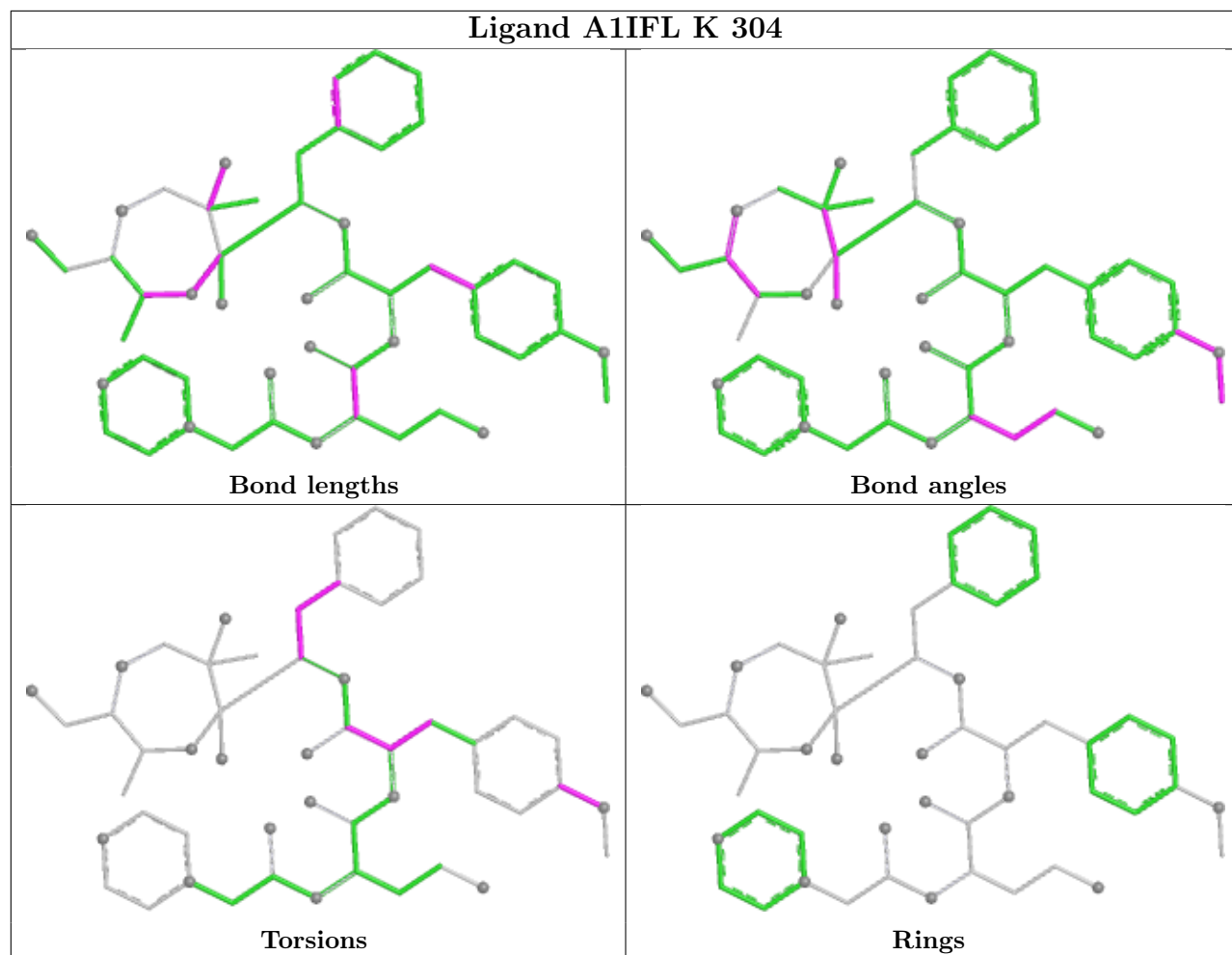
Ligand A1IFL Y 304

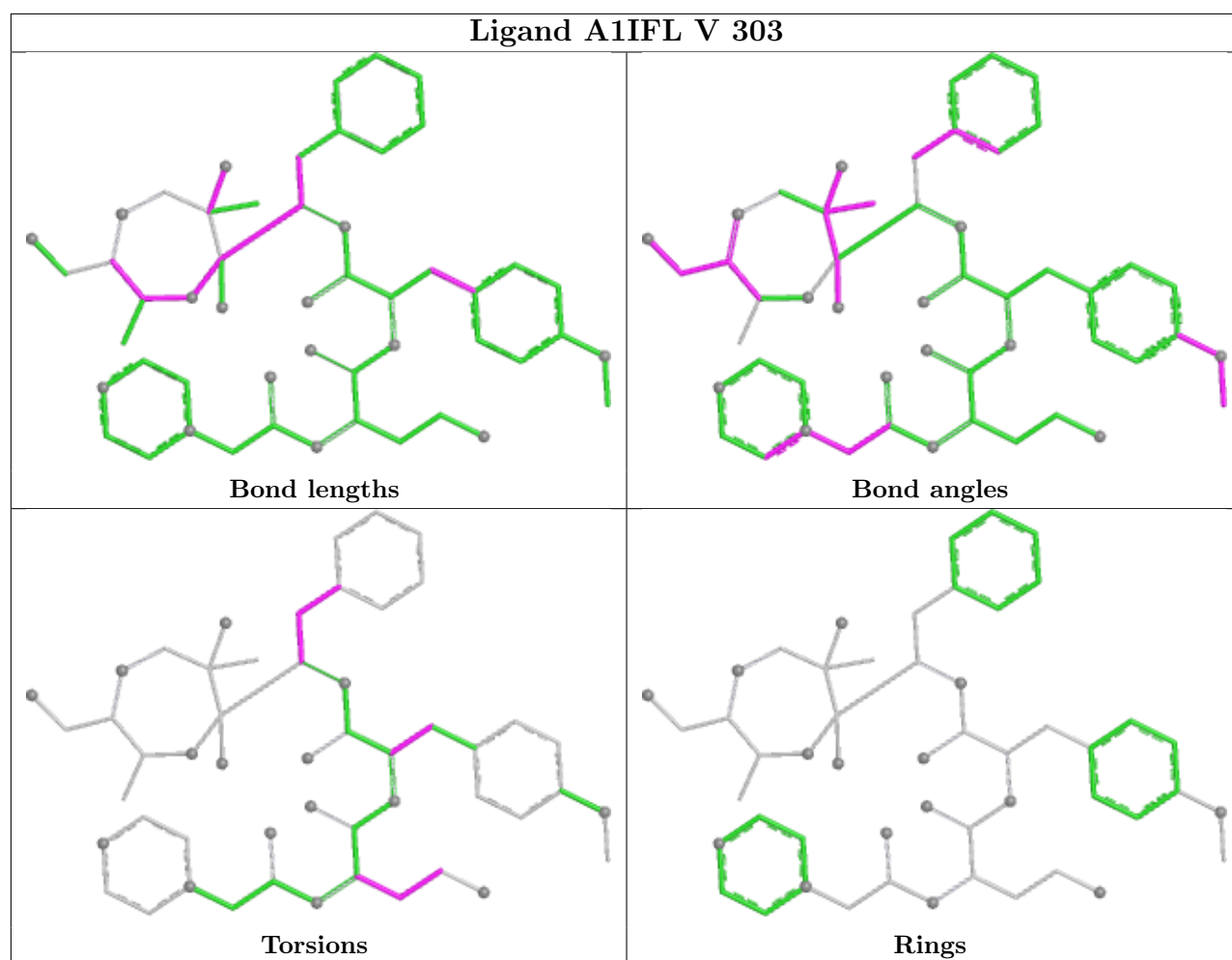


Ligand A1IFL H 302



Ligand A1IFL K 304





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%)	0.29	9 (3%) 46 44	49, 64, 99, 127	0
1	O	250/250 (100%)	0.35	11 (4%) 39 38	54, 74, 108, 127	0
2	B	244/258 (94%)	0.47	11 (4%) 38 37	53, 69, 107, 149	0
2	P	244/258 (94%)	0.45	11 (4%) 38 37	57, 72, 118, 144	0
3	C	240/254 (94%)	0.49	13 (5%) 31 31	53, 73, 131, 143	0
3	Q	240/254 (94%)	0.70	24 (10%) 12 12	58, 83, 150, 160	0
4	D	235/260 (90%)	0.26	7 (2%) 52 50	54, 71, 93, 123	0
4	R	235/260 (90%)	0.55	10 (4%) 40 38	59, 77, 106, 131	0
5	E	231/234 (98%)	0.36	3 (1%) 75 75	56, 73, 100, 121	0
5	S	231/234 (98%)	0.62	9 (3%) 43 40	59, 80, 115, 131	0
6	F	243/288 (84%)	0.37	4 (1%) 70 69	49, 68, 107, 130	0
6	T	243/288 (84%)	0.32	8 (3%) 49 47	54, 72, 108, 139	0
7	G	241/252 (95%)	0.26	4 (1%) 69 67	49, 64, 90, 126	0
7	U	241/252 (95%)	0.21	4 (1%) 69 67	53, 68, 91, 126	0
8	H	225/225 (100%)	0.22	7 (3%) 51 49	49, 60, 86, 162	0
8	V	222/225 (98%)	0.25	3 (1%) 73 73	51, 62, 84, 141	0
9	I	204/205 (99%)	0.26	1 (0%) 87 87	45, 60, 78, 96	0
9	W	204/205 (99%)	0.06	1 (0%) 87 87	49, 60, 77, 97	0
10	J	195/198 (98%)	0.29	4 (2%) 63 61	50, 61, 82, 104	0
10	X	195/198 (98%)	0.23	5 (2%) 57 55	53, 64, 82, 120	0
11	K	211/211 (100%)	0.08	0 100 100	49, 59, 78, 87	0
11	Y	211/211 (100%)	0.21	1 (0%) 87 87	52, 62, 83, 98	0
12	L	222/222 (100%)	0.22	1 (0%) 87 87	47, 61, 85, 100	0
12	Z	222/222 (100%)	0.16	1 (0%) 87 87	50, 62, 87, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	0.22	4 (1%)	69	67	30, 60, 79, 90	1 (0%)
13	a	233/246 (94%)	0.29	2 (0%)	81	81	29, 61, 76, 84	1 (0%)
14	N	196/196 (100%)	0.11	2 (1%)	79	79	48, 57, 78, 101	0
14	b	196/196 (100%)	0.18	2 (1%)	79	79	48, 59, 83, 106	0
All	All	6337/6598 (96%)	0.31	162 (2%)	57	55	29, 66, 104, 162	2 (0%)

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	51	VAL	7.4
3	Q	50	LEU	6.1
3	Q	49	THR	5.8
8	V	223	ILE	5.5
1	O	229	THR	5.3
2	P	1	GLY	4.8
3	Q	204	GLY	4.7
1	A	229	THR	4.7
1	O	1	MET	4.6
8	H	223	ILE	4.5
4	R	112	ALA	4.3
2	P	51	VAL	4.2
4	R	113	LEU	4.1
1	O	52	SER	4.1
1	A	201	GLU	4.0
13	M	1	THR	4.0
13	M	190[A]	ARG	3.8
13	a	69	ASP	3.7
10	J	1	MET	3.7
7	G	3	TYR	3.6
3	C	52	LEU	3.6
13	a	1	THR	3.5
3	C	204	GLY	3.5
2	B	2	SER	3.5
1	A	227	ILE	3.4
3	Q	47	ARG	3.4
2	P	219	ALA	3.4
7	U	2	GLY	3.4
12	L	136	CYS	3.4
1	O	228	PRO	3.3
2	B	1	GLY	3.1
3	C	50	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	2	THR	3.0
7	G	2	GLY	3.0
4	D	117	GLU	2.9
1	A	4	ARG	2.8
5	S	178	PHE	2.8
10	J	2	ASP	2.8
14	b	192	GLU	2.8
2	P	50	LYS	2.8
7	U	242	GLN	2.8
1	O	227	ILE	2.8
2	P	60	THR	2.8
3	C	240	GLU	2.8
2	B	53	SER	2.7
1	O	2	THR	2.7
4	D	240	ALA	2.7
6	T	243	ILE	2.7
5	E	207	VAL	2.7
1	A	228	PRO	2.7
10	X	1	MET	2.7
3	C	49	THR	2.7
4	D	209	ALA	2.7
5	E	122	TYR	2.7
4	R	68	CYS	2.7
3	C	47	ARG	2.7
10	X	11	ASP	2.7
13	M	69	ASP	2.7
3	Q	53	GLN	2.6
4	R	125	LEU	2.6
1	A	202	GLY	2.6
2	B	222	GLY	2.6
9	W	130	ASP	2.6
8	H	225	GLU	2.6
6	T	3	GLY	2.6
14	N	116	GLY	2.6
1	A	1	MET	2.5
9	I	192	ASP	2.5
2	B	3	ARG	2.5
5	S	122	TYR	2.5
4	R	115	PHE	2.5
6	F	62	LYS	2.5
6	F	215	CYS	2.5
3	C	3	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
7	G	40	ASP	2.5
2	B	218	GLY	2.5
4	R	99	ILE	2.4
3	Q	44	CYS	2.4
4	R	1	ASP	2.4
3	Q	201	VAL	2.4
10	J	195	PHE	2.4
5	S	210	LEU	2.4
14	b	196	LEU	2.4
10	X	174	MET	2.4
3	C	51	LYS	2.4
2	B	125	GLY	2.4
3	Q	34	VAL	2.4
13	M	81	ALA	2.4
2	B	52	THR	2.4
3	C	59	PRO	2.4
3	Q	59	PRO	2.4
1	O	4	ARG	2.4
2	B	8	ARG	2.4
10	J	25	ILE	2.3
3	Q	51	LYS	2.3
2	P	218	GLY	2.3
1	O	209	ILE	2.3
12	Z	106	TYR	2.3
3	Q	61	LYS	2.3
4	D	242	GLU	2.3
6	T	244	ASN	2.3
7	G	242	GLN	2.3
3	Q	186	VAL	2.3
3	Q	189	CYS	2.3
8	H	218	VAL	2.3
6	T	178	HIS	2.3
5	E	3	ASN	2.3
2	B	7	SER	2.3
4	D	2	ARG	2.3
5	S	233	ILE	2.2
3	Q	58	THR	2.2
6	T	2	THR	2.2
14	N	151	THR	2.2
3	Q	177	TYR	2.2
2	P	125	GLY	2.2
8	H	224	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
8	H	222	ASP	2.2
3	Q	52	LEU	2.2
11	Y	31	VAL	2.2
3	Q	234	ILE	2.2
10	X	25	ILE	2.2
1	O	93	ALA	2.2
8	V	169	SER	2.2
5	S	65	CYS	2.2
4	D	3	GLY	2.2
3	C	231	VAL	2.2
3	Q	205	ALA	2.1
4	D	169	GLU	2.1
6	T	205	GLU	2.1
2	P	241	THR	2.1
2	P	180	LYS	2.1
5	S	3	ASN	2.1
3	Q	48	SER	2.1
3	C	5	ALA	2.1
3	Q	5	ALA	2.1
5	S	207	VAL	2.1
6	T	201	GLU	2.1
2	P	52	THR	2.1
3	C	44	CYS	2.1
3	Q	57	ILE	2.1
8	H	217	ILE	2.1
1	O	62	SER	2.1
6	F	185	ALA	2.1
1	O	61	LEU	2.1
8	H	219	ASN	2.1
4	R	154	GLY	2.1
1	A	209	ILE	2.1
2	P	225	TYR	2.1
7	U	3	TYR	2.1
7	U	183	ASP	2.0
10	X	195	PHE	2.1
3	Q	184	ALA	2.0
6	F	244	ASN	2.0
4	R	117	GLU	2.0
6	T	53	LYS	2.0
5	S	204	SER	2.0
8	V	30	SER	2.0
3	Q	203	THR	2.0

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Mol	Chain	Res	Type	RSRZ
5	S	185	PRO	2.0
3	C	208	ILE	2.0
3	Q	190	VAL	2.0
4	R	114	ARG	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($\text{\AA}^2$)	Q<0.9
15	MG	Z	301	1/1	0.77	0.18	73,73,73,73	0
17	MES	V	302	12/12	0.87	0.18	55,58,59,59	12
15	MG	I	301	1/1	0.88	0.25	87,87,87,87	0
17	MES	Y	302	12/12	0.88	0.21	47,51,53,56	12
18	A1IFL	H	302	51/51	0.88	0.13	56,61,72,73	0
18	A1IFL	V	303	51/51	0.88	0.13	60,64,69,69	0
18	A1IFL	K	304	51/51	0.90	0.12	49,51,59,60	0
19	SO4	N	202	5/5	0.90	0.18	81,83,84,85	5
19	SO4	b	201	5/5	0.91	0.18	64,64,67,71	5
17	MES	H	301	12/12	0.92	0.17	50,51,51,52	12
16	CL	U	301	1/1	0.93	0.10	55,55,55,55	0
15	MG	N	201	1/1	0.93	0.11	64,64,64,64	0
17	MES	K	302	12/12	0.93	0.16	45,47,50,50	12
18	A1IFL	Y	304	51/51	0.93	0.10	53,54,65,66	0
15	MG	Y	301	1/1	0.93	0.09	70,70,70,70	0
19	SO4	Y	303	5/5	0.93	0.17	92,93,97,102	0
15	MG	G	301	1/1	0.93	0.08	61,61,61,61	0
15	MG	K	301	1/1	0.94	0.07	65,65,65,65	0
16	CL	G	302	1/1	0.94	0.11	49,49,49,49	0

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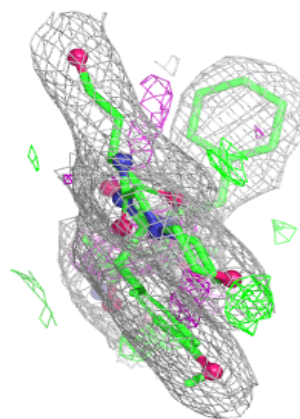
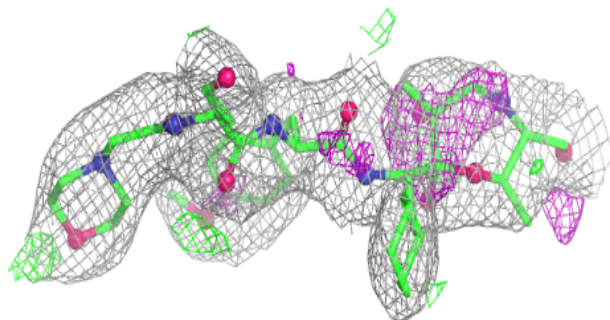
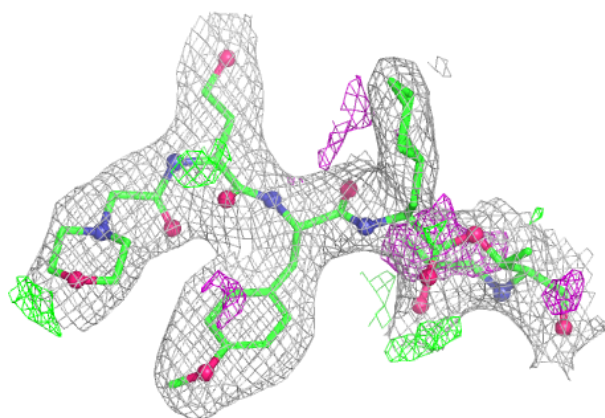
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	CL	N	203	1/1	0.94	0.17	79,79,79,79	0
15	MG	W	301	1/1	0.96	0.09	66,66,66,66	0
15	MG	V	301	1/1	0.96	0.07	75,75,75,75	0
19	SO4	K	303	5/5	0.96	0.20	92,95,95,96	0

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.

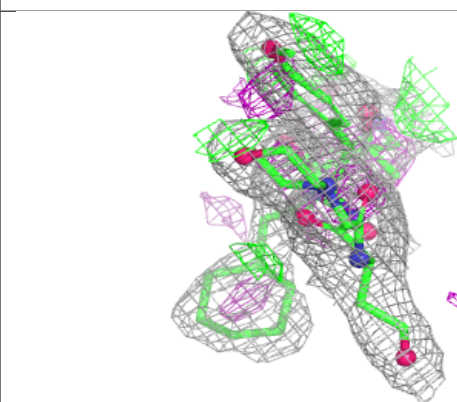
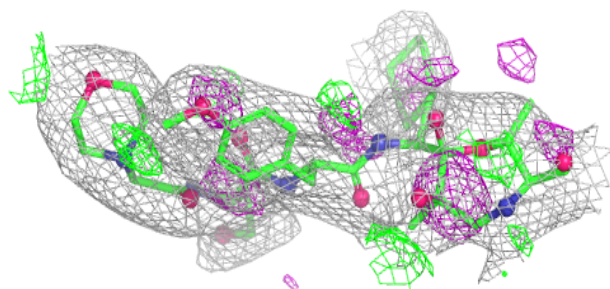
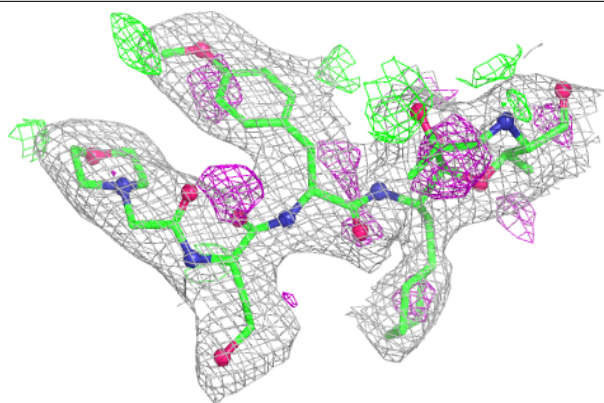
Electron density around A1IFL H 302:

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

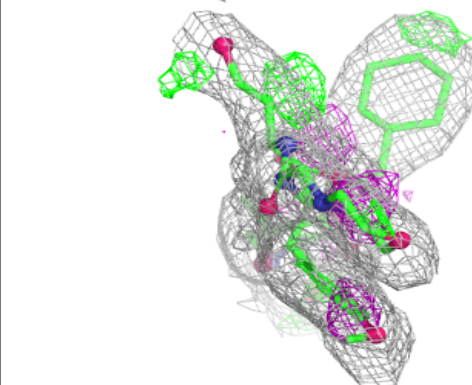
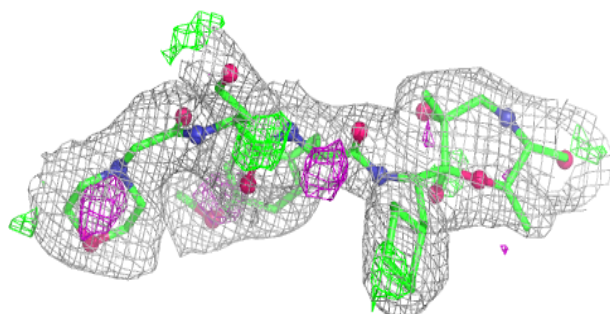
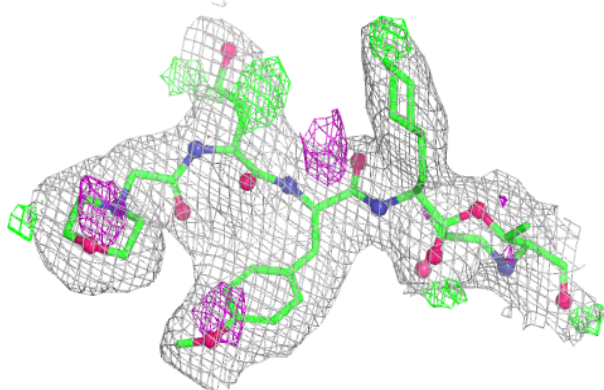


Electron density around A1IFL V 303:

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

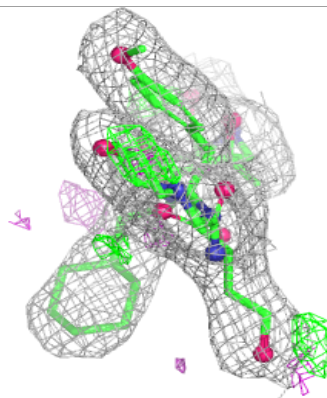
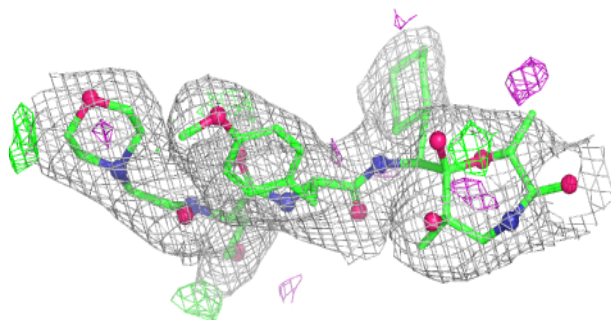
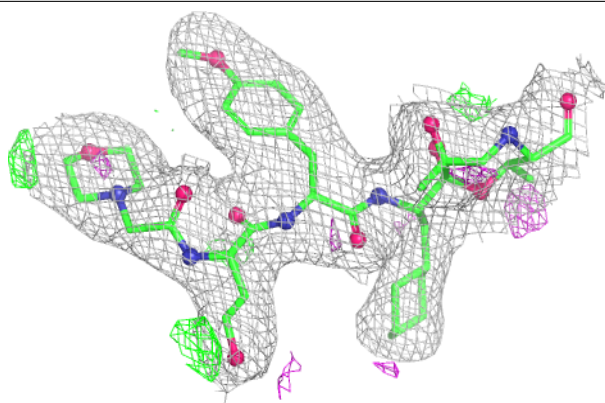
**Electron density around A1IFL K 304:**

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



Electron density around A1IFL Y 304:

$2mF_o-DF_c$ (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.