



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:10 AM UTC

PDB ID : 8OHZ / pdb_00008ohz
Title : Yeast 20S proteasome in complex with a photoswitchable cepafungin derivative (transCep1)
Authors : Morstein, J.; Amatuni, A.; Schuster, A.; Kuttanlochner, W.; Ko, T.; Groll, M.; Adibekian, A.; Renata, H.; Trauner, D.H.
Deposited on : 2023-03-21
Resolution : 2.65 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:

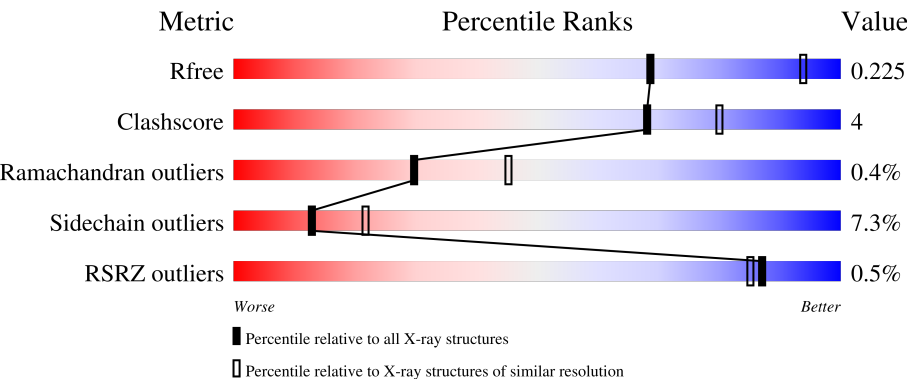
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.65 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.



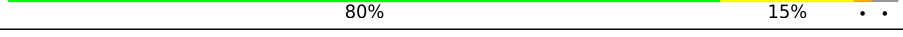
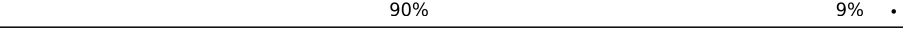
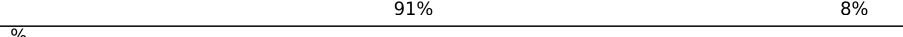
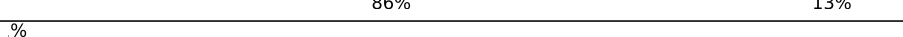
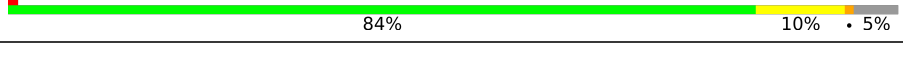
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	91%8%
1	O	250	90%10%
2	B	258	% 77%16%5%
2	P	258	2% 80%14%5%

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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	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49742 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	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).

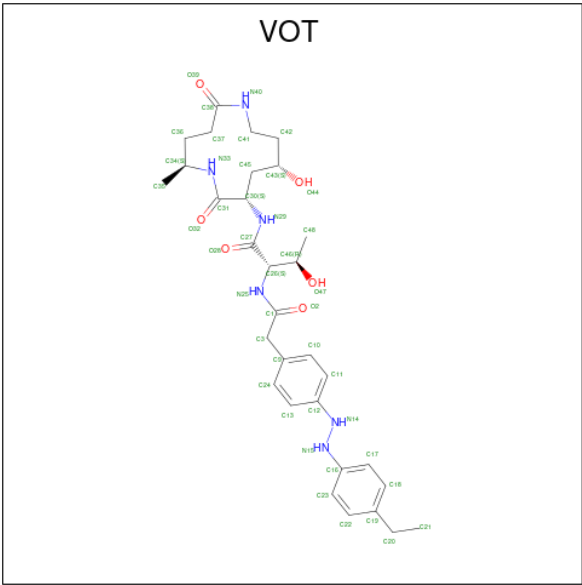
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	I	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	J	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	V	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 {S},3 {R})-2-[2-[4-[2-(4-ethylphenyl)hydrazinyl]phenyl]ethanoylamino]- {N}-[(5 {S},8 {S},10 {S})-5-methyl-10-oxidanyl-2,7-bis(oxidanylidene)-1,6-diazacyclododec-8-yl]-3-oxidanyl-butanamide (CCD ID: VOT) (formula: C₃₁H₄₄N₆O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	H	1	Total	C	N	O	0	0
			43	31	6	6		
16	K	1	Total	C	N	O	0	0
			43	31	6	6		
16	V	1	Total	C	N	O	0	0
			43	31	6	6		
16	Y	1	Total	C	N	O	0	0
			43	31	6	6		

- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	N	1	Total Cl 1 1	0	0
17	b	1	Total Cl 1 1	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	4	Total O 4 4	0	0
18	B	12	Total O 12 12	0	0
18	C	7	Total O 7 7	0	0
18	D	4	Total O 4 4	0	0
18	E	2	Total O 2 2	0	0
18	F	8	Total O 8 8	0	0
18	G	4	Total O 4 4	0	0
18	H	8	Total O 8 8	0	0
18	I	3	Total O 3 3	0	0
18	J	9	Total O 9 9	0	0
18	K	9	Total O 9 9	0	0
18	L	7	Total O 7 7	0	0
18	M	10	Total O 10 10	0	0
18	N	6	Total O 6 6	0	0
18	O	1	Total O 1 1	0	0
18	P	8	Total O 8 8	0	0
18	Q	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	R	2	Total 2	O 2	0	0
18	S	3	Total 3	O 3	0	0
18	T	12	Total 12	O 12	0	0
18	U	5	Total 5	O 5	0	0
18	V	13	Total 13	O 13	0	0
18	W	5	Total 5	O 5	0	0
18	X	11	Total 11	O 11	0	0
18	Y	5	Total 5	O 5	0	0
18	Z	8	Total 8	O 8	0	0
18	a	11	Total 11	O 11	0	0
18	b	9	Total 9	O 9	0	0

3 Residue-property plots

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

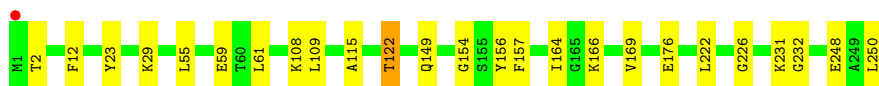
- Molecule 1: Proteasome subunit alpha type-2

Chain A: 



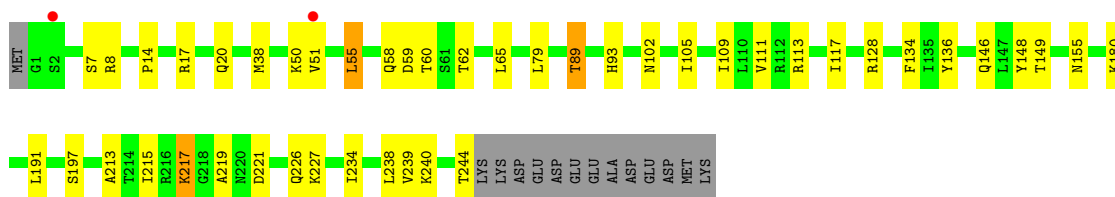
- Molecule 1: Proteasome subunit alpha type-2

Chain O: 



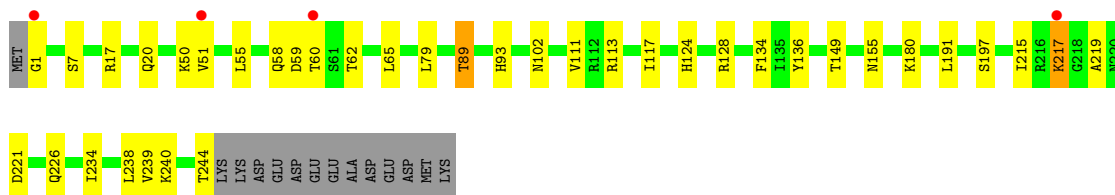
- Molecule 2: Proteasome subunit alpha type-3

Chain B: 

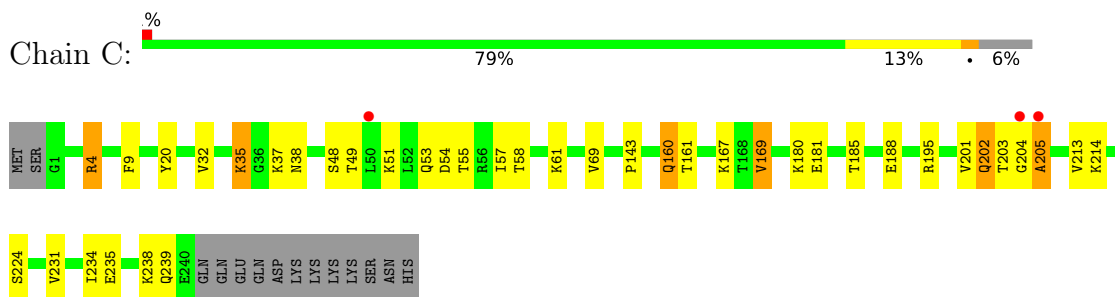


- Molecule 2: Proteasome subunit alpha type-3

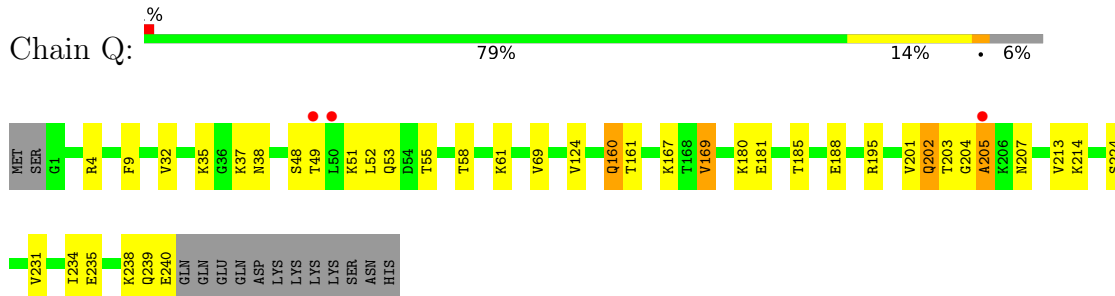
Chain P: 



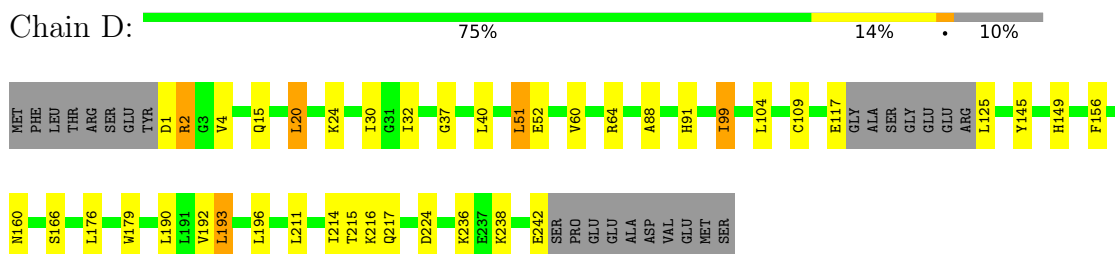
- Molecule 3: Proteasome subunit alpha type-4



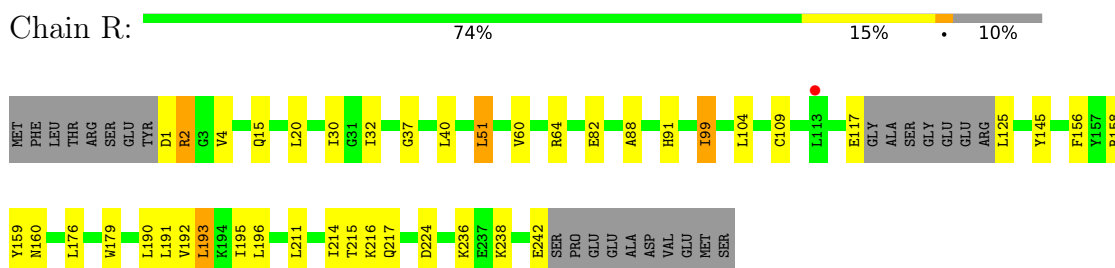
- Molecule 3: Proteasome subunit alpha type-4



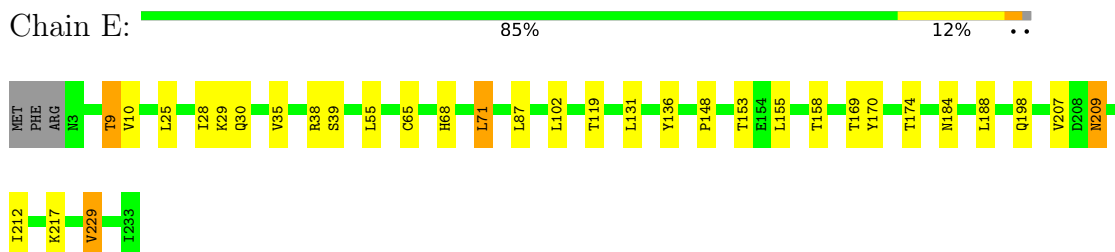
- Molecule 4: Proteasome subunit alpha type-5



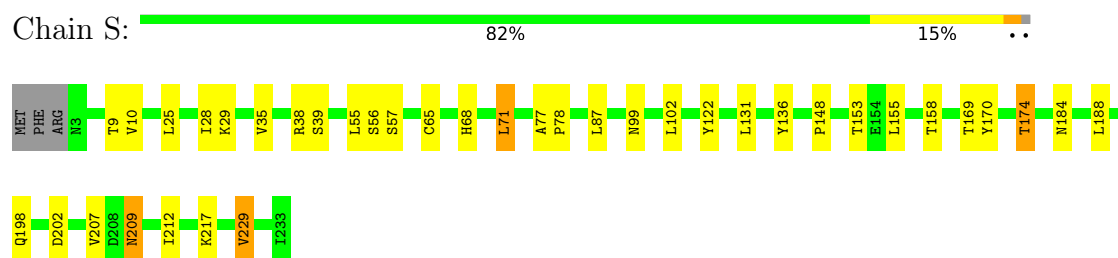
- Molecule 4: Proteasome subunit alpha type-5



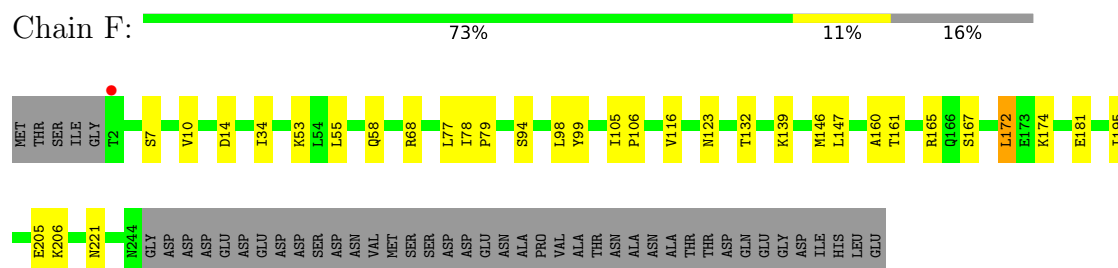
- Molecule 5: Proteasome subunit alpha type-6



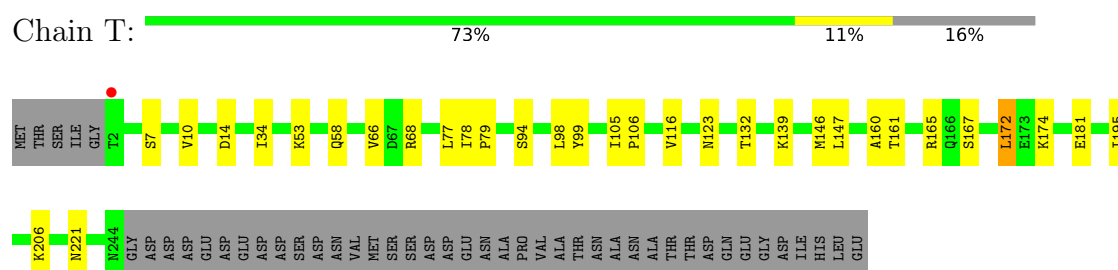
- Molecule 5: Proteasome subunit alpha type-6



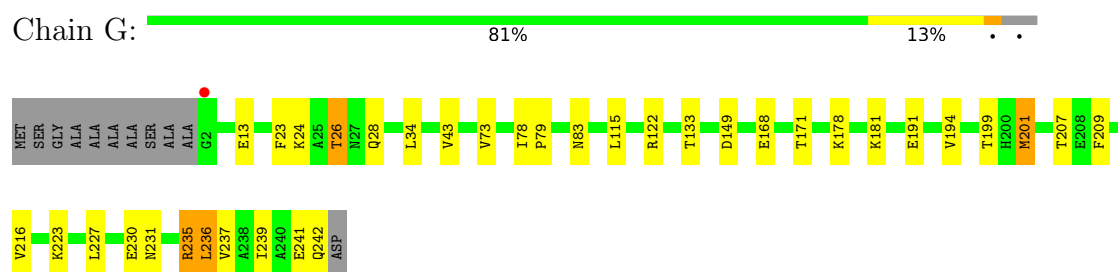
- Molecule 6: Probable proteasome subunit alpha type-7



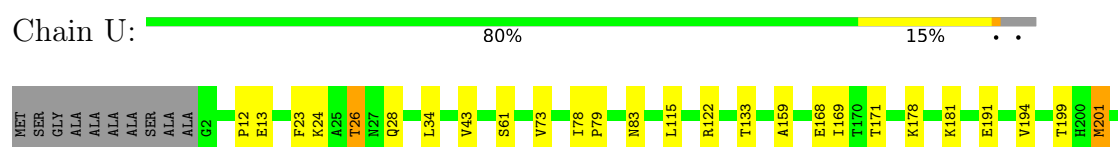
- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 7: Proteasome subunit alpha type-1



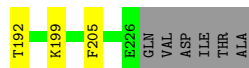
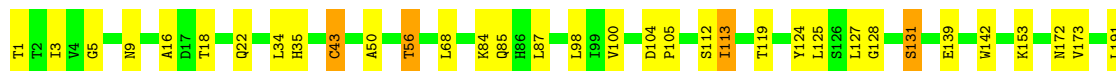
- Molecule 7: Proteasome subunit alpha type-1





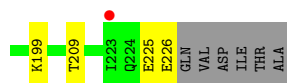
• Molecule 8: Proteasome subunit beta type-2

Chain H: 81% 14% . .



• Molecule 8: Proteasome subunit beta type-2

Chain V: 80% 15% . .



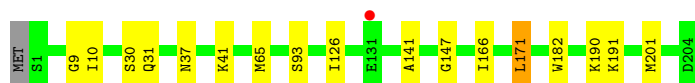
• Molecule 9: Proteasome subunit beta type-3

Chain I: 90% 9% .



• Molecule 9: Proteasome subunit beta type-3

Chain W: 91% 8%



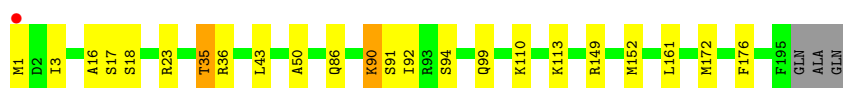
• Molecule 10: Proteasome subunit beta type-4

Chain J: 89% 9% . .



• Molecule 10: Proteasome subunit beta type-4

Chain X: 87% 11% . .



• Molecule 11: Proteasome subunit beta type-5

Chain K: 81% 18%



• Molecule 11: Proteasome subunit beta type-5

Chain Y: 83% 16%



• Molecule 12: Proteasome subunit beta type-6

Chain L: 86% 14%



• Molecule 12: Proteasome subunit beta type-6

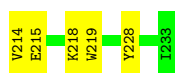
Chain Z: 86% 13%



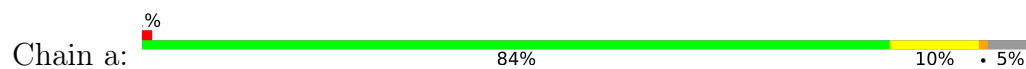
• Molecule 13: Proteasome subunit beta type-7

Chain M: 83% 11% 5%

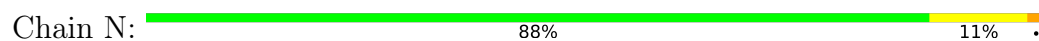




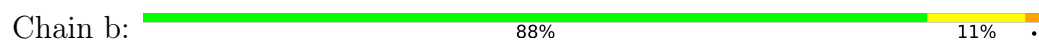
• Molecule 13: Proteasome subunit beta type-7



• 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	135.51 Å 300.79 Å 144.77 Å 90.00° 113.41° 90.00°	Depositor
Resolution (Å)	30.00 – 2.65 30.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	96.0 (30.00-2.65) 96.0 (30.00-2.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.64 Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.180 , 0.222 0.184 , 0.225	Depositor DCC
R_{free} test set	14721 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.805	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	49742	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: VOT, MG, CL

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	1.40	0/2642
1	O	1.03	0/1952	1.40	0/2642
2	B	1.02	0/1934	1.43	0/2618
2	P	1.02	0/1934	1.42	0/2618
3	C	1.02	0/1910	1.44	2/2586 (0.1%)
3	Q	1.03	0/1910	1.45	2/2586 (0.1%)
4	D	1.02	0/1837	1.46	0/2475
4	R	1.03	0/1837	1.47	0/2475
5	E	1.02	0/1800	1.42	4/2433 (0.2%)
5	S	1.03	0/1800	1.42	2/2433 (0.1%)
6	F	1.01	0/1932	1.42	2/2609 (0.1%)
6	T	1.01	0/1932	1.43	2/2609 (0.1%)
7	G	1.01	1/1945 (0.1%)	1.42	2/2634 (0.1%)
7	U	1.01	0/1945	1.43	2/2634 (0.1%)
8	H	1.03	0/1750	1.40	0/2373
8	V	1.03	0/1750	1.40	0/2373
9	I	1.01	0/1611	1.39	0/2174
9	W	1.01	0/1611	1.39	0/2174
10	J	0.99	0/1589	1.38	0/2142
10	X	0.99	0/1589	1.39	0/2142
11	K	1.01	0/1681	1.40	0/2274
11	Y	1.01	0/1681	1.39	0/2274
12	L	1.01	0/1795	1.37	2/2420 (0.1%)
12	Z	1.00	0/1795	1.37	2/2420 (0.1%)
13	M	1.01	0/1855	1.36	0/2514
13	a	1.00	0/1855	1.37	0/2514
14	N	1.00	0/1541	1.39	1/2087 (0.0%)
14	b	1.01	0/1541	1.41	1/2087 (0.0%)
All	All	1.01	1/50264 (0.0%)	1.41	24/67962 (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	5.31	1.49	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	216	VAL	CA-C-N	5.84	125.62	121.65
7	U	216	VAL	C-N-CA	5.84	125.62	121.65
7	G	216	VAL	CA-C-N	5.62	125.47	121.65
7	G	216	VAL	C-N-CA	5.62	125.47	121.65
6	T	77	LEU	CA-C-N	5.54	124.76	120.33
6	T	77	LEU	C-N-CA	5.54	124.76	120.33
5	S	35	VAL	CA-C-N	5.53	125.41	121.65
5	S	35	VAL	C-N-CA	5.53	125.41	121.65
14	b	20	THR	CB-CA-C	5.45	119.20	110.16
6	F	77	LEU	CA-C-N	5.43	124.67	120.33
6	F	77	LEU	C-N-CA	5.43	124.67	120.33
5	E	35	VAL	CA-C-N	5.39	125.31	121.65
5	E	35	VAL	C-N-CA	5.39	125.31	121.65
14	N	20	THR	CB-CA-C	5.24	118.86	110.16
5	E	30	GLN	CA-C-N	5.20	125.04	120.10
5	E	30	GLN	C-N-CA	5.20	125.04	120.10
12	L	119	LYS	CA-C-N	5.12	124.83	119.92
12	L	119	LYS	C-N-CA	5.12	124.83	119.92
3	Q	32	VAL	CA-C-N	5.07	125.10	121.65
3	Q	32	VAL	C-N-CA	5.07	125.10	121.65
12	Z	119	LYS	CA-C-N	5.06	124.78	119.92
12	Z	119	LYS	C-N-CA	5.06	124.78	119.92
3	C	32	VAL	CA-C-N	5.03	125.07	121.65
3	C	32	VAL	C-N-CA	5.03	125.07	121.65

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	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1915	0	1929	11	0
2	B	1904	0	1904	20	0
2	P	1904	0	1904	14	0
3	C	1881	0	1895	15	0
3	Q	1881	0	1895	10	0
4	D	1813	0	1797	20	0
4	R	1813	0	1797	21	0
5	E	1773	0	1775	13	0
5	S	1773	0	1775	19	0
6	F	1892	0	1883	11	0
6	T	1892	0	1883	13	0
7	G	1907	0	1901	11	0
7	U	1907	0	1901	13	0
8	H	1719	0	1718	22	0
8	V	1719	0	1718	23	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	6	0
10	X	1561	0	1569	8	0
11	K	1644	0	1594	23	0
11	Y	1644	0	1594	21	0
12	L	1757	0	1711	15	0
12	Z	1757	0	1711	13	0
13	M	1824	0	1832	16	0
13	a	1824	0	1832	17	0
14	N	1512	0	1481	13	0
14	b	1512	0	1481	13	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	J	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	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	H	43	0	0	0	0
16	K	43	0	0	1	0
16	V	43	0	0	0	0
16	Y	43	0	0	0	0
17	N	1	0	0	0	0
17	b	1	0	0	0	0
18	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	B	12	0	0	0	0
18	C	7	0	0	0	0
18	D	4	0	0	0	0
18	E	2	0	0	0	0
18	F	8	0	0	0	0
18	G	4	0	0	0	0
18	H	8	0	0	0	0
18	I	3	0	0	0	0
18	J	9	0	0	0	0
18	K	9	0	0	0	0
18	L	7	0	0	0	0
18	M	10	0	0	1	0
18	N	6	0	0	1	0
18	O	1	0	0	0	0
18	P	8	0	0	0	0
18	Q	8	0	0	1	0
18	R	2	0	0	0	0
18	S	3	0	0	0	0
18	T	12	0	0	0	0
18	U	5	0	0	0	0
18	V	13	0	0	0	0
18	W	5	0	0	0	0
18	X	11	0	0	0	0
18	Y	5	0	0	0	0
18	Z	8	0	0	0	0
18	a	11	0	0	1	0
18	b	9	0	0	0	0
All	All	49742	0	49126	356	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 (356) 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)
6:T:68:ARG:HH21	13:a:71:VAL:HG12	1.26	0.99
6:T:68:ARG:HH21	13:a:71:VAL:CG1	1.86	0.88
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.55	0.87
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.55	0.85
6:T:68:ARG:NH2	13:a:71:VAL:CG1	2.46	0.78
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:68:ARG:NH1	13:M:72:THR:OG1	2.23	0.71
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.55	0.71
14:b:152:VAL:HA	14:b:175:MET:HE1	1.73	0.71
7:U:23:PHE:O	7:U:26:THR:HB	1.92	0.70
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.57	0.70
7:G:23:PHE:O	7:G:26:THR:HB	1.91	0.70
14:N:14:LEU:HD11	14:N:100:ALA:HB3	1.74	0.69
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.57	0.67
14:N:152:VAL:HA	14:N:175:MET:HE1	1.74	0.67
11:K:44:THR:HG21	11:K:100:MET:HE2	1.76	0.67
14:b:14:LEU:HD11	14:b:100:ALA:HB3	1.76	0.67
11:Y:44:THR:HG21	11:Y:100:MET:HE2	1.76	0.66
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.78	0.65
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.78	0.65
8:V:113:ILE:HD12	8:V:119:THR:HG22	1.79	0.64
8:H:113:ILE:HD12	8:H:119:THR:HG22	1.78	0.64
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.80	0.64
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.79	0.64
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.79	0.63
14:b:35:THR:OG1	14:b:43:CYS:SG	2.57	0.62
8:H:84:LYS:HA	8:H:113:ILE:HD11	1.82	0.62
8:V:3:ILE:HG13	8:V:99:ILE:HD12	1.82	0.61
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.82	0.61
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.82	0.60
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.84	0.60
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.67	0.60
14:N:35:THR:OG1	14:N:43:CYS:SG	2.60	0.59
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.85	0.59
5:S:71:LEU:HD22	5:S:71:LEU:C	2.28	0.59
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.84	0.58
8:V:84:LYS:HA	8:V:113:ILE:HD11	1.83	0.58
11:Y:40:PHE:CD1	11:Y:73:ARG:CZ	2.87	0.58
8:V:98:LEU:HB2	8:V:113:ILE:CG2	2.33	0.58
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.85	0.58
8:H:98:LEU:HB2	8:H:113:ILE:CG2	2.33	0.58
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.86	0.57
5:E:71:LEU:C	5:E:71:LEU:HD22	2.30	0.56
8:H:113:ILE:HD12	8:H:119:THR:CG2	2.35	0.56
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.70	0.56
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.88	0.56
11:K:4:LEU:C	11:K:4:LEU:CD2	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:40:PHE:CD1	11:K:73:ARG:CZ	2.88	0.56
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.71	0.55
8:H:128:GLY:O	8:H:131:SER:HB3	2.07	0.55
8:V:113:ILE:HD12	8:V:119:THR:CG2	2.36	0.55
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.89	0.55
11:K:53:GLN:O	11:K:57:THR:HG23	2.07	0.55
11:K:4:LEU:C	11:K:4:LEU:HD22	2.32	0.54
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.54	0.54
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.43	0.54
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.07	0.54
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.90	0.54
5:E:68:HIS:HE1	5:E:102:LEU:O	1.91	0.54
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.88	0.54
12:L:8:ASN:HA	12:L:30:ILE:O	2.07	0.54
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.08	0.53
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.39	0.53
6:T:146:MET:HE3	6:T:161:THR:HB	1.91	0.53
6:T:68:ARG:NH2	13:a:71:VAL:HG11	2.23	0.53
6:F:146:MET:HE3	6:F:161:THR:HB	1.91	0.52
11:Y:51:ASP:HB3	11:Y:97:MET:HE2	1.92	0.52
4:R:82:GLU:OE2	11:Y:69:ARG:NH1	2.42	0.52
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.45	0.52
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.43	0.52
14:N:83:LYS:HG3	14:N:119:VAL:HG22	1.92	0.52
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.91	0.52
11:K:51:ASP:HB3	11:K:97:MET:HE2	1.92	0.52
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.83	0.52
12:L:113:GLY:HA2	12:L:207:VAL:HG11	1.92	0.52
4:R:1:ASP:O	4:R:2:ARG:HB2	2.11	0.51
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.25	0.51
5:S:68:HIS:HE1	5:S:102:LEU:O	1.94	0.51
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.91	0.51
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.91	0.51
6:F:146:MET:CE	6:F:161:THR:HB	2.40	0.51
2:P:93:HIS:HB3	2:P:113:ARG:NH2	2.26	0.51
6:T:146:MET:CE	6:T:161:THR:HB	2.40	0.51
4:R:51:LEU:C	4:R:51:LEU:HD12	2.36	0.51
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.40	0.51
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.35	0.50
5:E:155:LEU:HD13	5:E:158:THR:HB	1.93	0.50
11:K:4:LEU:HD22	11:K:4:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLN:O	1:A:156:TYR:HA	2.12	0.50
10:J:50:ALA:O	11:K:91:LYS:NZ	2.44	0.50
3:Q:185:THR:OG1	3:Q:188:GLU:HB2	2.12	0.50
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.93	0.50
1:O:149:GLN:O	1:O:156:TYR:HA	2.11	0.49
4:D:51:LEU:HD12	4:D:51:LEU:C	2.37	0.49
8:H:18:THR:HG21	8:H:172:ASN:HB2	1.95	0.49
5:E:65:CYS:SG	5:E:71:LEU:HD12	2.51	0.49
13:M:228:TYR:HE2	14:b:35:THR:HG21	1.78	0.49
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.94	0.49
7:G:78:ILE:N	7:G:79:PRO:CD	2.76	0.49
7:U:78:ILE:N	7:U:79:PRO:CD	2.75	0.49
6:F:98:LEU:HD23	6:F:99:TYR:CZ	2.47	0.49
14:N:35:THR:HG21	13:a:228:TYR:HE2	1.78	0.49
2:B:93:HIS:HB3	2:B:113:ARG:NH2	2.27	0.49
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.48	0.49
8:V:18:THR:HG21	8:V:172:ASN:HB2	1.94	0.49
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.27	0.49
14:b:83:LYS:HG3	14:b:119:VAL:HG22	1.93	0.49
5:S:155:LEU:HD13	5:S:158:THR:HB	1.94	0.49
4:D:1:ASP:O	4:D:2:ARG:HB2	2.12	0.48
8:V:43:CYS:HB2	8:V:100:VAL:HA	1.95	0.48
11:Y:7:ARG:NH1	11:Y:110:PRO:O	2.41	0.48
8:H:139:GLU:OE1	13:a:187:ARG:NH1	2.45	0.48
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.48	0.48
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.95	0.48
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.13	0.48
4:R:91:HIS:CG	4:R:99:ILE:HB	2.48	0.48
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.96	0.48
4:R:193:LEU:HD22	4:R:211:LEU:HD11	1.96	0.48
13:M:2:GLN:NE2	18:M:301:HOH:O	2.46	0.48
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.48	0.48
10:J:35:THR:HG23	10:J:43:LEU:HD11	1.96	0.48
1:O:12:PHE:H	2:P:20:GLN:HE22	1.62	0.48
3:C:201:VAL:O	3:C:202:GLN:HB3	2.12	0.48
6:F:34:ILE:HG22	6:F:160:ALA:HB2	1.96	0.48
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.48	0.48
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.79	0.47
6:T:34:ILE:HG22	6:T:160:ALA:HB2	1.96	0.47
12:L:147:MET:N	12:L:148:PRO:HD2	2.29	0.47
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:113:GLY:HA2	12:Z:207:VAL:HG11	1.95	0.47
3:C:185:THR:OG1	3:C:188:GLU:HB2	2.14	0.47
8:V:18:THR:HG23	8:V:172:ASN:O	2.14	0.47
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.97	0.47
4:D:193:LEU:HD22	4:D:211:LEU:HD11	1.96	0.47
5:S:65:CYS:SG	5:S:71:LEU:HD12	2.55	0.47
10:X:35:THR:HG23	10:X:43:LEU:HD11	1.97	0.47
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.49	0.47
4:D:91:HIS:CG	4:D:99:ILE:HB	2.50	0.47
9:I:65:MET:HE1	9:I:93:SER:HB3	1.95	0.47
11:K:86:LEU:C	11:K:86:LEU:HD13	2.39	0.47
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.49	0.47
8:H:87:LEU:HD12	8:H:113:ILE:HG12	1.97	0.47
6:T:98:LEU:HD23	6:T:99:TYR:CZ	2.50	0.47
14:b:35:THR:HG21	14:b:45:ARG:HE	1.80	0.47
11:K:19:ARG:O	11:K:33:LYS:NZ	2.42	0.47
7:U:73:VAL:HG12	7:U:133:THR:HB	1.96	0.47
7:U:227:LEU:HB3	7:U:231:ASN:HB2	1.97	0.47
12:Z:100:LYS:HD3	12:Z:105:TYR:CZ	2.50	0.47
2:B:38:MET:HE1	3:C:54:ASP:OD2	2.15	0.46
1:A:12:PHE:H	2:B:20:GLN:HE22	1.63	0.46
7:G:227:LEU:HB3	7:G:231:ASN:HB2	1.95	0.46
4:R:91:HIS:CD2	4:R:99:ILE:HB	2.50	0.46
4:R:158:ARG:O	5:S:57:SER:N	2.41	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.97	0.46
8:V:84:LYS:HE2	8:V:119:THR:HG23	1.97	0.46
8:V:84:LYS:HG3	8:V:85:GLN:N	2.31	0.46
3:C:161:THR:HG21	3:C:169:VAL:HG22	1.97	0.46
4:R:158:ARG:HB3	5:S:57:SER:HB3	1.97	0.46
6:T:78:ILE:HB	6:T:79:PRO:HD3	1.98	0.46
13:a:161:ARG:HG3	13:a:161:ARG:HH11	1.81	0.46
2:B:134:PHE:O	2:B:149:THR:HA	2.15	0.46
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.81	0.46
16:K:301:VOT:C23	12:L:104:PRO:HG2	2.46	0.46
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.29	0.45
8:H:50:ALA:HB2	9:I:128:CYS:HB2	1.99	0.45
8:H:84:LYS:HG3	8:H:85:GLN:N	2.30	0.45
8:H:142:TRP:O	13:a:218:LYS:HE2	2.16	0.45
4:R:193:LEU:CD2	4:R:211:LEU:HD11	2.47	0.45
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.51	0.45
8:V:128:GLY:O	8:V:131:SER:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:73:VAL:HG12	7:G:133:THR:HB	1.97	0.45
5:S:38:ARG:HD2	5:S:39:SER:O	2.16	0.45
1:O:55:LEU:HB3	7:U:159:ALA:O	2.16	0.45
11:Y:44:THR:O	11:Y:99:THR:OG1	2.33	0.45
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.99	0.45
2:P:134:PHE:O	2:P:149:THR:HA	2.17	0.45
3:Q:52:LEU:N	18:Q:301:HOH:O	2.48	0.45
5:S:212:ILE:HD12	5:S:229:VAL:HG12	1.98	0.45
8:V:87:LEU:HD12	8:V:113:ILE:HG12	1.98	0.45
9:W:65:MET:HE1	9:W:93:SER:HB3	1.97	0.45
11:Y:20:ALA:CB	11:Y:31:VAL:HG21	2.46	0.45
4:D:109:CYS:SG	4:D:156:PHE:HB3	2.57	0.45
7:G:34:LEU:C	7:G:34:LEU:HD23	2.41	0.45
8:H:3:ILE:HG22	8:H:16:ALA:HB2	1.99	0.45
2:P:1:GLY:HA3	5:S:122:TYR:CD1	2.52	0.45
2:B:89:THR:HG21	2:B:117:ILE:CD1	2.48	0.44
11:K:7:ARG:NH1	11:K:110:PRO:O	2.44	0.44
4:R:109:CYS:SG	4:R:156:PHE:HB3	2.57	0.44
5:S:170:TYR:HB2	5:S:198:GLN:HG3	2.00	0.44
14:b:163:ILE:HG23	14:b:170:GLY:HA2	2.00	0.44
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.31	0.44
6:T:105:ILE:N	6:T:106:PRO:CD	2.80	0.44
5:E:209:ASN:C	5:E:209:ASN:ND2	2.76	0.44
6:F:116:VAL:HG21	6:F:147:LEU:HD21	2.00	0.44
13:a:2:GLN:CD	18:a:301:HOH:O	2.59	0.44
4:D:193:LEU:CD2	4:D:211:LEU:HD11	2.47	0.44
6:F:78:ILE:HB	6:F:79:PRO:HD3	1.99	0.44
11:K:44:THR:O	11:K:99:THR:OG1	2.36	0.44
1:A:66:LEU:C	1:A:66:LEU:HD23	2.43	0.44
8:V:2:THR:O	8:V:159:ILE:HD12	2.17	0.44
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.43	0.44
10:J:18:SER:HB2	10:J:176:PHE:HB2	2.00	0.44
3:Q:161:THR:HG21	3:Q:169:VAL:HG22	1.99	0.44
7:U:191:GLU:O	7:U:235:ARG:HD3	2.18	0.44
5:E:212:ILE:HD12	5:E:229:VAL:HG12	1.98	0.43
3:Q:195:ARG:HG2	3:Q:234:ILE:HG21	2.00	0.43
8:H:84:LYS:HE2	8:H:119:THR:HG23	2.01	0.43
2:P:89:THR:HG21	2:P:117:ILE:CD1	2.48	0.43
13:a:129:TYR:O	13:a:136:THR:HA	2.18	0.43
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.99	0.43
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:204:GLY:HA3	3:Q:231:VAL:HG11	2.01	0.43
6:F:7:SER:HB3	6:F:10:VAL:HG21	1.99	0.43
8:H:43:CYS:HB2	8:H:100:VAL:HA	1.99	0.43
11:K:46:ALA:HB3	11:K:98:GLY:O	2.18	0.43
12:L:160:TYR:CD2	12:L:166:GLY:HA2	2.53	0.43
12:L:152:ASN:O	12:L:156:PHE:HA	2.19	0.43
4:R:30:ILE:HD12	4:R:196:LEU:HG	2.01	0.43
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	2.01	0.43
13:a:27:LEU:HB2	13:a:192:SER:HB3	2.01	0.43
3:C:35:LYS:NZ	4:D:52:GLU:OE1	2.47	0.43
4:D:91:HIS:CD2	4:D:99:ILE:HB	2.54	0.43
8:V:192:THR:HG22	8:V:192:THR:O	2.19	0.43
11:Y:19:ARG:O	11:Y:33:LYS:NZ	2.42	0.43
12:Z:16:ALA:O	12:Z:135:GLN:NE2	2.52	0.43
3:C:195:ARG:HG2	3:C:234:ILE:HG21	2.01	0.43
4:D:104:LEU:C	4:D:104:LEU:HD13	2.44	0.43
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.01	0.43
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.54	0.43
6:T:7:SER:HB3	6:T:10:VAL:HG21	2.00	0.43
2:B:215:ILE:HG12	2:B:226:GLN:HG3	2.01	0.43
5:E:170:TYR:HB2	5:E:198:GLN:HG3	2.00	0.43
7:G:78:ILE:HG22	7:G:79:PRO:HD3	2.00	0.43
9:I:171:LEU:HD11	9:I:201:MET:HB3	2.01	0.43
11:K:35:ILE:HD13	11:K:56:GLU:OE1	2.19	0.43
1:O:226:GLY:HA3	8:V:186:TYR:O	2.19	0.43
10:X:18:SER:HB2	10:X:176:PHE:HB2	2.00	0.43
11:K:20:ALA:CB	11:K:31:VAL:HG21	2.46	0.42
14:N:59:VAL:HG22	14:N:81:VAL:HG12	2.01	0.42
11:Y:35:ILE:HD13	11:Y:56:GLU:OE1	2.19	0.42
4:D:30:ILE:HD12	4:D:196:LEU:HG	2.02	0.42
7:U:78:ILE:HG22	7:U:79:PRO:HD3	2.00	0.42
13:M:27:LEU:HB2	13:M:192:SER:HB3	2.01	0.42
6:F:105:ILE:N	6:F:106:PRO:CD	2.82	0.42
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.54	0.42
12:L:145:LEU:O	9:W:147:GLY:HA3	2.18	0.42
3:C:9:PHE:H	4:D:15:GLN:HE22	1.66	0.42
4:D:20:LEU:HD12	4:D:20:LEU:HA	1.93	0.42
4:D:32:ILE:HD12	4:D:192:VAL:HG23	2.02	0.42
2:P:215:ILE:HG12	2:P:226:GLN:HG3	2.02	0.42
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.53	0.42
8:V:173:VAL:HB	8:V:191:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:171:LEU:HD12	9:W:171:LEU:HA	1.89	0.42
2:B:238:LEU:HD12	2:B:238:LEU:HA	1.93	0.42
7:U:43:VAL:HG11	7:U:194:VAL:HA	2.02	0.42
8:V:98:LEU:HB2	8:V:113:ILE:HG22	2.01	0.42
4:D:160:ASN:HB3	4:D:179:TRP:CZ2	2.55	0.42
8:H:205:PHE:CE1	9:I:168:GLN:HG3	2.55	0.42
2:P:1:GLY:HA3	5:S:122:TYR:CE1	2.55	0.42
4:R:32:ILE:HD12	4:R:192:VAL:HG23	2.02	0.42
3:C:204:GLY:HA3	3:C:231:VAL:HG11	2.02	0.42
5:E:38:ARG:HD2	5:E:39:SER:O	2.18	0.42
13:M:182:ARG:HG3	13:M:214:VAL:HG13	2.02	0.42
14:N:163:ILE:HG23	14:N:170:GLY:HA2	2.01	0.42
1:O:61:LEU:HD23	1:O:61:LEU:C	2.44	0.42
3:Q:205:ALA:C	3:Q:207:ASN:H	2.28	0.42
4:R:104:LEU:HD13	4:R:104:LEU:C	2.45	0.42
5:S:28:ILE:HD11	5:S:148:PRO:CD	2.50	0.42
5:E:9:THR:HG21	5:E:119:THR:HA	2.02	0.42
5:S:77:ALA:N	5:S:78:PRO:CD	2.83	0.42
11:K:6:PHE:HA	11:K:125:ASP:O	2.20	0.42
12:L:36:ASN:HB3	13:M:137:TYR:CE1	2.54	0.42
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.20	0.42
7:G:73:VAL:CG1	7:G:133:THR:HB	2.50	0.41
9:I:31:GLN:HB3	9:I:32:SER:H	1.77	0.41
6:T:116:VAL:HG21	6:T:147:LEU:HD21	2.00	0.41
3:C:204:GLY:O	3:C:205:ALA:O	2.38	0.41
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.50	0.41
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.02	0.41
14:N:35:THR:HG21	14:N:45:ARG:HE	1.85	0.41
2:P:111:VAL:HG22	2:P:136:TYR:CG	2.55	0.41
9:W:171:LEU:HD11	9:W:201:MET:HB3	2.02	0.41
10:X:149:ARG:O	10:X:152:MET:HG3	2.20	0.41
12:Z:160:TYR:CD2	12:Z:166:GLY:HA2	2.55	0.41
2:B:105:ILE:HD11	2:B:109:ILE:HG22	2.02	0.41
12:L:4:PRO:O	13:M:104:ARG:NH1	2.44	0.41
11:Y:8:PHE:CE1	11:Y:13:ILE:HG12	2.55	0.41
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.55	0.41
9:I:7:ASN:HA	9:I:29:GLY:O	2.19	0.41
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.85	0.41
4:R:160:ASN:HB3	4:R:179:TRP:CZ2	2.56	0.41
10:X:92:ILE:HD12	10:X:92:ILE:HA	1.94	0.41
2:B:111:VAL:HG22	2:B:136:TYR:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:8:PHE:CE1	11:K:13:ILE:HG12	2.55	0.41
13:M:26:ASN:HA	13:M:39:VAL:O	2.20	0.41
7:U:34:LEU:HD12	7:U:169:ILE:CG2	2.51	0.41
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.63	0.41
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.86	0.41
7:G:201:MET:HG2	7:G:209:PHE:CE2	2.56	0.41
8:H:173:VAL:HB	8:H:191:LEU:HB2	2.03	0.41
13:M:218:LYS:HE2	8:V:142:TRP:O	2.20	0.41
13:a:26:ASN:HA	13:a:39:VAL:O	2.20	0.41
2:B:234:ILE:O	2:B:238:LEU:HB2	2.20	0.41
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.51	0.41
2:B:213:ALA:HA	2:B:227:LYS:O	2.21	0.41
1:O:250:LEU:HD13	1:O:250:LEU:C	2.46	0.41
7:U:61:SER:OG	7:U:215:GLU:OE2	2.27	0.41
10:X:86:GLN:O	10:X:90:LYS:HB2	2.21	0.41
1:A:250:LEU:HD13	1:A:250:LEU:C	2.46	0.41
3:C:35:LYS:HE3	3:C:143:PRO:O	2.20	0.41
7:G:43:VAL:HG11	7:G:194:VAL:HA	2.02	0.41
7:G:191:GLU:O	7:G:235:ARG:HD3	2.21	0.41
11:K:12:ILE:HB	11:K:180:VAL:HB	2.02	0.41
11:K:38:ASN:OD1	11:K:38:ASN:C	2.63	0.41
9:W:126:ILE:HD13	9:W:126:ILE:HA	1.87	0.41
10:X:91:SER:HA	10:X:94:SER:OG	2.21	0.41
12:Z:36:ASN:HB3	13:a:137:TYR:CE1	2.56	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.02	0.41
2:P:234:ILE:O	2:P:238:LEU:HB2	2.21	0.41
5:S:170:TYR:O	5:S:174:THR:OG1	2.36	0.41
1:A:61:LEU:HD23	1:A:61:LEU:C	2.47	0.40
13:M:129:TYR:O	13:M:136:THR:HA	2.20	0.40
5:S:99:ASN:HB2	13:a:94:GLU:HG2	2.02	0.40
7:U:73:VAL:CG1	7:U:133:THR:HB	2.51	0.40
2:B:148:TYR:OH	3:C:57:ILE:HB	2.21	0.40
5:E:136:TYR:CE1	5:E:217:LYS:HA	2.55	0.40
8:H:5:GLY:O	8:H:124:TYR:HA	2.22	0.40
8:H:98:LEU:HB2	8:H:113:ILE:HG22	2.02	0.40
14:N:107:LYS:HG3	18:N:303:HOH:O	2.22	0.40
1:O:115:ALA:HB1	1:O:154:GLY:O	2.21	0.40
4:R:191:LEU:O	4:R:195:ILE:HG13	2.21	0.40
13:a:127:LEU:HG	13:a:142:LEU:HD12	2.03	0.40
14:b:59:VAL:HG22	14:b:81:VAL:HG12	2.03	0.40
4:D:149:HIS:O	4:D:156:PHE:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:71:LEU:HD23	5:S:131:LEU:HD22	2.03	0.40
5:S:136:TYR:CE1	5:S:217:LYS:HA	2.56	0.40
5:S:209:ASN:C	5:S:209:ASN:ND2	2.78	0.40
7:U:201:MET:HG2	7:U:209:PHE:CE2	2.56	0.40
11:Y:4:LEU:HD22	11:Y:4:LEU:O	2.21	0.40
12:Z:147:MET:N	12:Z:148:PRO:CD	2.84	0.40
4:D:24:LYS:O	4:D:166:SER:HA	2.21	0.40
5:E:71:LEU:HD23	5:E:131:LEU:HD22	2.03	0.40
11:K:113:TYR:CE1	11:K:123:LYS:HB2	2.57	0.40
2:P:217:LYS:HE3	2:P:217:LYS:HA	2.03	0.40
8:V:225:GLU:HG2	8:V:226:GLU:N	2.36	0.40
1:A:64:VAL:HG11	1:A:212:ALA:HB3	2.02	0.40
2:B:217:LYS:HA	2:B:217:LYS:HE3	2.04	0.40
5:E:155:LEU:CD2	6:F:55:LEU:HD23	2.51	0.40
7:G:236:LEU:HD12	7:G:236:LEU:HA	1.95	0.40
8:H:192:THR:HG22	8:H:192:THR:O	2.21	0.40
10:J:1:MET:HB2	10:J:34:LYS:HE3	2.04	0.40
11:K:4:LEU:HD13	11:K:161:ILE:HD11	2.04	0.40
13:M:11:VAL:O	13:M:143:ALA:HA	2.21	0.40
14:N:133:PHE:HA	14:b:132:THR:O	2.22	0.40
11:Y:100:MET:HE2	11:Y:100:MET:HB2	1.98	0.40
14:b:9:LYS:HD3	14:b:9:LYS:HA	1.89	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%)	241 (97%)	5 (2%)	2 (1%)	16	27
1	O	248/250 (99%)	241 (97%)	5 (2%)	2 (1%)	16	27
2	B	242/258 (94%)	227 (94%)	10 (4%)	5 (2%)	5	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	242/258 (94%)	228 (94%)	9 (4%)	5 (2%)	5	9
3	C	238/254 (94%)	228 (96%)	8 (3%)	2 (1%)	16	27
3	Q	238/254 (94%)	228 (96%)	8 (3%)	2 (1%)	16	27
4	D	231/260 (89%)	225 (97%)	5 (2%)	1 (0%)	30	45
4	R	231/260 (89%)	224 (97%)	6 (3%)	1 (0%)	30	45
5	E	229/234 (98%)	216 (94%)	13 (6%)	0	100	100
5	S	229/234 (98%)	217 (95%)	11 (5%)	1 (0%)	30	45
6	F	241/288 (84%)	230 (95%)	10 (4%)	1 (0%)	30	45
6	T	241/288 (84%)	230 (95%)	11 (5%)	0	100	100
7	G	239/252 (95%)	231 (97%)	8 (3%)	0	100	100
7	U	239/252 (95%)	233 (98%)	6 (2%)	0	100	100
8	H	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
8	V	224/232 (97%)	220 (98%)	4 (2%)	0	100	100
9	I	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
9	W	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
10	J	193/198 (98%)	183 (95%)	10 (5%)	0	100	100
10	X	193/198 (98%)	183 (95%)	10 (5%)	0	100	100
11	K	210/212 (99%)	204 (97%)	4 (2%)	2 (1%)	12	20
11	Y	210/212 (99%)	204 (97%)	4 (2%)	2 (1%)	12	20
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/246 (94%)	220 (95%)	11 (5%)	0	100	100
13	a	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6284/6614 (95%)	6043 (96%)	215 (3%)	26 (0%)	30	45

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	51	VAL
3	C	205	ALA

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Mol	Chain	Res	Type
4	D	2	ARG
11	K	209	ASN
1	O	2	THR
2	P	51	VAL
3	Q	205	ALA
4	R	2	ARG
11	Y	209	ASN
2	B	219	ALA
2	P	219	ALA
1	A	166	LYS
2	B	60	THR
2	B	221	ASP
3	C	202	GLN
11	K	106	ARG
1	O	166	LYS
2	P	60	THR
2	P	221	ASP
3	Q	202	GLN
11	Y	106	ARG
2	B	59	ASP
2	P	59	ASP
6	F	205	GLU
5	S	202	ASP

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%)	198 (95%)	11 (5%)	20	35
1	O	209/209 (100%)	198 (95%)	11 (5%)	20	35
2	B	203/216 (94%)	185 (91%)	18 (9%)	9	15
2	P	203/216 (94%)	185 (91%)	18 (9%)	9	15
3	C	212/226 (94%)	188 (89%)	24 (11%)	5	8
3	Q	212/226 (94%)	187 (88%)	25 (12%)	5	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	194/215 (90%)	174 (90%)	20 (10%)	7	10
4	R	194/215 (90%)	174 (90%)	20 (10%)	7	10
5	E	190/193 (98%)	175 (92%)	15 (8%)	11	19
5	S	190/193 (98%)	175 (92%)	15 (8%)	11	19
6	F	201/239 (84%)	187 (93%)	14 (7%)	14	24
6	T	201/239 (84%)	186 (92%)	15 (8%)	12	21
7	G	206/210 (98%)	184 (89%)	22 (11%)	6	9
7	U	206/210 (98%)	184 (89%)	22 (11%)	6	9
8	H	185/190 (97%)	173 (94%)	12 (6%)	15	27
8	V	185/190 (97%)	170 (92%)	15 (8%)	11	18
9	I	172/173 (99%)	164 (95%)	8 (5%)	23	40
9	W	172/173 (99%)	164 (95%)	8 (5%)	23	40
10	J	173/175 (99%)	162 (94%)	11 (6%)	16	28
10	X	173/175 (99%)	162 (94%)	11 (6%)	16	28
11	K	169/169 (100%)	162 (96%)	7 (4%)	27	46
11	Y	169/169 (100%)	162 (96%)	7 (4%)	27	46
12	L	185/185 (100%)	174 (94%)	11 (6%)	18	30
12	Z	185/185 (100%)	173 (94%)	12 (6%)	15	27
13	M	199/208 (96%)	189 (95%)	10 (5%)	22	37
13	a	199/208 (96%)	189 (95%)	10 (5%)	22	37
14	N	162/162 (100%)	155 (96%)	7 (4%)	26	44
14	b	162/162 (100%)	155 (96%)	7 (4%)	26	44
All	All	5320/5540 (96%)	4934 (93%)	386 (7%)	13	22

All (386) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	59	GLU
1	A	108	LYS
1	A	109	LEU
1	A	122	THR
1	A	157	PHE
1	A	164	ILE

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Mol	Chain	Res	Type
1	A	169	VAL
1	A	176	GLU
1	A	231	LYS
1	A	248	GLU
2	B	7	SER
2	B	17	ARG
2	B	50	LYS
2	B	55	LEU
2	B	58	GLN
2	B	62	THR
2	B	65	LEU
2	B	79	LEU
2	B	89	THR
2	B	102	ASN
2	B	155	ASN
2	B	180	LYS
2	B	191	LEU
2	B	197	SER
2	B	217	LYS
2	B	239	VAL
2	B	240	LYS
2	B	244	THR
3	C	4	ARG
3	C	35	LYS
3	C	37	LYS
3	C	38	ASN
3	C	48	SER
3	C	49	THR
3	C	51	LYS
3	C	53	GLN
3	C	55	THR
3	C	58	THR
3	C	61	LYS
3	C	69	VAL
3	C	160	GLN
3	C	167	LYS
3	C	169	VAL
3	C	180	LYS
3	C	181	GLU
3	C	203	THR
3	C	213	VAL
3	C	214	LYS

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Mol	Chain	Res	Type
3	C	224	SER
3	C	235	GLU
3	C	238	LYS
3	C	239	GLN
4	D	4	VAL
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	60	VAL
4	D	64	ARG
4	D	99	ILE
4	D	117	GLU
4	D	125	LEU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	214	ILE
4	D	215	THR
4	D	216	LYS
4	D	217	GLN
4	D	224	ASP
4	D	236	LYS
4	D	238	LYS
4	D	242	GLU
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	87	LEU
5	E	153	THR
5	E	169	THR
5	E	174	THR
5	E	184	ASN
5	E	188	LEU
5	E	207	VAL
5	E	209	ASN
5	E	229	VAL
6	F	14	ASP
6	F	53	LYS
6	F	58	GLN

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Mol	Chain	Res	Type
6	F	94	SER
6	F	123	ASN
6	F	132	THR
6	F	139	LYS
6	F	165	ARG
6	F	167	SER
6	F	172	LEU
6	F	174	LYS
6	F	181	GLU
6	F	206	LYS
6	F	221	ASN
7	G	13	GLU
7	G	24	LYS
7	G	26	THR
7	G	28	GLN
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	168	GLU
7	G	171	THR
7	G	178	LYS
7	G	181	LYS
7	G	199	THR
7	G	201	MET
7	G	207	THR
7	G	223	LYS
7	G	230	GLU
7	G	235	ARG
7	G	236	LEU
7	G	237	VAL
7	G	239	ILE
7	G	241	GLU
7	G	242	GLN
8	H	1	THR
8	H	9	ASN
8	H	22	GLN
8	H	34	LEU
8	H	43	CYS
8	H	56	THR
8	H	68	LEU
8	H	113	ILE
8	H	127	LEU

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Mol	Chain	Res	Type
8	H	131	SER
8	H	153	LYS
8	H	199	LYS
9	I	30	SER
9	I	31	GLN
9	I	37	ASN
9	I	166	ILE
9	I	171	LEU
9	I	182	TRP
9	I	190	LYS
9	I	191	LYS
10	J	1	MET
10	J	3	ILE
10	J	17	SER
10	J	23	ARG
10	J	35	THR
10	J	36	ARG
10	J	90	LYS
10	J	99	GLN
10	J	110	LYS
10	J	113	LYS
10	J	172	MET
11	K	4	LEU
11	K	9	GLN
11	K	99	THR
11	K	148	LEU
11	K	181	THR
11	K	186	ILE
11	K	211	ILE
12	L	18	GLU
12	L	23	LEU
12	L	43	VAL
12	L	49	ASN
12	L	70	ASN
12	L	85	SER
12	L	130	SER
12	L	172	LEU
12	L	173	LYS
12	L	189	THR
12	L	209	LYS
13	M	2	GLN
13	M	10	SER

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Mol	Chain	Res	Type
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	157	LYS
13	M	161	ARG
13	M	190	ARG
13	M	215	GLU
14	N	9	LYS
14	N	20	THR
14	N	92	ASN
14	N	105	LYS
14	N	107	LYS
14	N	119	VAL
14	N	178	LEU
1	O	29	LYS
1	O	59	GLU
1	O	108	LYS
1	O	109	LEU
1	O	122	THR
1	O	157	PHE
1	O	164	ILE
1	O	169	VAL
1	O	176	GLU
1	O	231	LYS
1	O	248	GLU
2	P	7	SER
2	P	17	ARG
2	P	50	LYS
2	P	55	LEU
2	P	58	GLN
2	P	62	THR
2	P	65	LEU
2	P	79	LEU
2	P	89	THR
2	P	102	ASN
2	P	155	ASN
2	P	180	LYS
2	P	191	LEU
2	P	197	SER
2	P	217	LYS
2	P	239	VAL

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Mol	Chain	Res	Type
2	P	240	LYS
2	P	244	THR
3	Q	4	ARG
3	Q	35	LYS
3	Q	37	LYS
3	Q	38	ASN
3	Q	48	SER
3	Q	49	THR
3	Q	51	LYS
3	Q	53	GLN
3	Q	55	THR
3	Q	58	THR
3	Q	61	LYS
3	Q	69	VAL
3	Q	160	GLN
3	Q	167	LYS
3	Q	169	VAL
3	Q	180	LYS
3	Q	181	GLU
3	Q	203	THR
3	Q	213	VAL
3	Q	214	LYS
3	Q	224	SER
3	Q	235	GLU
3	Q	238	LYS
3	Q	239	GLN
3	Q	240	GLU
4	R	4	VAL
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	60	VAL
4	R	64	ARG
4	R	99	ILE
4	R	117	GLU
4	R	125	LEU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	214	ILE
4	R	215	THR
4	R	216	LYS

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Mol	Chain	Res	Type
4	R	217	GLN
4	R	224	ASP
4	R	236	LYS
4	R	238	LYS
4	R	242	GLU
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	87	LEU
5	S	153	THR
5	S	169	THR
5	S	174	THR
5	S	184	ASN
5	S	188	LEU
5	S	207	VAL
5	S	209	ASN
5	S	229	VAL
6	T	14	ASP
6	T	53	LYS
6	T	58	GLN
6	T	66	VAL
6	T	94	SER
6	T	123	ASN
6	T	132	THR
6	T	139	LYS
6	T	165	ARG
6	T	167	SER
6	T	172	LEU
6	T	174	LYS
6	T	181	GLU
6	T	206	LYS
6	T	221	ASN
7	U	13	GLU
7	U	24	LYS
7	U	26	THR
7	U	28	GLN
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG

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Mol	Chain	Res	Type
7	U	168	GLU
7	U	171	THR
7	U	178	LYS
7	U	181	LYS
7	U	199	THR
7	U	201	MET
7	U	207	THR
7	U	223	LYS
7	U	230	GLU
7	U	235	ARG
7	U	236	LEU
7	U	237	VAL
7	U	239	ILE
7	U	241	GLU
7	U	242	GLN
8	V	1	THR
8	V	3	ILE
8	V	9	ASN
8	V	22	GLN
8	V	34	LEU
8	V	38	SER
8	V	43	CYS
8	V	56	THR
8	V	68	LEU
8	V	113	ILE
8	V	127	LEU
8	V	131	SER
8	V	153	LYS
8	V	199	LYS
8	V	209	THR
9	W	30	SER
9	W	31	GLN
9	W	37	ASN
9	W	166	ILE
9	W	171	LEU
9	W	182	TRP
9	W	190	LYS
9	W	191	LYS
10	X	1	MET
10	X	3	ILE
10	X	17	SER
10	X	23	ARG

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Mol	Chain	Res	Type
10	X	35	THR
10	X	36	ARG
10	X	90	LYS
10	X	99	GLN
10	X	110	LYS
10	X	113	LYS
10	X	172	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	99	THR
11	Y	148	LEU
11	Y	181	THR
11	Y	186	ILE
11	Y	211	ILE
12	Z	18	GLU
12	Z	23	LEU
12	Z	43	VAL
12	Z	49	ASN
12	Z	70	ASN
12	Z	85	SER
12	Z	128	VAL
12	Z	130	SER
12	Z	172	LEU
12	Z	173	LYS
12	Z	189	THR
12	Z	209	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	157	LYS
13	a	161	ARG
13	a	190	ARG
13	a	215	GLU
14	b	9	LYS
14	b	20	THR
14	b	92	ASN
14	b	105	LYS
14	b	107	LYS
14	b	119	VAL

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Mol	Chain	Res	Type
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (159) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
2	B	20	GLN
2	B	95	GLN
2	B	102	ASN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	17	GLN
3	C	147	GLN
3	C	160	GLN
3	C	239	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	106	GLN
4	D	146	GLN
4	D	160	ASN
4	D	225	ASN
5	E	3	ASN
5	E	4	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	209	ASN
6	F	58	GLN
6	F	86	ASN
6	F	117	GLN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN

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Mol	Chain	Res	Type
7	G	166	GLN
7	G	175	ASN
7	G	184	HIS
7	G	186	ASN
7	G	242	GLN
8	H	30	ASN
8	H	66	HIS
8	H	189	ASN
8	H	200	GLN
9	I	37	ASN
9	I	63	ASN
9	I	71	ASN
9	I	88	GLN
10	J	55	GLN
10	J	63	ASN
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	190	ASN
11	K	208	ASN
12	L	3	ASN
12	L	29	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	135	GLN
12	L	153	GLN
12	L	159	GLN
12	L	197	GLN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	194	ASN
13	M	203	ASN
13	M	211	ASN
13	M	213	GLN
14	N	38	HIS

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Mol	Chain	Res	Type
1	O	149	GLN
2	P	20	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	220	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	233	GLN
3	Q	239	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	3	ASN
5	S	4	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	209	ASN
6	T	58	GLN
6	T	86	ASN
6	T	117	GLN
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	166	GLN
7	U	184	HIS
7	U	186	ASN
7	U	242	GLN
8	V	30	ASN
8	V	66	HIS
8	V	165	ASN

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Mol	Chain	Res	Type
8	V	189	ASN
8	V	200	GLN
9	W	37	ASN
9	W	63	ASN
9	W	88	GLN
10	X	55	GLN
10	X	63	ASN
10	X	86	GLN
10	X	112	ASN
10	X	191	GLN
11	Y	9	GLN
11	Y	24	ASN
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
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	94	GLN
12	Z	153	GLN
12	Z	159	GLN
12	Z	197	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	194	ASN
13	a	203	ASN
13	a	211	ASN
13	a	213	GLN
14	b	38	HIS
14	b	141	ASN
14	b	145	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	VOT	K	301	11	45,45,45	2.40	10 (22%)	58,60,60	1.38	9 (15%)
16	VOT	H	301	8	45,45,45	2.40	9 (20%)	58,60,60	1.14	6 (10%)
16	VOT	V	301	8	45,45,45	2.54	9 (20%)	58,60,60	1.23	6 (10%)
16	VOT	Y	301	11	45,45,45	2.29	8 (17%)	58,60,60	1.22	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
16	VOT	K	301	11	-	11/50/50/50	0/2/3/3
16	VOT	H	301	8	-	8/50/50/50	0/2/3/3
16	VOT	V	301	8	-	11/50/50/50	0/2/3/3
16	VOT	Y	301	11	-	10/50/50/50	0/2/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	301	VOT	C3-C9	-10.13	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	301	VOT	C3-C9	-9.35	1.36	1.51
16	Y	301	VOT	C3-C9	-8.73	1.37	1.51
16	K	301	VOT	C3-C9	-8.67	1.37	1.51
16	V	301	VOT	C37-C38	-8.32	1.34	1.51
16	H	301	VOT	C37-C38	-8.17	1.35	1.51
16	K	301	VOT	C37-C38	-7.09	1.37	1.51
16	Y	301	VOT	C37-C38	-6.96	1.37	1.51
16	Y	301	VOT	C30-C31	-6.16	1.37	1.52
16	V	301	VOT	C30-C31	-5.79	1.38	1.52
16	K	301	VOT	C36-C34	-5.64	1.44	1.53
16	H	301	VOT	C30-C31	-5.47	1.39	1.52
16	K	301	VOT	C30-C31	-5.46	1.39	1.52
16	V	301	VOT	C20-C19	-4.34	1.37	1.52
16	H	301	VOT	C20-C19	-4.11	1.38	1.52
16	K	301	VOT	C20-C19	-3.98	1.38	1.52
16	Y	301	VOT	C20-C19	-3.81	1.39	1.52
16	V	301	VOT	C36-C34	-3.21	1.48	1.53
16	V	301	VOT	C36-C37	-2.93	1.44	1.52
16	Y	301	VOT	C36-C34	-2.79	1.48	1.53
16	H	301	VOT	C16-N15	-2.57	1.31	1.39
16	K	301	VOT	C42-C43	-2.55	1.45	1.52
16	V	301	VOT	C31-N33	2.48	1.39	1.34
16	K	301	VOT	C42-C41	-2.36	1.44	1.52
16	H	301	VOT	C12-N14	-2.31	1.32	1.39
16	V	301	VOT	C16-N15	-2.30	1.32	1.39
16	V	301	VOT	C12-N14	-2.28	1.32	1.39
16	K	301	VOT	C38-N40	2.27	1.38	1.33
16	K	301	VOT	C16-N15	-2.26	1.32	1.39
16	Y	301	VOT	C46-C26	-2.25	1.47	1.53
16	H	301	VOT	C36-C37	-2.25	1.46	1.52
16	H	301	VOT	C3-C1	-2.23	1.47	1.52
16	K	301	VOT	C12-N14	-2.22	1.32	1.39
16	Y	301	VOT	C12-N14	-2.17	1.32	1.39
16	Y	301	VOT	C16-N15	-2.09	1.32	1.39
16	H	301	VOT	C42-C43	-2.00	1.46	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	301	VOT	C37-C36-C34	-3.74	108.16	114.04
16	V	301	VOT	C37-C36-C34	-3.65	108.30	114.04
16	K	301	VOT	C26-N25-C1	3.10	127.91	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	H	301	VOT	C12-N14-N15	-3.03	111.02	119.14
16	V	301	VOT	C12-N14-N15	-2.99	111.14	119.14
16	V	301	VOT	O32-C31-N33	-2.99	117.61	122.96
16	K	301	VOT	C35-C34-C36	-2.95	106.11	111.48
16	K	301	VOT	C48-C46-C26	-2.94	106.47	112.29
16	Y	301	VOT	C34-N33-C31	-2.85	117.25	123.91
16	Y	301	VOT	C48-C46-C26	-2.76	106.84	112.29
16	H	301	VOT	O32-C31-N33	-2.71	118.11	122.96
16	K	301	VOT	C46-C26-N25	-2.63	104.72	111.70
16	K	301	VOT	C3-C1-N25	-2.62	111.79	115.88
16	K	301	VOT	O32-C31-N33	-2.59	118.31	122.96
16	K	301	VOT	C34-N33-C31	-2.56	117.93	123.91
16	H	301	VOT	C37-C36-C34	-2.45	110.20	114.04
16	Y	301	VOT	C36-C34-N33	2.41	114.56	110.42
16	K	301	VOT	C46-C26-C27	-2.38	106.12	111.32
16	Y	301	VOT	O32-C31-N33	-2.38	118.70	122.96
16	H	301	VOT	C35-C34-C36	-2.36	107.18	111.48
16	V	301	VOT	C35-C34-C36	-2.33	107.22	111.48
16	H	301	VOT	C34-N33-C31	-2.31	118.50	123.91
16	Y	301	VOT	C46-C26-C27	-2.31	106.27	111.32
16	H	301	VOT	O2-C1-N25	2.27	126.80	122.95
16	Y	301	VOT	C35-C34-C36	-2.19	107.48	111.48
16	V	301	VOT	C34-N33-C31	-2.13	118.94	123.91
16	Y	301	VOT	C26-N25-C1	2.06	125.87	121.80
16	Y	301	VOT	C46-C26-N25	-2.05	106.25	111.70
16	V	301	VOT	C3-C9-C24	-2.04	117.89	120.89

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	H	301	VOT	C27-C26-N25-C1
16	H	301	VOT	C41-C42-C43-O44
16	H	301	VOT	N29-C30-C45-C43
16	K	301	VOT	C41-C42-C43-O44
16	K	301	VOT	N29-C30-C45-C43
16	V	301	VOT	O44-C43-C45-C30
16	V	301	VOT	N29-C30-C45-C43
16	Y	301	VOT	C27-C26-N25-C1
16	Y	301	VOT	C41-C42-C43-O44
16	Y	301	VOT	N29-C30-C45-C43
16	V	301	VOT	C31-C30-C45-C43

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Mol	Chain	Res	Type	Atoms
16	K	301	VOT	C31-C30-C45-C43
16	V	301	VOT	C27-C26-N25-C1
16	H	301	VOT	C31-C30-C45-C43
16	Y	301	VOT	C31-C30-C45-C43
16	H	301	VOT	C11-C12-N14-N15
16	Y	301	VOT	C17-C16-N15-N14
16	Y	301	VOT	C23-C16-N15-N14
16	K	301	VOT	C41-C42-C43-C45
16	Y	301	VOT	C41-C42-C43-C45
16	K	301	VOT	C27-C26-N25-C1
16	H	301	VOT	C13-C12-N14-N15
16	V	301	VOT	C13-C12-N14-N15
16	V	301	VOT	C11-C12-N14-N15
16	H	301	VOT	C34-C36-C37-C38
16	V	301	VOT	C34-C36-C37-C38
16	V	301	VOT	C1-C3-C9-C10
16	V	301	VOT	C1-C3-C9-C24
16	H	301	VOT	C41-C42-C43-C45
16	K	301	VOT	C34-C36-C37-C38
16	V	301	VOT	C42-C43-C45-C30
16	Y	301	VOT	C1-C3-C9-C10
16	Y	301	VOT	C1-C3-C9-C24
16	K	301	VOT	C1-C3-C9-C10
16	V	301	VOT	C41-C42-C43-O44
16	K	301	VOT	C1-C3-C9-C24
16	Y	301	VOT	C34-C36-C37-C38
16	K	301	VOT	O44-C43-C45-C30
16	K	301	VOT	N29-C30-C31-O32
16	K	301	VOT	N29-C30-C31-N33

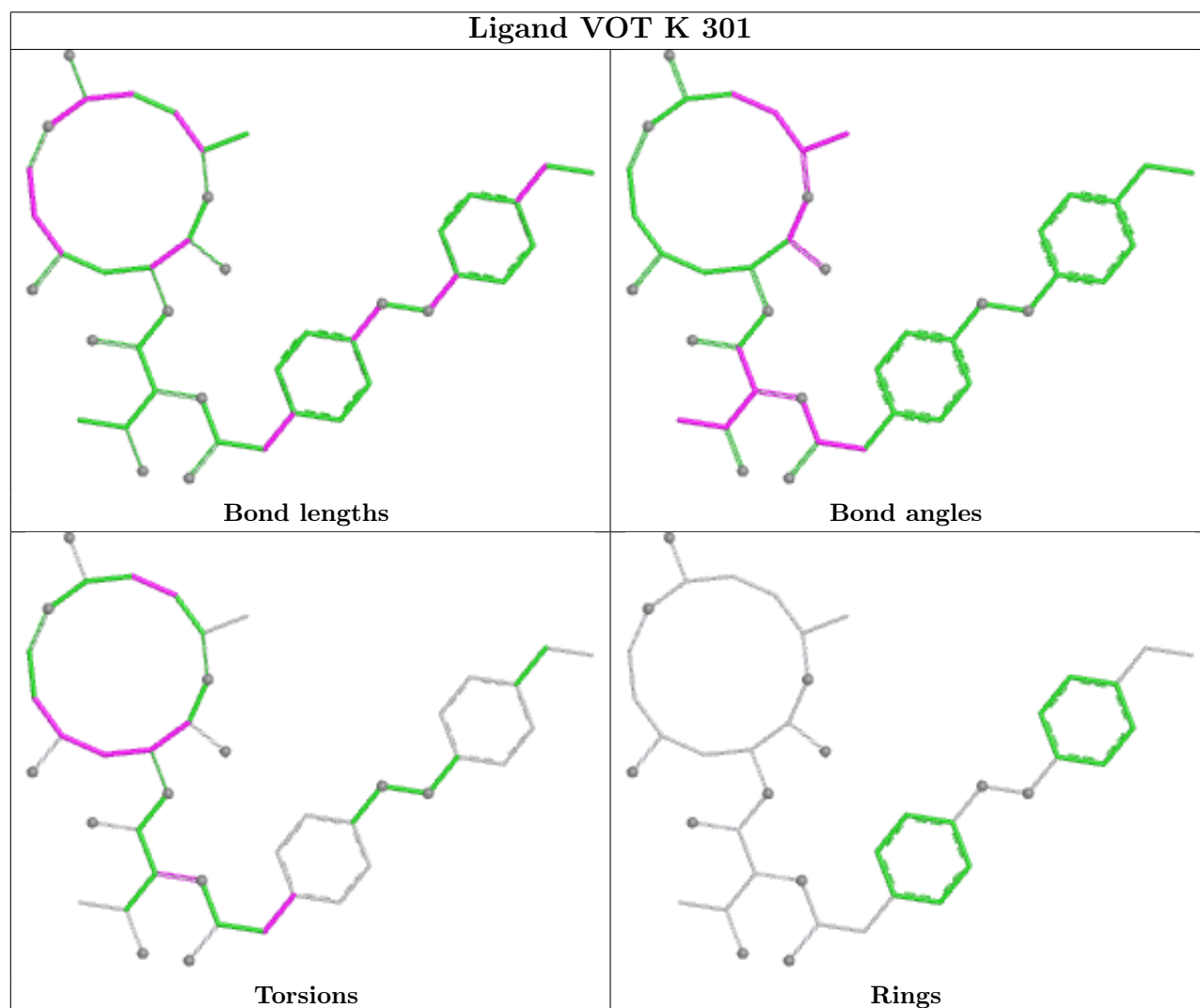
There are no ring outliers.

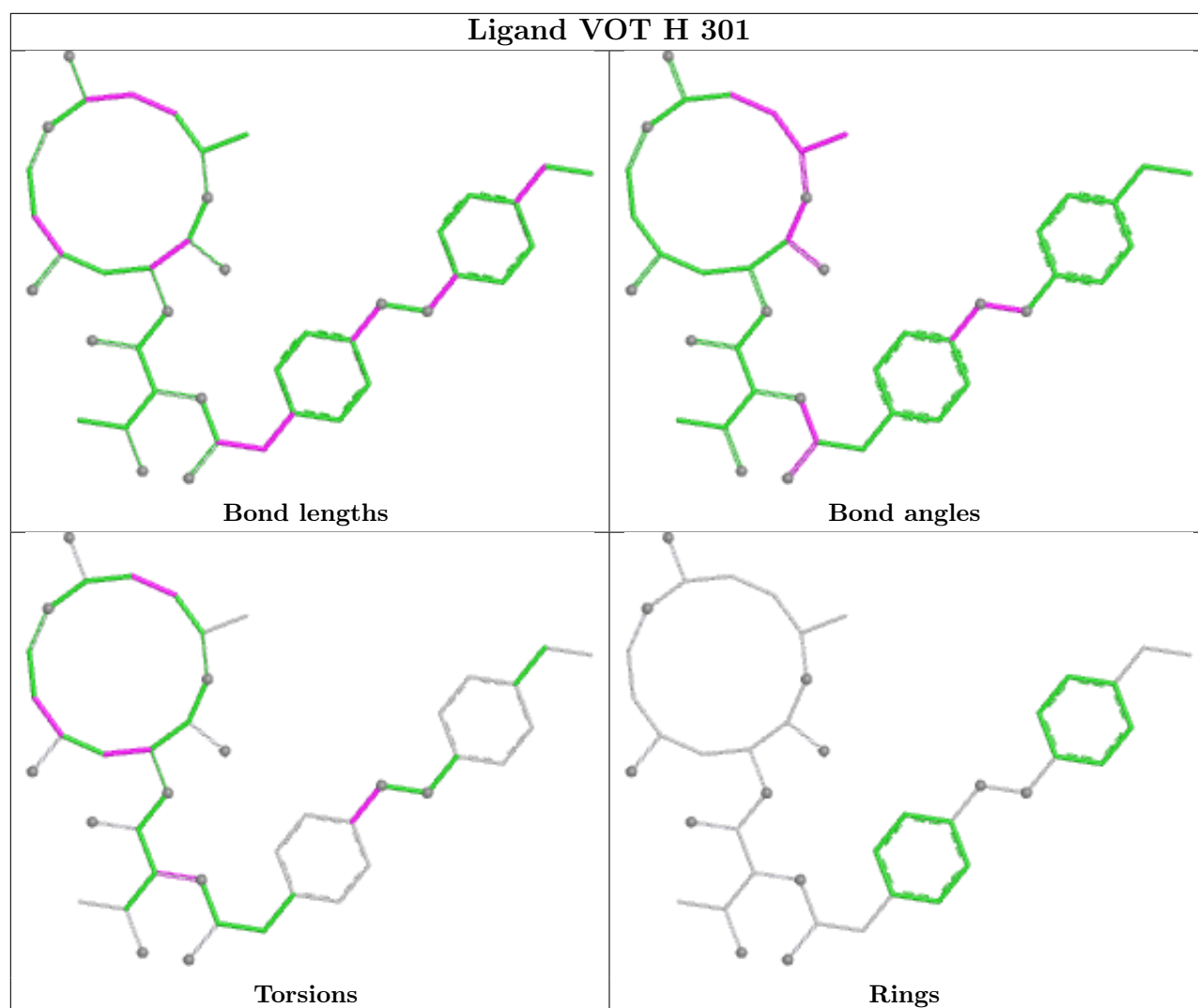
1 monomer is involved in 1 short contact:

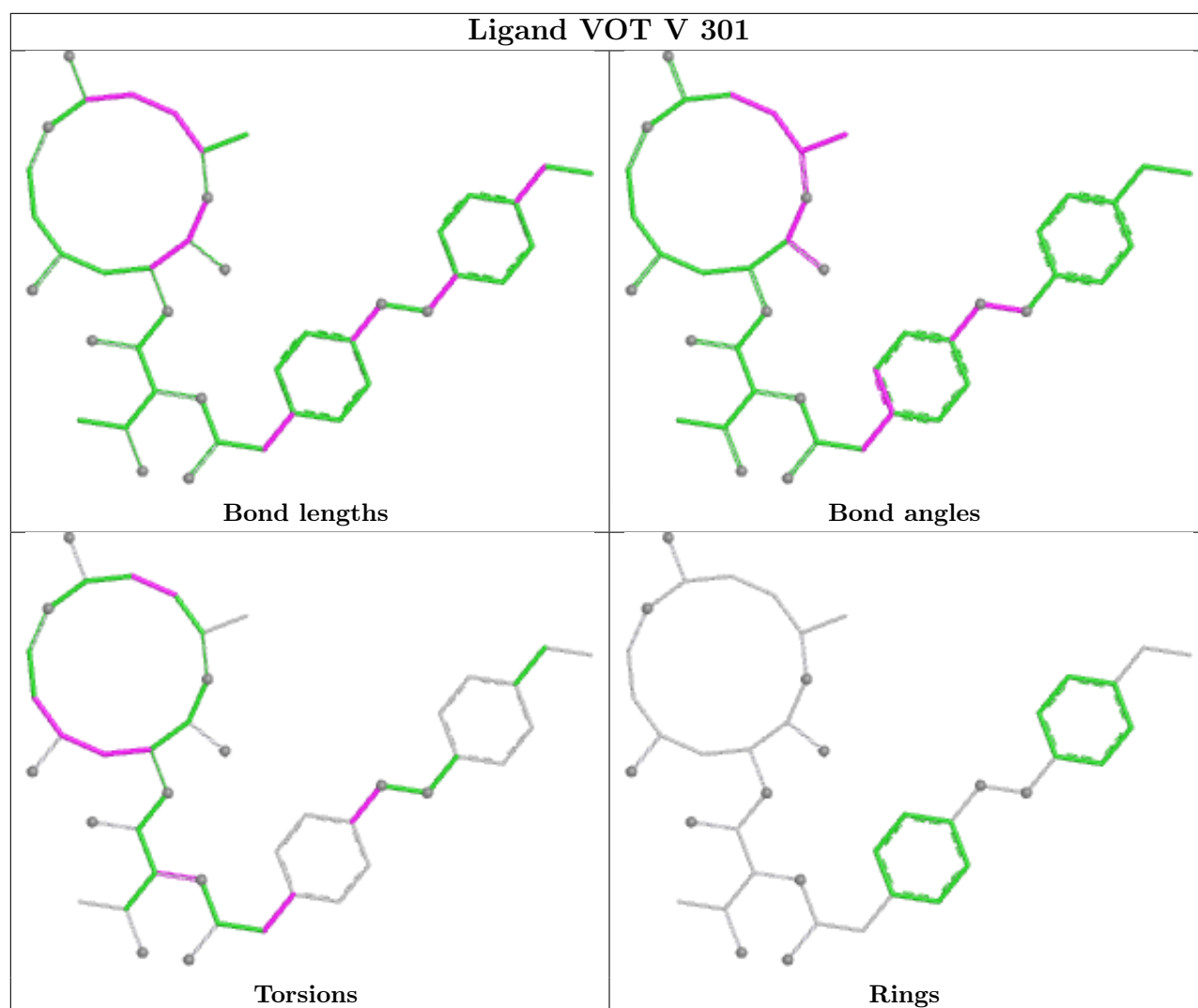
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	301	VOT	1	0

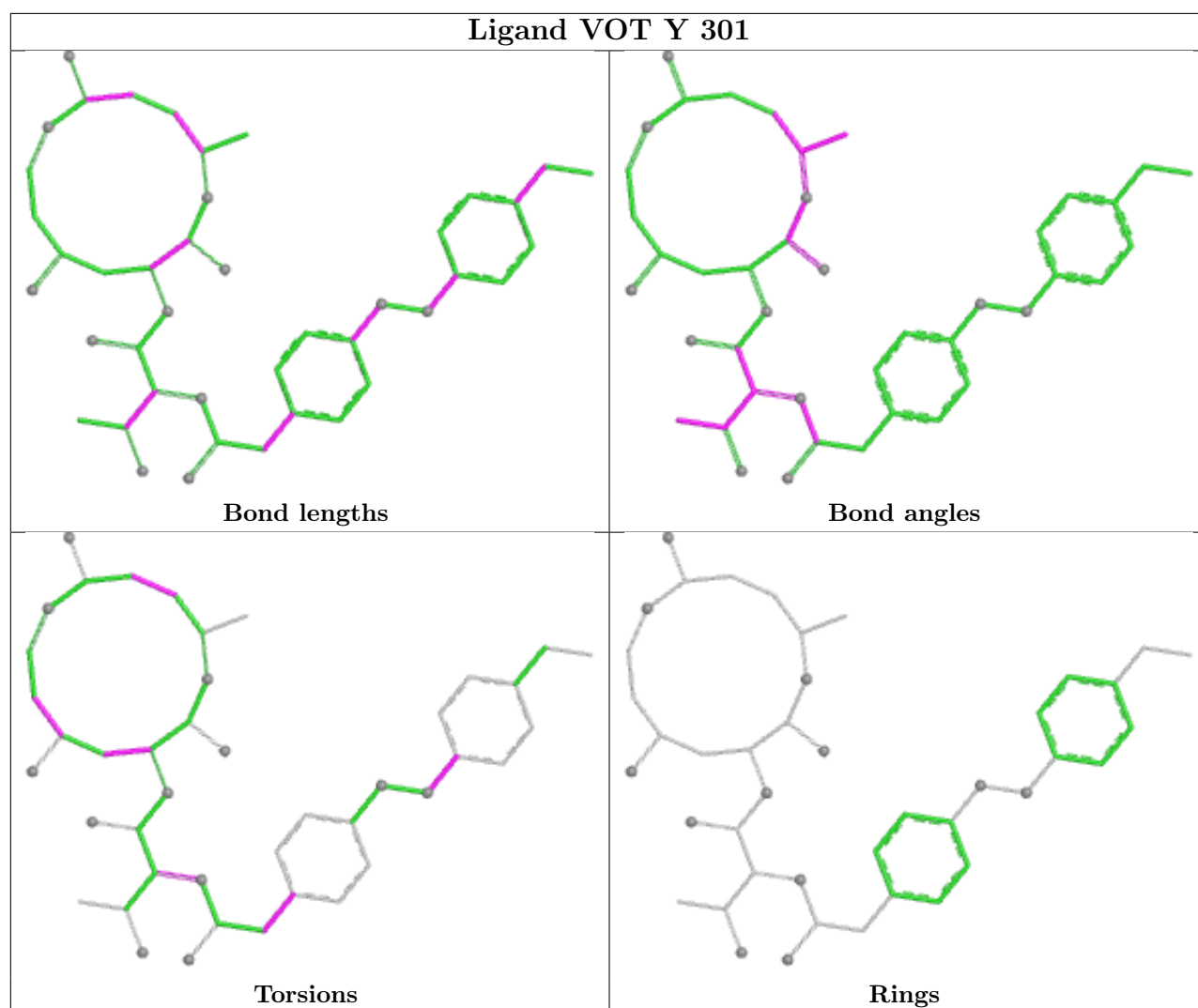
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	250/250 (100%)	-0.36	1 (0%) 88 87	56, 73, 105, 159	0
1	O	250/250 (100%)	-0.41	1 (0%) 88 87	62, 82, 115, 159	0
2	B	244/258 (94%)	-0.18	2 (0%) 82 79	58, 80, 129, 163	0
2	P	244/258 (94%)	-0.20	4 (1%) 70 66	64, 83, 137, 177	0
3	C	240/254 (94%)	-0.20	3 (1%) 75 71	57, 82, 135, 159	0
3	Q	240/254 (94%)	-0.07	3 (1%) 75 71	62, 98, 159, 171	0
4	D	235/260 (90%)	-0.30	0 100 100	61, 83, 113, 152	0
4	R	235/260 (90%)	-0.22	1 (0%) 88 87	65, 89, 123, 153	0
5	E	231/234 (98%)	-0.17	0 100 100	65, 85, 116, 146	0
5	S	231/234 (98%)	-0.14	0 100 100	64, 96, 134, 157	0
6	F	243/288 (84%)	-0.34	1 (0%) 88 87	55, 77, 121, 147	0
6	T	243/288 (84%)	-0.31	1 (0%) 88 87	58, 88, 132, 153	0
7	G	241/252 (95%)	-0.45	1 (0%) 88 87	56, 71, 100, 147	0
7	U	241/252 (95%)	-0.44	1 (0%) 88 87	57, 76, 106, 131	0
8	H	226/232 (97%)	-0.36	0 100 100	52, 67, 104, 167	0
8	V	226/232 (97%)	-0.37	1 (0%) 88 87	57, 70, 105, 172	0
9	I	204/205 (99%)	-0.40	0 100 100	54, 71, 97, 129	0
9	W	204/205 (99%)	-0.46	1 (0%) 87 85	56, 71, 98, 129	0
10	J	195/198 (98%)	-0.38	1 (0%) 87 85	55, 74, 102, 140	0
10	X	195/198 (98%)	-0.46	1 (0%) 87 85	58, 76, 100, 139	0
11	K	212/212 (100%)	-0.31	1 (0%) 87 85	56, 75, 106, 128	0
11	Y	212/212 (100%)	-0.30	1 (0%) 87 85	61, 77, 111, 128	0
12	L	222/222 (100%)	-0.40	0 100 100	57, 71, 105, 118	0
12	Z	222/222 (100%)	-0.31	1 (0%) 87 85	56, 73, 110, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.43	2 (0%) 81 78	53, 70, 92, 105	0
13	a	233/246 (94%)	-0.45	2 (0%) 81 78	54, 70, 90, 103	0
14	N	196/196 (100%)	-0.48	0 100 100	52, 65, 91, 120	0
14	b	196/196 (100%)	-0.46	0 100 100	54, 67, 93, 115	0
All	All	6344/6614 (95%)	-0.33	30 (0%) 87 85	52, 76, 121, 177	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	50	LEU	4.7
10	X	1	MET	4.6
10	J	1	MET	3.9
1	A	1	MET	3.8
11	K	211	ILE	3.5
2	P	60	THR	3.4
11	Y	211	ILE	3.4
3	Q	49	THR	3.1
2	P	51	VAL	2.8
1	O	1	MET	2.8
13	M	1	THR	2.5
4	R	113	LEU	2.5
7	U	242	GLN	2.5
2	P	1	GLY	2.4
6	F	2	THR	2.4
3	C	204	GLY	2.4
12	Z	172	LEU	2.3
13	a	1	THR	2.3
6	T	2	THR	2.3
2	B	2	SER	2.3
8	V	223	ILE	2.3
2	B	51	VAL	2.2
3	Q	205	ALA	2.1
7	G	2	GLY	2.1
13	M	38	GLY	2.1
9	W	131	GLU	2.1
3	C	50	LEU	2.1
13	a	38	GLY	2.1
3	C	205	ALA	2.1
2	P	217	LYS	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](#)

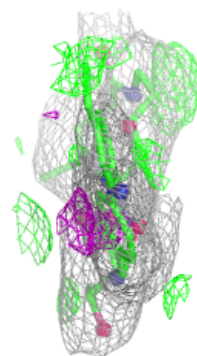
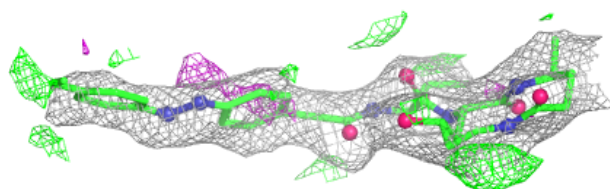
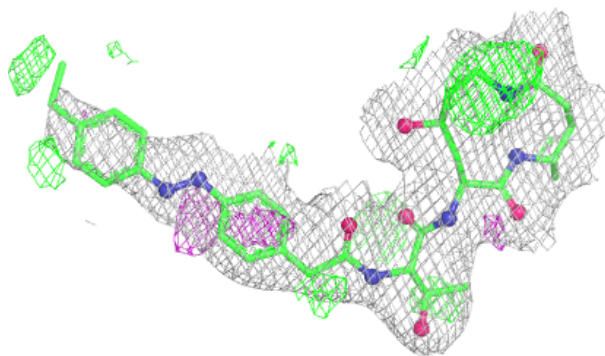
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
16	VOT	K	301	43/43	0.91	0.14	58,74,126,133	0
16	VOT	V	301	43/43	0.92	0.12	63,77,105,110	0
16	VOT	H	301	43/43	0.93	0.11	63,70,109,114	0
16	VOT	Y	301	43/43	0.93	0.11	65,73,128,131	0
15	MG	Y	302	1/1	0.94	0.04	81,81,81,81	0
17	CL	b	201	1/1	0.95	0.12	89,89,89,89	0
15	MG	Z	301	1/1	0.96	0.06	73,73,73,73	0
15	MG	I	301	1/1	0.96	0.17	86,86,86,86	0
15	MG	J	201	1/1	0.98	0.07	61,61,61,61	0
15	MG	V	302	1/1	0.98	0.05	83,83,83,83	0
15	MG	G	301	1/1	0.98	0.06	81,81,81,81	0
15	MG	K	302	1/1	0.99	0.06	70,70,70,70	0
17	CL	N	202	1/1	0.99	0.04	74,74,74,74	0
15	MG	N	201	1/1	0.99	0.03	59,59,59,59	0

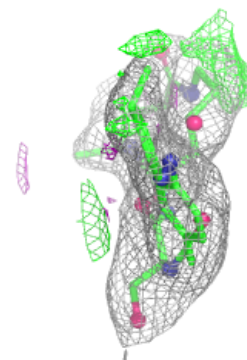
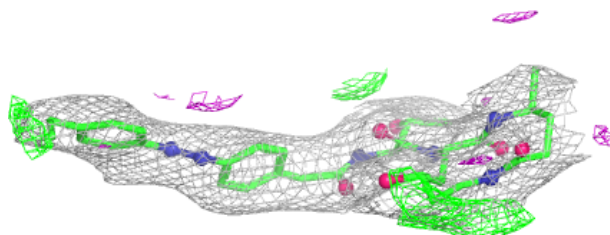
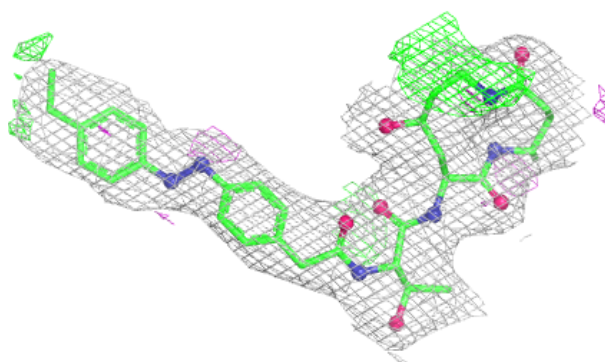
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VOT K 301:

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

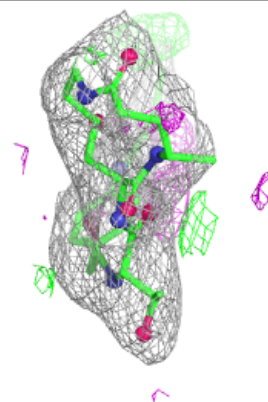
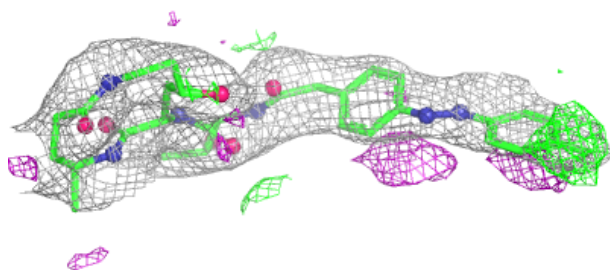
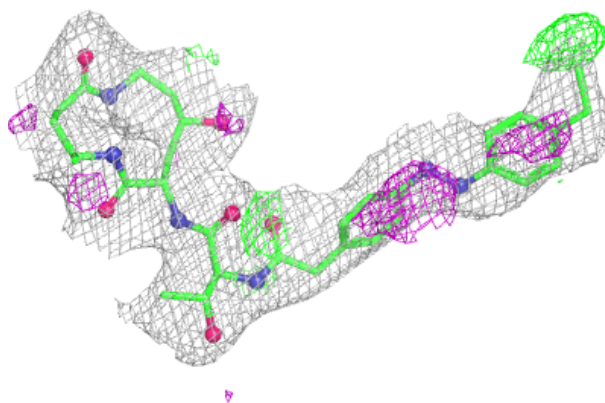
**Electron density around VOT V 301:**

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

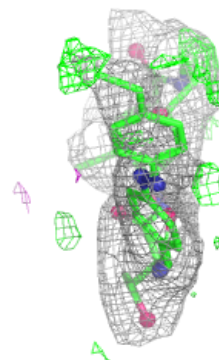
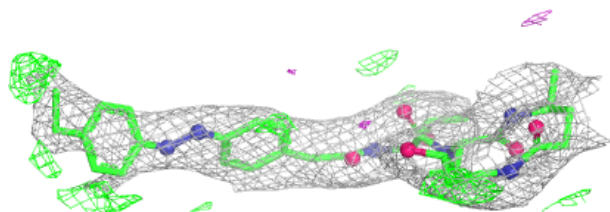
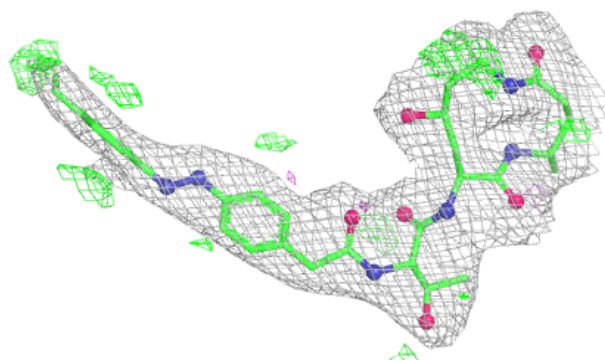


Electron density around VOT H 301:

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

**Electron density around VOT Y 301:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.