



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:25 AM UTC

PDB ID : 4HRC / pdb_00004hrc
Title : Crystal structure of yeast 20S proteasome in complex with epoxyketone carma-
phyacin analogue 3
Authors : Trivella, D.B.B.; Stein, M.; Groll, M.
Deposited on : 2012-10-27
Resolution : 2.80 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

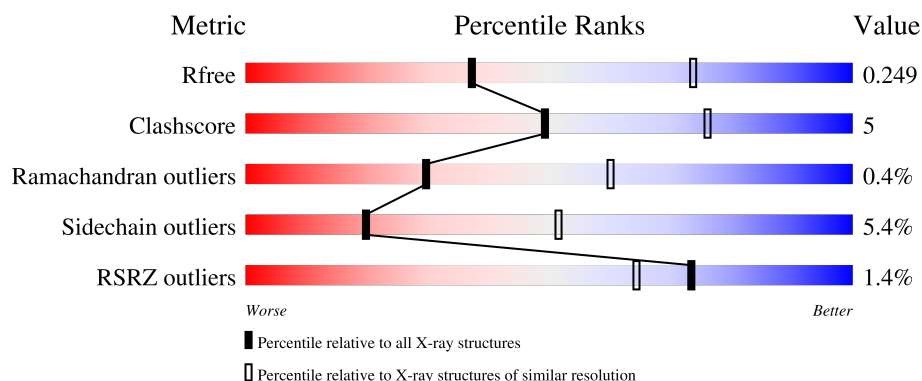
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

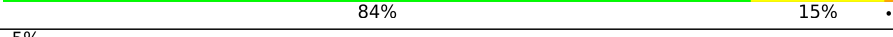
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	249	
1	O	249	
2	B	244	
2	P	244	
3	C	241	

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Mol	Chain	Length	Quality of chain
3	Q	241	4% 83% 15% .
4	D	242	3% 85% 14% .
4	R	242	5% 83% 15% .
5	E	233	% 85% 13% .
5	S	233	2% 84% 14% .
6	F	244	76% 22% .
6	T	244	% 84% 14% .
7	G	243	89% 10% .
7	U	243	% 86% 13% .
8	H	222	86% 13%
8	V	222	% 79% 19% .
9	I	204	88% 12%
9	W	204	86% 14%
10	J	198	2% 88% 12%
10	X	198	2% 89% 9% .
11	K	212	83% 15% .
11	Y	212	84% 15% .
12	L	222	86% 13%
12	Z	222	86% 12% .
13	M	233	2% 83% 15% .
13	a	233	83% 16% .
14	N	196	84% 16% .
14	b	196	88% 11% .

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50159 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 component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			
1	O	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			

- Molecule 2 is a protein called Proteasome component Y13.

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 component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			
4	R	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
6	T	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called Proteasome component PUP1.

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

- Molecule 9 is a protein called Proteasome component PUP3.

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 component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called Proteasome component PRE2.

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 component C5.

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			

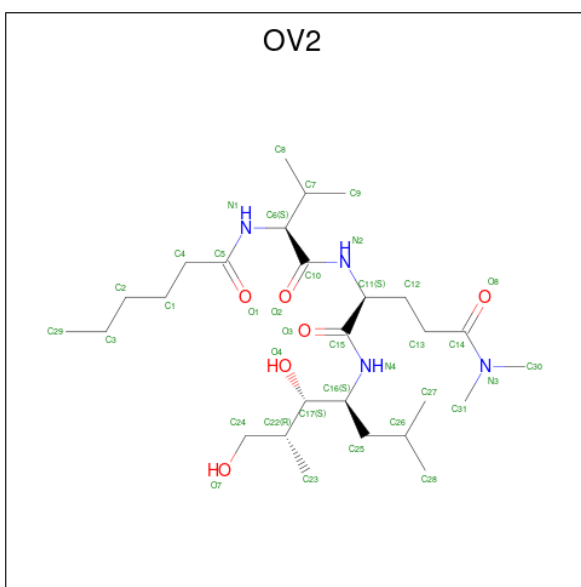
- Molecule 13 is a protein called Proteasome component PRE4.

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 component PRE3.

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 N-hexanoyl-L-valyl-N 1 -[(2R,3S,4S)-1,3-dihydroxy-2,6-dimethylheptan-4-yl]-N 5 ,N 5 -dimethyl-L-glutamamide (CCD ID: OV2) (formula: C₂₇H₅₂N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			37	27	4	6		
15	K	1	Total	C	N	O	0	0
			37	27	4	6		
15	N	1	Total	C	N	O	0	0
			37	27	4	6		
15	V	1	Total	C	N	O	0	0
			37	27	4	6		
15	Y	1	Total	C	N	O	0	0
			37	27	4	6		
15	b	1	Total	C	N	O	0	0
			37	27	4	6		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	10	Total	O	0	0
			10	10		
16	B	20	Total	O	0	0
			20	20		
16	C	13	Total	O	0	0
			13	13		
16	D	17	Total	O	0	0
			17	17		
16	E	18	Total	O	0	0
			18	18		
16	F	15	Total	O	0	0
			15	15		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	18	Total O 18 18	0	0
16	H	12	Total O 12 12	0	0
16	I	19	Total O 19 19	0	0
16	J	19	Total O 19 19	0	0
16	K	13	Total O 13 13	0	0
16	L	22	Total O 22 22	0	0
16	M	22	Total O 22 22	0	0
16	N	16	Total O 16 16	0	0
16	O	19	Total O 19 19	0	0
16	P	4	Total O 4 4	0	0
16	Q	13	Total O 13 13	0	0
16	R	8	Total O 8 8	0	0
16	S	8	Total O 8 8	0	0
16	T	11	Total O 11 11	0	0
16	U	9	Total O 9 9	0	0
16	V	19	Total O 19 19	0	0
16	W	13	Total O 13 13	0	0
16	X	15	Total O 15 15	0	0
16	Y	15	Total O 15 15	0	0
16	Z	18	Total O 18 18	0	0
16	a	11	Total O 11 11	0	0

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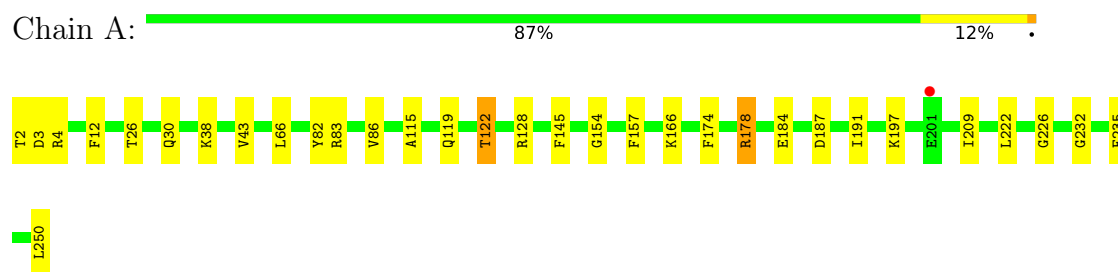
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	b	18	Total	O	0	0
			18	18		

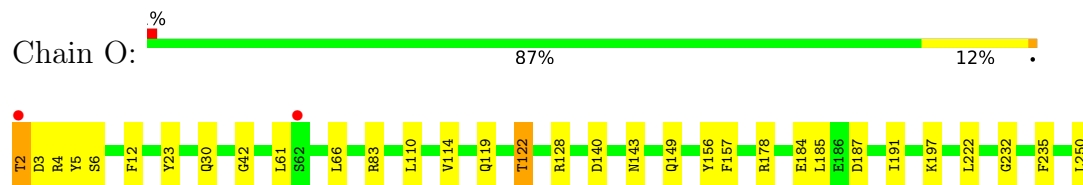
3 Residue-property plots [i](#)

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

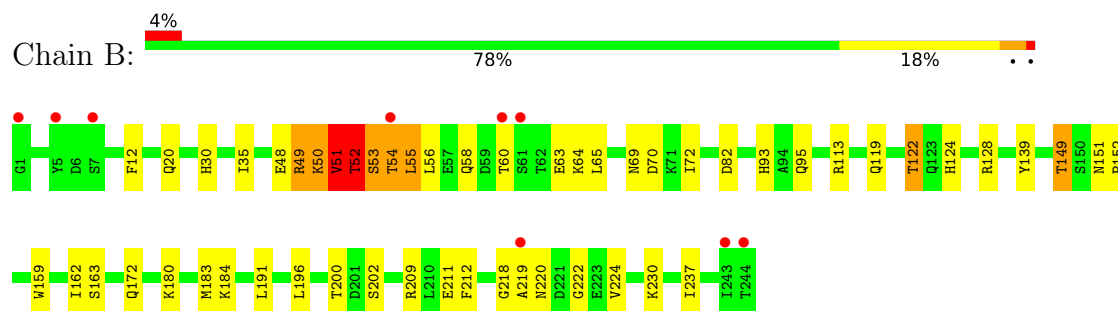
- Molecule 1: Proteasome component Y7



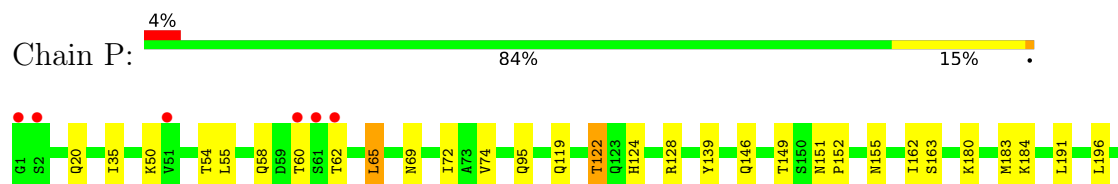
- Molecule 1: Proteasome component Y7

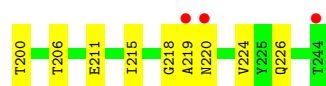


- Molecule 2: Proteasome component Y13

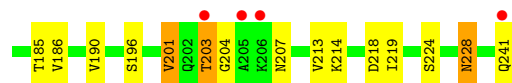
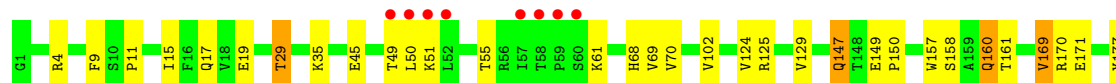
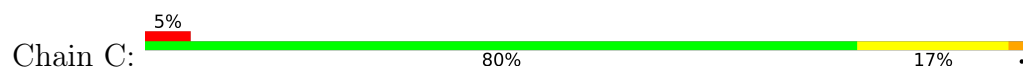


- Molecule 2: Proteasome component Y13

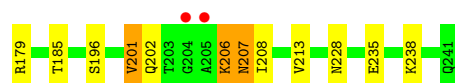
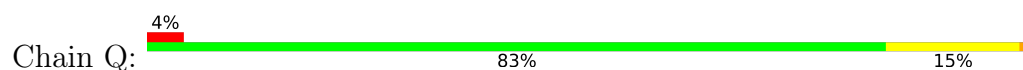




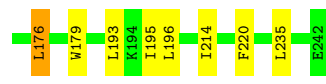
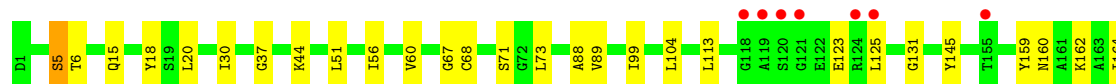
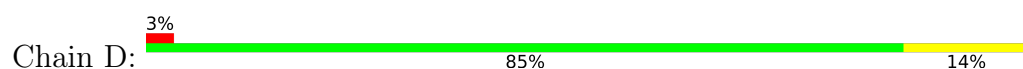
• Molecule 3: Proteasome component PRE6



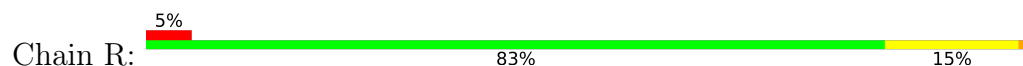
• Molecule 3: Proteasome component PRE6



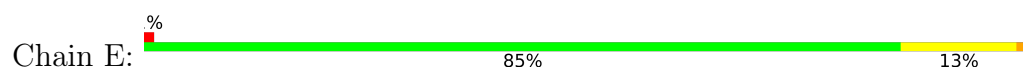
• Molecule 4: Proteasome component PUP2

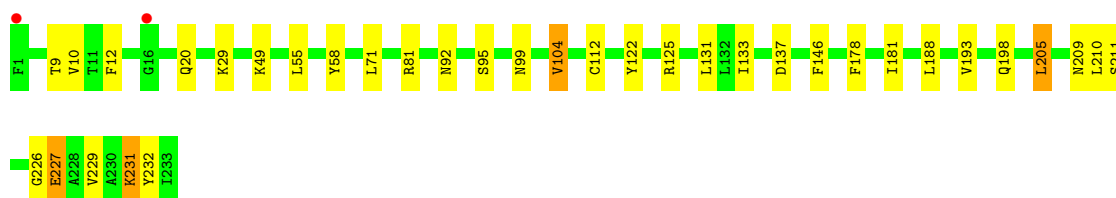


• Molecule 4: Proteasome component PUP2

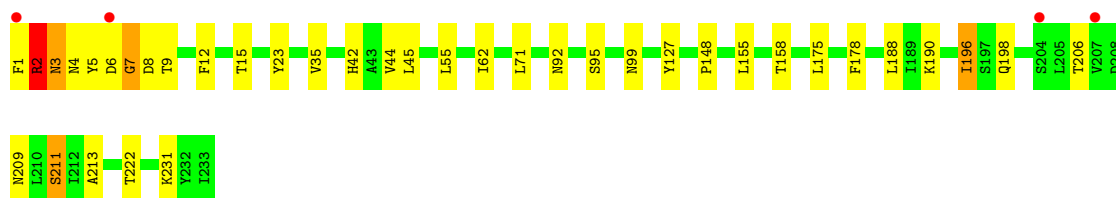
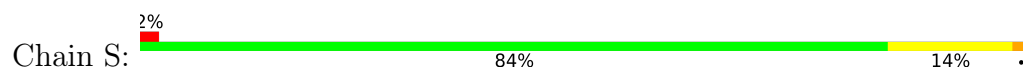


• Molecule 5: Proteasome component PRE5

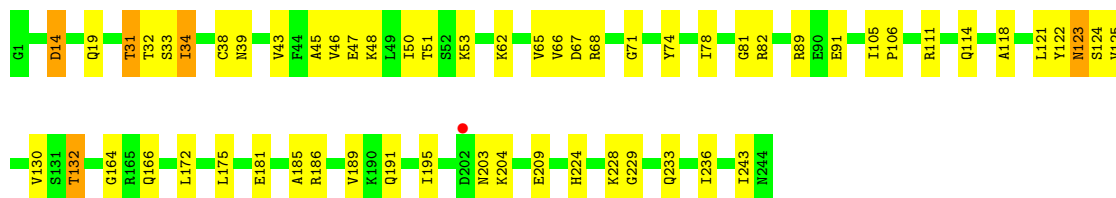
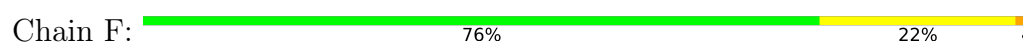




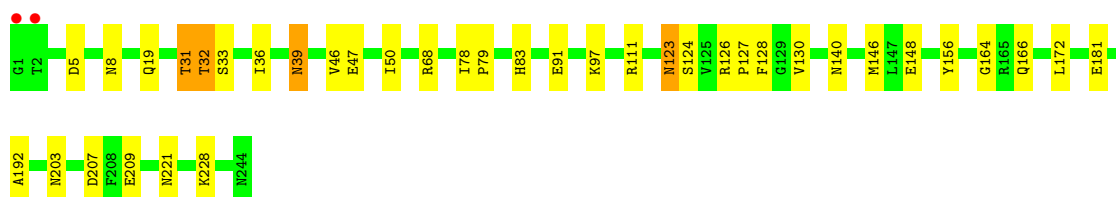
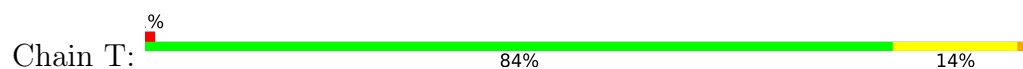
• Molecule 5: Proteasome component PRE5



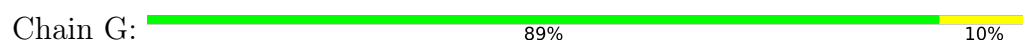
• Molecule 6: Proteasome component C1



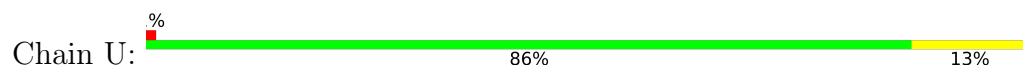
• Molecule 6: Proteasome component C1

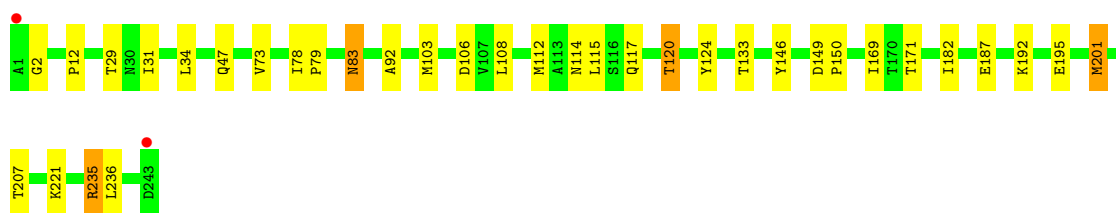


• Molecule 7: Proteasome component C7-alpha



• Molecule 7: Proteasome component C7-alpha





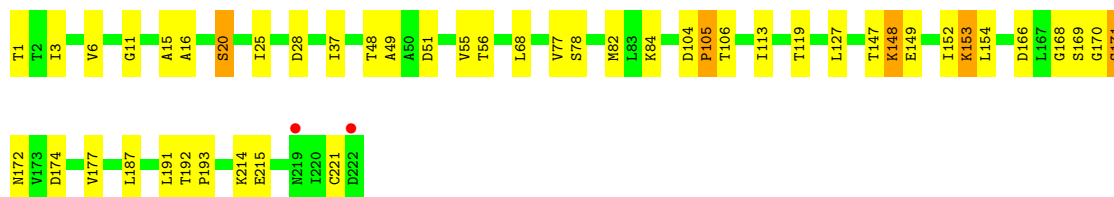
• Molecule 8: Proteasome component PUP1

Chain H: 86% 13%



• Molecule 8: Proteasome component PUP1

Chain V: 79% 19%



• Molecule 9: Proteasome component PUP3

Chain I: 88% 12%



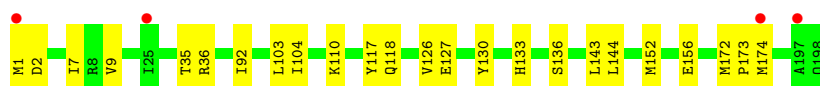
• Molecule 9: Proteasome component PUP3

Chain W: 86% 14%



• Molecule 10: Proteasome component C11

Chain J: 88% 12%



• Molecule 10: Proteasome component C11

Chain X: 89% 9%



• Molecule 11: Proteasome component PRE2

Chain K: 83% 15%



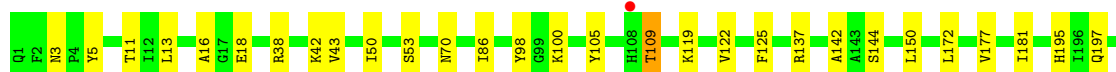
• Molecule 11: Proteasome component PRE2

Chain Y: 84% 15%



• Molecule 12: Proteasome component C5

Chain L: 86% 13%



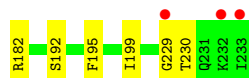
• Molecule 12: Proteasome component C5

Chain Z: 86% 12%

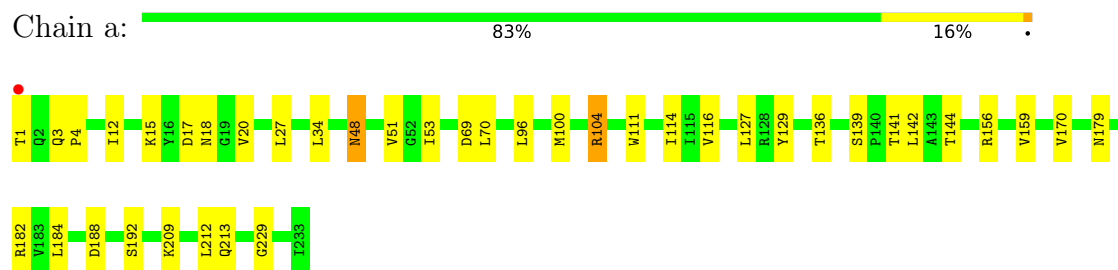


• Molecule 13: Proteasome component PRE4

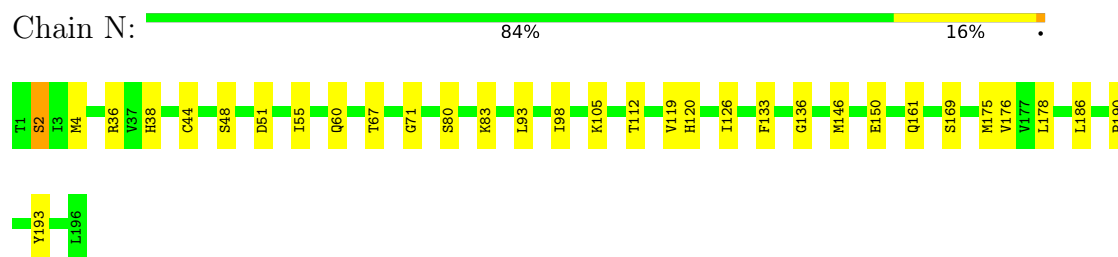
Chain M: 83% 15%



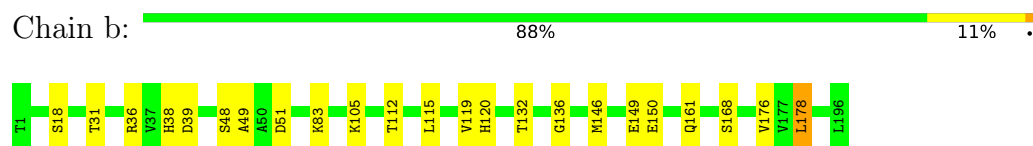
- Molecule 13: Proteasome component PRE4



- Molecule 14: Proteasome component PRE3



- Molecule 14: Proteasome component PRE3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.35Å 300.88Å 144.25Å 90.00° 112.74° 90.00°	Depositor
Resolution (Å)	48.00 – 2.80 48.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.00-2.80) 98.0 (48.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.243 0.215 , 0.249	Depositor DCC
R_{free} test set	12670 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50159	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: OV2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/1944	0.77	0/2632
1	O	0.46	0/1944	0.79	0/2632
2	B	0.50	0/1934	0.82	1/2618 (0.0%)
2	P	0.44	0/1934	0.78	0/2618
3	C	0.45	0/1919	0.82	0/2598
3	Q	0.45	0/1919	0.80	1/2598 (0.0%)
4	D	0.44	0/1886	0.81	0/2541
4	R	0.45	0/1886	0.80	0/2541
5	E	0.45	0/1823	0.81	0/2463
5	S	0.52	0/1823	0.82	2/2463 (0.1%)
6	F	0.49	1/1936 (0.1%)	0.82	0/2614
6	T	0.44	0/1936	0.82	0/2614
7	G	0.44	0/1959	0.78	0/2652
7	U	0.44	0/1959	0.77	0/2652
8	H	0.46	0/1715	0.77	0/2326
8	V	0.52	0/1715	0.81	2/2326 (0.1%)
9	I	0.45	0/1611	0.78	0/2174
9	W	0.47	0/1611	0.81	0/2174
10	J	0.44	0/1613	0.82	0/2173
10	X	0.44	0/1613	0.75	0/2173
11	K	0.45	0/1681	0.80	0/2274
11	Y	0.47	0/1681	0.79	1/2274 (0.0%)
12	L	0.45	0/1795	0.78	0/2420
12	Z	0.46	0/1795	0.78	0/2420
13	M	0.46	0/1855	0.79	0/2514
13	a	0.45	0/1855	0.75	0/2514
14	N	0.44	0/1541	0.75	0/2087
14	b	0.41	0/1541	0.76	0/2087
All	All	0.46	1/50424 (0.0%)	0.79	7/68172 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
8	V	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	78	ILE	CA-CB	5.64	1.56	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	2	ARG	N-CA-C	-9.93	100.29	111.71
8	V	11	GLY	N-CA-C	5.89	117.98	110.20
5	S	3	ASN	N-CA-C	-5.84	101.65	110.24
2	B	51	VAL	N-CA-C	5.67	116.41	110.62
3	Q	201	VAL	N-CA-C	5.39	116.87	111.00
8	V	37	ILE	N-CA-C	-5.10	106.71	111.45
11	Y	189	GLY	N-CA-C	5.09	119.10	112.68

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	50	LYS	Peptide
8	V	1	THR	Peptide

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	1907	0	1917	20	0
1	O	1907	0	1917	24	0
2	B	1904	0	1904	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1904	0	1904	19	0
3	C	1890	0	1903	28	0
3	Q	1890	0	1903	25	0
4	D	1861	0	1839	19	0
4	R	1861	0	1839	18	0
5	E	1795	0	1800	24	0
5	S	1795	0	1800	36	0
6	F	1896	0	1889	31	0
6	T	1896	0	1889	18	0
7	G	1921	0	1913	15	0
7	U	1921	0	1913	25	0
8	H	1684	0	1685	20	0
8	V	1684	0	1685	28	0
9	I	1581	0	1574	14	0
9	W	1581	0	1574	15	0
10	J	1585	0	1590	10	0
10	X	1585	0	1590	10	0
11	K	1644	0	1592	26	0
11	Y	1644	0	1592	25	0
12	L	1757	0	1711	21	0
12	Z	1757	0	1711	16	0
13	M	1824	0	1832	19	0
13	a	1824	0	1832	20	0
14	N	1512	0	1478	19	0
14	b	1512	0	1478	13	0
15	H	37	0	50	2	0
15	K	37	0	50	3	0
15	N	37	0	50	0	0
15	V	37	0	50	5	0
15	Y	37	0	50	1	0
15	b	37	0	50	2	0
16	A	10	0	0	0	0
16	B	20	0	0	1	0
16	C	13	0	0	0	0
16	D	17	0	0	1	0
16	E	18	0	0	0	0
16	F	15	0	0	1	0
16	G	18	0	0	0	0
16	H	12	0	0	0	0
16	I	19	0	0	1	0
16	J	19	0	0	0	0
16	K	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	L	22	0	0	0	0
16	M	22	0	0	2	0
16	N	16	0	0	2	0
16	O	19	0	0	1	0
16	P	4	0	0	0	0
16	Q	13	0	0	1	0
16	R	8	0	0	0	0
16	S	8	0	0	0	0
16	T	11	0	0	0	0
16	U	9	0	0	0	0
16	V	19	0	0	1	0
16	W	13	0	0	0	0
16	X	15	0	0	0	0
16	Y	15	0	0	0	0
16	Z	18	0	0	0	0
16	a	11	0	0	0	0
16	b	18	0	0	0	0
All	All	50159	0	49554	533	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 (533) 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)
2:B:51:VAL:C	2:B:52:THR:HG23	1.59	1.24
11:Y:4:LEU:HD23	11:Y:4:LEU:C	1.61	1.19
5:S:2:ARG:HG3	5:S:2:ARG:HH11	0.95	1.04
5:S:2:ARG:HH11	5:S:2:ARG:CG	1.71	1.04
2:B:51:VAL:O	2:B:52:THR:HG23	1.56	1.04
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.30	1.03
5:S:2:ARG:HG3	5:S:2:ARG:NH1	1.61	1.03
2:B:30:HIS:O	2:B:50:LYS:HE3	1.58	1.01
2:B:51:VAL:C	2:B:52:THR:CG2	2.33	1.00
5:S:2:ARG:CD	5:S:2:ARG:H	1.75	0.98
5:S:5:TYR:OH	6:T:5:ASP:OD2	1.88	0.91
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.36	0.90
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.39	0.86
7:G:92:ALA:HA	7:G:103:MET:HE2	1.57	0.85
11:Y:4:LEU:HD23	11:Y:4:LEU:O	1.75	0.85
5:S:2:ARG:HD2	5:S:2:ARG:N	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.39	0.85
2:B:51:VAL:HA	2:B:209:ARG:HH12	1.44	0.83
5:S:2:ARG:CD	5:S:2:ARG:N	2.37	0.83
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.24	0.82
2:B:49:ARG:HG2	2:B:49:ARG:HH11	1.43	0.81
2:B:50:LYS:O	2:B:52:THR:HG22	1.81	0.81
5:S:3:ASN:O	5:S:4:ASN:HB2	1.80	0.81
2:B:51:VAL:HA	2:B:209:ARG:NH1	1.95	0.80
2:B:51:VAL:O	2:B:52:THR:CG2	2.29	0.80
7:U:92:ALA:HA	7:U:103:MET:HE2	1.64	0.79
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.48	0.78
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.64	0.77
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.50	0.76
1:O:12:PHE:H	2:P:20:GLN:HE22	1.34	0.75
2:B:49:ARG:HG2	2:B:49:ARG:NH1	2.00	0.75
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.69	0.74
1:O:3:ASP:C	1:O:3:ASP:OD2	2.30	0.74
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.00	0.73
3:C:9:PHE:H	4:D:15:GLN:HE22	1.37	0.73
2:B:222:GLY:HA3	16:B:315:HOH:O	1.87	0.72
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.52	0.72
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.73	0.71
1:A:12:PHE:H	2:B:20:GLN:HE22	1.37	0.71
14:b:18:SER:HB2	14:b:31:THR:H	1.56	0.71
10:X:147:HIS:HB3	10:X:160:LEU:HD11	1.72	0.71
5:S:2:ARG:O	5:S:3:ASN:C	2.33	0.70
3:C:204:GLY:HA3	3:C:207:ASN:HB2	1.73	0.69
5:E:81:ARG:HG3	5:E:81:ARG:HH11	1.58	0.69
10:J:1:MET:HG2	10:J:2:ASP:H	1.58	0.69
8:V:148:LYS:O	8:V:148:LYS:HG2	1.92	0.68
11:Y:4:LEU:HD23	11:Y:5:ALA:N	2.09	0.68
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.75	0.67
12:L:109:THR:HG23	12:L:125:PHE:HB2	1.77	0.67
1:O:83:ARG:HE	7:U:114:ASN:HD21	1.40	0.67
5:S:1:PHE:HB3	5:S:2:ARG:HD3	1.76	0.67
5:S:2:ARG:H	5:S:2:ARG:HD3	1.56	0.67
11:Y:4:LEU:CD2	11:Y:4:LEU:O	2.37	0.67
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.41	0.67
2:B:48:GLU:OE2	2:B:209:ARG:NH2	2.28	0.67
6:F:191:GLN:O	6:F:195:ILE:HG12	1.94	0.66
5:E:99:ASN:HB2	13:M:94:GLU:HG2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.77	0.66
11:Y:1:THR:HG22	11:Y:3:THR:HG23	1.78	0.66
11:K:99:THR:HG22	11:K:115:VAL:HB	1.78	0.65
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.77	0.65
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.77	0.65
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.77	0.65
16:Q:311:HOH:O	4:R:51:LEU:HD22	1.98	0.64
11:Y:209:ASN:N	11:Y:209:ASN:HD22	1.96	0.64
1:A:83:ARG:HE	7:G:114:ASN:HD21	1.46	0.63
8:H:215:GLU:HG3	9:I:197:ARG:HG2	1.81	0.63
5:S:3:ASN:O	5:S:4:ASN:CB	2.47	0.63
1:A:119:GLN:O	1:A:122:THR:HB	1.99	0.63
5:S:12:PHE:H	6:T:19:GLN:HE22	1.47	0.62
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.82	0.62
6:T:31:THR:HG21	6:T:47:GLU:O	2.00	0.61
8:V:172:ASN:HD22	8:V:192:THR:HA	1.64	0.61
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.65	0.61
13:M:35:ARG:HG2	16:M:313:HOH:O	1.99	0.61
1:O:3:ASP:OD2	1:O:5:TYR:N	2.30	0.61
1:A:83:ARG:HE	7:G:114:ASN:ND2	1.97	0.61
2:B:51:VAL:O	2:B:52:THR:CB	2.48	0.61
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.47	0.61
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.01	0.61
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.82	0.61
2:P:122:THR:HG22	3:Q:125:ARG:HH21	1.66	0.60
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.49	0.60
1:A:128:ARG:HH21	7:G:120:THR:CG2	2.14	0.60
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.66	0.60
6:T:31:THR:HG23	6:T:47:GLU:HB3	1.83	0.60
1:O:2:THR:HA	16:O:312:HOH:O	2.00	0.59
5:E:92:ASN:ND2	12:L:70:ASN:HD21	1.98	0.59
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.83	0.59
14:N:36:ARG:HH21	14:N:60:GLN:HE21	1.50	0.59
2:B:200:THR:HG22	2:B:202:SER:H	1.68	0.58
1:O:83:ARG:HE	7:U:114:ASN:ND2	2.01	0.58
1:O:128:ARG:HH21	7:U:120:THR:CG2	2.14	0.58
1:O:83:ARG:HH21	7:U:114:ASN:HD22	1.48	0.58
2:B:122:THR:HG22	3:C:125:ARG:HH21	1.69	0.58
1:O:5:TYR:HE2	7:U:124:TYR:HA	1.68	0.58
9:W:62:LEU:HD12	9:W:104:VAL:HG11	1.85	0.58
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:5:TYR:HD2	7:U:124:TYR:HB3	1.69	0.57
9:I:148:MET:SD	12:Z:148:PRO:HB2	2.44	0.57
11:Y:18:SER:HB2	11:Y:31:VAL:H	1.67	0.57
2:B:30:HIS:O	2:B:50:LYS:CE	2.43	0.57
3:C:160:GLN:HE21	3:C:161:THR:H	1.52	0.57
6:F:31:THR:HG21	6:F:47:GLU:O	2.04	0.57
14:N:136:GLY:HA2	14:b:161:GLN:NE2	2.17	0.57
4:D:71:SER:HB3	4:D:164:ILE:HD12	1.85	0.57
6:F:32:THR:HB	6:F:164:GLY:H	1.68	0.57
11:K:37:ILE:HB	11:K:41:LEU:HB3	1.86	0.57
13:a:129:TYR:HE1	13:a:144:THR:HG22	1.69	0.57
2:P:35:ILE:HD12	2:P:196:LEU:HG	1.87	0.57
8:V:6:VAL:HG11	8:V:154:LEU:HD23	1.85	0.57
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.87	0.56
1:O:187:ASP:O	1:O:191:ILE:HD12	2.05	0.56
6:F:74:TYR:HB3	6:F:132:THR:HG23	1.86	0.56
5:E:104:VAL:HG23	5:E:137:ASP:OD1	2.06	0.56
1:O:140:ASP:OD1	1:O:143:ASN:HB2	2.05	0.56
2:B:122:THR:CG2	3:C:125:ARG:HH21	2.18	0.56
8:H:165:ASN:HD22	13:a:156:ARG:HH11	1.53	0.56
13:a:209:LYS:HB3	13:a:212:LEU:HD11	1.87	0.56
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.87	0.56
8:V:153:LYS:HE3	16:V:412:HOH:O	2.06	0.56
14:b:48:SER:HB3	14:b:51:ASP:HB2	1.88	0.56
7:G:103:MET:HE3	7:G:108:LEU:HD13	1.88	0.56
12:L:38:ARG:HD3	12:L:200:ASP:OD1	2.07	0.55
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.54	0.55
5:S:2:ARG:O	5:S:5:TYR:N	2.30	0.55
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.42	0.55
11:K:33:LYS:HA	11:K:45:MET:HE2	1.88	0.55
1:O:119:GLN:O	1:O:122:THR:HB	2.07	0.55
3:C:201:VAL:HG11	3:C:207:ASN:HB3	1.87	0.55
6:T:33:SER:HB3	6:T:46:VAL:HG23	1.89	0.55
11:Y:1:THR:CG2	11:Y:3:THR:HG23	2.37	0.55
11:K:49:ALA:HB2	15:K:301:OV2:H19	1.89	0.54
14:N:67:THR:HA	14:N:71:GLY:O	2.08	0.54
12:Z:90:ALA:HA	12:Z:125:PHE:HZ	1.72	0.54
6:F:66:VAL:HG22	6:F:89:ARG:HG3	1.90	0.54
6:T:32:THR:HB	6:T:164:GLY:H	1.73	0.54
5:S:6:ASP:O	5:S:7:GLY:C	2.51	0.54
2:B:12:PHE:H	3:C:17:GLN:HE22	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:224:SER:O	3:C:228:ASN:HB2	2.08	0.54
11:K:38:ASN:HB2	11:K:39:PRO:HD2	1.90	0.54
4:R:1:ASP:O	4:R:2:ARG:HB2	2.07	0.54
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.88	0.54
8:H:148:LYS:O	8:H:152:ILE:HG12	2.08	0.54
1:A:83:ARG:HH21	7:G:114:ASN:HD22	1.56	0.54
13:M:27:LEU:HB2	13:M:192:SER:HB2	1.90	0.54
13:M:162:GLU:O	13:M:165:ILE:HG12	2.08	0.54
8:V:147:THR:C	8:V:149:GLU:H	2.15	0.54
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.21	0.54
9:I:22:ILE:HG12	9:I:42:ILE:HD12	1.90	0.53
10:J:104:ILE:HB	10:J:117:TYR:HB2	1.89	0.53
14:N:44:CYS:HB2	14:N:98:ILE:HB	1.89	0.53
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.90	0.53
1:O:42:GLY:HA3	1:O:185:LEU:HD13	1.89	0.53
7:G:117:GLN:O	7:G:120:THR:HB	2.09	0.53
5:S:45:LEU:HB2	5:S:213:ALA:HB3	1.90	0.53
6:T:91:GLU:HG3	6:T:111:ARG:HH11	1.72	0.53
8:V:15:ALA:HA	8:V:174:ASP:O	2.09	0.53
10:X:119:ILE:HG12	10:X:125:LYS:HG3	1.89	0.53
13:a:53:ILE:HG12	13:a:114:ILE:HG12	1.89	0.53
3:C:29:THR:HB	3:C:45:GLU:HG3	1.90	0.53
2:B:119:GLN:O	2:B:122:THR:HB	2.09	0.53
5:S:1:PHE:CD2	5:S:2:ARG:CD	2.91	0.53
2:B:50:LYS:O	2:B:52:THR:CG2	2.53	0.53
7:U:103:MET:HE3	7:U:108:LEU:HD13	1.90	0.53
8:V:78:SER:O	8:V:82:MET:HG3	2.09	0.53
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.44	0.52
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.91	0.52
11:Y:209:ASN:HD22	11:Y:209:ASN:H	1.57	0.52
14:N:161:GLN:NE2	14:b:136:GLY:HA2	2.18	0.52
12:Z:4:PRO:O	13:a:104:ARG:NH1	2.39	0.52
3:C:68:HIS:CD2	3:C:69:VAL:HG23	2.44	0.52
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.90	0.52
11:K:3:THR:HB	11:K:16:VAL:HG12	1.92	0.52
8:V:170:GLY:O	8:V:171:SER:HB2	2.10	0.52
7:G:195:GLU:HG3	7:G:235:ARG:HG3	1.92	0.52
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.92	0.52
8:V:166:ASP:HB3	8:V:169:SER:HB2	1.91	0.52
9:W:106:PRO:HD2	9:W:123:PHE:HB2	1.92	0.52
6:F:48:LYS:HB2	6:F:209:GLU:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:201:LYS:HG3	11:K:206:SER:O	2.10	0.51
5:S:42:HIS:HB2	5:S:188:LEU:HD12	1.91	0.51
5:S:1:PHE:CD2	5:S:2:ARG:HD2	2.45	0.51
8:V:3:ILE:HG22	8:V:16:ALA:HB2	1.92	0.51
12:Z:109:THR:HG23	12:Z:125:PHE:HB2	1.91	0.51
6:F:175:LEU:HD21	6:F:191:GLN:NE2	2.25	0.51
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.91	0.51
11:K:99:THR:CG2	11:K:115:VAL:HB	2.41	0.51
2:P:180:LYS:O	2:P:183:MET:HG3	2.11	0.51
10:J:174:MET:CE	10:X:174:MET:HE3	2.40	0.51
12:L:18:GLU:O	12:L:119:LYS:HA	2.10	0.51
10:X:33:ASP:OD2	10:X:35:THR:HG22	2.11	0.51
1:A:26:THR:O	1:A:30:GLN:HG2	2.10	0.51
6:F:31:THR:HG23	6:F:47:GLU:HB3	1.92	0.51
6:F:175:LEU:HD21	6:F:191:GLN:HE21	1.75	0.51
14:N:38:HIS:HD2	16:N:404:HOH:O	1.93	0.51
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.09	0.51
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.41	0.51
3:C:160:GLN:NE2	3:C:161:THR:H	2.08	0.51
6:F:123:ASN:HD22	6:F:124:SER:N	2.09	0.51
5:S:44:VAL:HG21	5:S:188:LEU:HB3	1.92	0.51
2:B:69:ASN:ND2	2:B:70:ASP:H	2.09	0.50
14:N:38:HIS:CD2	16:N:404:HOH:O	2.64	0.50
7:U:117:GLN:O	7:U:120:THR:HB	2.10	0.50
5:S:1:PHE:O	5:S:2:ARG:C	2.53	0.50
2:B:52:THR:OG1	2:B:53:SER:N	2.40	0.50
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.92	0.50
4:R:176:LEU:HD22	5:S:55:LEU:HD13	1.94	0.50
5:E:12:PHE:H	6:F:19:GLN:HE22	1.58	0.50
8:H:49:ALA:HB2	15:H:301:OV2:H19	1.94	0.50
9:I:189:ILE:HG23	9:I:194:VAL:HG22	1.91	0.50
11:K:158:LYS:HD3	11:K:196:LEU:HD11	1.93	0.50
12:L:195:HIS:HD2	12:L:197:GLN:H	1.58	0.50
9:W:62:LEU:CD1	9:W:104:VAL:HG11	2.42	0.50
12:L:3:ASN:ND2	12:L:5:TYR:H	2.10	0.50
5:S:1:PHE:O	5:S:3:ASN:O	2.30	0.50
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	1.92	0.50
8:H:172:ASN:HD22	8:H:192:THR:HA	1.75	0.50
2:B:35:ILE:HD12	2:B:196:LEU:HG	1.92	0.50
4:R:191:LEU:O	4:R:195:ILE:HD12	2.12	0.50
12:Z:207:VAL:HG22	12:Z:212:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:71:GLY:HA3	6:F:224:HIS:CD2	2.47	0.50
14:N:4:MET:HB3	14:N:126:ILE:HG22	1.93	0.49
3:Q:146:TYR:CE1	3:Q:156:SER:HB3	2.47	0.49
1:A:187:ASP:O	1:A:191:ILE:HD12	2.12	0.49
2:B:49:ARG:HH11	2:B:49:ARG:CG	2.14	0.49
2:B:65:LEU:HD22	2:B:211:GLU:HB3	1.94	0.49
12:Z:93:ILE:HA	12:Z:96:LEU:HD12	1.93	0.49
11:K:1:THR:HG22	11:K:3:THR:HG23	1.94	0.49
5:S:1:PHE:C	5:S:3:ASN:N	2.66	0.49
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.47	0.49
13:a:15:LYS:HB3	13:a:20:VAL:HG12	1.94	0.49
4:D:73:LEU:HD12	4:D:131:GLY:HA3	1.94	0.49
1:O:110:LEU:O	1:O:114:VAL:HG23	2.12	0.49
2:P:218:GLY:C	2:P:220:ASN:H	2.20	0.49
2:B:53:SER:OG	2:B:54:THR:N	2.46	0.49
5:S:35:VAL:HG23	5:S:196:ILE:HD12	1.93	0.49
7:U:149:ASP:HB2	7:U:150:PRO:HD2	1.95	0.49
13:M:139:SER:HB3	13:M:141:THR:O	2.13	0.49
14:N:2:SER:OG	14:N:169:SER:OG	2.18	0.49
6:T:50:ILE:HD11	6:T:209:GLU:HB2	1.94	0.49
15:V:301:OV2:H39	9:W:124:ASP:HB3	1.95	0.49
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.94	0.48
3:C:35:LYS:HG2	3:C:158:SER:O	2.13	0.48
8:H:48:THR:HB	8:H:51:ASP:HB2	1.95	0.48
12:Z:18:GLU:O	12:Z:119:LYS:HA	2.13	0.48
2:B:93:HIS:CD2	2:B:113:ARG:HG2	2.49	0.48
2:P:146:GLN:HG2	3:Q:57:ILE:HG21	1.95	0.48
10:X:46:PHE:HD1	10:X:53:THR:HG1	1.61	0.48
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.95	0.48
5:E:193:VAL:HG21	5:E:232:TYR:HB3	1.96	0.48
11:K:115:VAL:HA	11:K:120:THR:O	2.14	0.48
13:M:14:MET:HG2	13:M:177:ILE:HD11	1.95	0.48
7:U:78:ILE:N	7:U:79:PRO:HD2	2.29	0.48
9:W:108:VAL:HG23	9:W:123:PHE:HE2	1.78	0.48
8:H:1:THR:HG22	8:H:3:ILE:HG23	1.96	0.48
13:M:179:ASN:HD22	13:M:182:ARG:NH1	2.12	0.48
6:F:118:ALA:HA	6:F:121:LEU:HD12	1.96	0.48
1:O:2:THR:O	1:O:2:THR:OG1	2.30	0.48
3:Q:206:LYS:HG3	3:Q:207:ASN:N	2.29	0.48
10:J:130:TYR:HB2	10:J:144:LEU:HD13	1.96	0.48
12:L:177:VAL:O	12:L:181:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.44	0.48
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.78	0.48
1:O:149:GLN:O	1:O:156:TYR:HA	2.13	0.47
4:R:73:LEU:HD12	4:R:131:GLY:HA3	1.95	0.47
6:T:123:ASN:HD22	6:T:124:SER:N	2.12	0.47
7:U:73:VAL:HG12	7:U:133:THR:HB	1.95	0.47
9:W:185:VAL:HG21	9:W:196:LYS:HE3	1.96	0.47
3:C:204:GLY:CA	3:C:207:ASN:HB2	2.42	0.47
5:E:231:LYS:H	5:E:231:LYS:HD2	1.79	0.47
6:T:83:HIS:HD2	6:T:128:PHE:HE2	1.63	0.47
7:U:83:ASN:C	7:U:83:ASN:HD22	2.22	0.47
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.96	0.47
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.95	0.47
8:V:147:THR:O	8:V:149:GLU:N	2.46	0.47
8:H:1:THR:HG23	8:H:33:LYS:HD3	1.97	0.47
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.49	0.47
4:R:60:VAL:HG21	4:R:81:ILE:HG13	1.96	0.47
10:X:18:SER:HB2	10:X:176:PHE:HB2	1.95	0.47
8:V:49:ALA:HA	15:V:301:OV2:H22	1.96	0.47
13:a:127:LEU:HG	13:a:142:LEU:HD12	1.96	0.47
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.50	0.47
6:F:14:ASP:OD2	6:F:14:ASP:N	2.46	0.47
11:K:33:LYS:HE2	15:K:301:OV2:H16	1.97	0.47
13:M:3:GLN:O	13:M:5:ILE:HD12	2.15	0.47
5:S:2:ARG:CG	5:S:2:ARG:NH1	2.40	0.47
6:F:233:GLN:HA	6:F:236:ILE:HD12	1.96	0.47
11:K:4:LEU:HD13	11:K:161:ILE:HD11	1.97	0.47
6:F:43:VAL:HG11	6:F:189:VAL:HA	1.97	0.47
13:M:21:ILE:HG12	13:M:199:ILE:HG12	1.96	0.47
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.63	0.47
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.45	0.47
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.78	0.47
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.96	0.47
2:P:162:ILE:HG13	2:P:163:SER:N	2.29	0.47
7:U:31:ILE:HG23	7:U:47:GLN:HB2	1.96	0.46
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.95	0.46
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.01	0.46
3:Q:30:CYS:H	3:Q:45:GLU:HG2	1.80	0.46
8:V:172:ASN:ND2	8:V:192:THR:HA	2.27	0.46
2:B:82:ASP:CG	2:B:128:ARG:HH22	2.23	0.46
2:P:69:ASN:HB3	2:P:72:ILE:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:62:ILE:HD12	5:S:211:SER:HB3	1.97	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.96	0.46
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.97	0.46
3:Q:206:LYS:C	3:Q:208:ILE:H	2.23	0.46
8:H:49:ALA:HA	15:H:301:OV2:H21	1.97	0.46
12:L:13:LEU:HD11	12:L:150:LEU:CD2	2.44	0.46
7:U:108:LEU:O	7:U:112:MET:HG2	2.15	0.46
14:b:112:THR:HG22	14:b:120:HIS:HB2	1.97	0.46
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.13	0.46
12:Z:124:SER:CB	12:Z:137:ARG:HG2	2.45	0.46
14:b:38:HIS:O	14:b:39:ASP:C	2.59	0.46
11:K:4:LEU:HD22	11:K:4:LEU:O	2.16	0.46
13:a:129:TYR:CE1	13:a:144:THR:HG22	2.50	0.46
2:B:51:VAL:O	2:B:52:THR:OG1	2.30	0.46
2:B:149:THR:HG22	2:B:159:TRP:HE1	1.80	0.46
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.98	0.46
4:D:89:VAL:HG21	11:K:65:LEU:HD13	1.98	0.46
4:D:113:LEU:HB2	16:D:301:HOH:O	2.16	0.46
9:I:204:ASP:HB3	11:Y:193:VAL:HG11	1.98	0.46
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.98	0.46
5:S:1:PHE:HD2	5:S:2:ARG:HE	1.63	0.46
2:B:53:SER:OG	2:B:55:LEU:N	2.50	0.45
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.46	0.45
1:A:226:GLY:HA3	8:H:186:TYR:HB3	1.98	0.45
11:K:25:TRP:CH2	12:L:144:SER:HA	2.51	0.45
11:K:162:LEU:HD13	11:K:196:LEU:HD23	1.99	0.45
12:L:11:THR:HG21	12:L:142:ALA:HB3	1.98	0.45
13:M:25:ASP:HA	13:M:195:PHE:HA	1.97	0.45
8:V:49:ALA:HA	15:V:301:OV2:C27	2.47	0.45
13:a:51:VAL:HG22	13:a:116:VAL:HG22	1.98	0.45
6:F:105:ILE:HB	6:F:106:PRO:HD3	1.98	0.45
7:U:83:ASN:C	7:U:83:ASN:ND2	2.74	0.45
2:B:162:ILE:HG13	2:B:163:SER:N	2.31	0.45
6:F:38:CYS:SG	6:F:185:ALA:HA	2.57	0.45
13:M:119:VAL:HG12	13:M:120:GLN:O	2.16	0.45
2:P:119:GLN:O	2:P:122:THR:HB	2.15	0.45
13:a:96:LEU:O	13:a:100:MET:HG2	2.16	0.45
4:R:29:ALA:HB3	4:R:164:ILE:HG13	1.99	0.45
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.99	0.45
10:J:173:PRO:HB3	10:X:22:THR:HG21	1.97	0.45
8:V:20:SER:HB3	8:V:28:ASP:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:120:ILE:HD12	9:I:136:ILE:HG12	1.98	0.45
11:K:81:LYS:HA	11:K:84:SER:HB3	1.99	0.45
3:C:214:LYS:HB2	3:C:218:ASP:HB3	1.98	0.44
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.13	0.44
3:Q:179:ARG:HH22	4:R:52:GLU:HA	1.82	0.44
9:I:141:ALA:HB2	9:I:177:ASP:HB2	1.99	0.44
5:S:1:PHE:CD2	5:S:2:ARG:NE	2.84	0.44
11:Y:20:ALA:HB3	11:Y:28:SER:HB3	1.99	0.44
11:Y:139:VAL:HG21	11:Y:163:ALA:CB	2.47	0.44
5:E:49:LYS:HB3	5:E:58:TYR:HB3	1.99	0.44
6:T:146:MET:HB3	6:T:156:TYR:CE1	2.53	0.44
7:U:29:THR:HB	7:U:31:ILE:HD12	1.99	0.44
13:a:129:TYR:O	13:a:136:THR:HA	2.16	0.44
3:C:11:PRO:HA	4:D:18:TYR:CE1	2.52	0.44
4:D:67:GLY:HA3	4:D:220:PHE:CE2	2.52	0.44
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.53	0.44
13:M:106:LYS:NZ	16:M:307:HOH:O	2.50	0.44
8:V:48:THR:HB	8:V:51:ASP:HB2	1.99	0.44
5:E:205:LEU:HD12	5:E:210:LEU:HD13	2.00	0.44
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.99	0.44
11:Y:107:LYS:H	11:Y:107:LYS:HD2	1.83	0.44
5:E:81:ARG:HH11	5:E:81:ARG:CG	2.24	0.44
16:I:302:HOH:O	11:Y:28:SER:HA	2.16	0.44
11:K:163:ALA:HB1	10:X:142:SER:HB2	2.00	0.44
11:Y:2:THR:HG21	11:Y:164:ALA:CB	2.48	0.44
11:K:4:LEU:HD11	11:K:161:ILE:HG12	2.00	0.44
5:S:127:TYR:O	5:S:148:PRO:HB3	2.16	0.44
8:V:148:LYS:HE3	8:V:177:VAL:HG11	1.99	0.44
6:T:39:ASN:HD22	6:T:39:ASN:C	2.25	0.44
6:T:126:ARG:HG2	6:T:127:PRO:O	2.18	0.44
1:A:174:PHE:O	1:A:178:ARG:HG2	2.17	0.43
5:E:49:LYS:HE2	5:E:211:SER:HB2	1.99	0.43
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.53	0.43
1:A:66:LEU:HD12	1:A:235:PHE:CD2	2.53	0.43
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.31	0.43
4:D:51:LEU:HD11	4:D:56:ILE:HD11	1.99	0.43
6:F:33:SER:HB3	6:F:46:VAL:HG23	2.00	0.43
6:F:62:LYS:HA	16:F:302:HOH:O	2.18	0.43
12:L:98:TYR:C	12:L:100:LYS:H	2.27	0.43
13:a:27:LEU:HB2	13:a:192:SER:HB2	2.00	0.43
7:G:73:VAL:CG1	7:G:133:THR:HB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.99	0.43
7:U:195:GLU:HG3	7:U:235:ARG:HG3	2.01	0.43
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.01	0.43
3:Q:65:ILE:HG21	3:Q:107:LEU:HD11	2.00	0.43
13:a:184:LEU:O	13:a:188:ASP:HB3	2.19	0.43
5:E:112:CYS:SG	6:F:82:ARG:HD3	2.58	0.43
10:J:172:MET:HE2	10:J:172:MET:HB3	1.93	0.43
7:U:34:LEU:HD23	7:U:201:MET:HE3	2.01	0.43
1:A:4:ARG:HD2	5:E:122:TYR:CE2	2.54	0.43
4:D:159:TYR:CE2	4:D:162:LYS:HD3	2.54	0.43
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.48	0.43
9:W:41:LYS:O	9:W:51:GLY:HA2	2.19	0.43
6:F:114:GLN:HE22	7:G:82:ARG:C	2.26	0.43
10:J:152:MET:HE2	10:J:156:GLU:HB3	2.01	0.43
5:S:155:LEU:HD13	5:S:158:THR:HB	2.01	0.43
8:V:215:GLU:HG3	9:W:197:ARG:HG2	2.00	0.43
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.46	0.43
5:E:205:LEU:HA	5:E:209:ASN:HD22	1.84	0.43
11:K:114:TYR:O	11:K:121:ARG:HA	2.19	0.43
13:M:95:TYR:O	13:M:99:VAL:HG23	2.19	0.43
1:O:5:TYR:CD2	7:U:124:TYR:HB3	2.52	0.43
5:E:227:GLU:CD	5:E:227:GLU:H	2.27	0.42
3:Q:83:LEU:HD22	3:Q:111:VAL:HG13	2.01	0.42
11:Y:33:LYS:HE2	15:Y:301:OV2:H16	2.01	0.42
4:D:176:LEU:HD22	5:E:55:LEU:HD13	2.01	0.42
5:E:131:LEU:HB2	5:E:146:PHE:HB3	2.01	0.42
5:E:178:PHE:HA	5:E:181:ILE:HG12	2.00	0.42
5:E:226:GLY:O	5:E:229:VAL:HG22	2.19	0.42
2:P:65:LEU:HD22	2:P:211:GLU:HB3	2.02	0.42
3:Q:77:ASN:HD22	3:Q:77:ASN:N	2.17	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.55	0.42
1:A:43:VAL:HG23	1:A:145:PHE:HB3	2.00	0.42
2:B:218:GLY:C	2:B:220:ASN:H	2.27	0.42
12:L:137:ARG:HH12	9:W:176:ARG:HH12	1.66	0.42
4:R:68:CYS:SG	4:R:134:LEU:HD22	2.60	0.42
10:X:1:MET:HG2	10:X:2:ASP:N	2.34	0.42
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	2.00	0.42
2:B:172:GLN:HG2	3:C:50:LEU:HD12	2.02	0.42
3:C:160:GLN:HA	3:C:160:GLN:NE2	2.33	0.42
11:K:107:LYS:H	11:K:107:LYS:HD2	1.84	0.42
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:66:LEU:HD12	1:O:235:PHE:CD2	2.55	0.42
4:R:105:THR:HG23	4:R:136:ILE:HD12	2.02	0.42
11:Y:78:ALA:O	11:Y:82:ILE:HG12	2.20	0.42
6:F:71:GLY:HA3	6:F:224:HIS:NE2	2.34	0.42
12:L:43:VAL:HG22	12:L:53:SER:HB2	2.00	0.42
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.01	0.42
14:N:146:MET:HE2	14:N:150:GLU:HB3	2.00	0.42
14:N:190:PRO:HA	14:N:193:TYR:CE2	2.55	0.42
3:Q:157:TRP:CZ3	4:R:48:SER:HB3	2.54	0.42
12:Z:100:LYS:O	12:Z:104:PRO:HA	2.19	0.42
8:H:35:HIS:CB	8:H:56:THR:HG21	2.47	0.42
2:P:215:ILE:HG12	2:P:226:GLN:HG2	2.01	0.42
10:X:53:THR:HG23	10:X:54:VAL:N	2.35	0.42
12:Z:28:ARG:NE	12:Z:200:ASP:OD2	2.52	0.42
6:T:78:ILE:HB	6:T:79:PRO:HD3	2.01	0.42
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.42
7:G:73:VAL:HG12	7:G:133:THR:HB	2.01	0.42
11:K:45:MET:HB3	11:K:52:CYS:HB3	2.02	0.42
11:Y:18:SER:HA	11:Y:33:LYS:HE3	2.02	0.42
4:D:6:THR:HG23	5:E:20:GLN:NE2	2.34	0.42
3:Q:201:VAL:CG1	3:Q:207:ASN:HB3	2.50	0.42
8:V:171:SER:O	8:V:193:PRO:HD2	2.20	0.42
15:V:301:OV2:H27	15:V:301:OV2:H13	1.85	0.42
9:W:65:MET:O	9:W:68:TYR:HB3	2.20	0.42
13:a:17:ASP:OD1	13:a:18:ASN:N	2.53	0.42
14:b:146:MET:HE2	14:b:150:GLU:HB3	2.01	0.42
13:M:48:ASN:N	13:M:48:ASN:HD22	2.17	0.41
14:N:133:PHE:HA	14:b:132:THR:O	2.19	0.41
3:C:147:GLN:HE21	3:C:160:GLN:HG2	1.85	0.41
11:K:148:LEU:HD23	11:K:153:ALA:HA	2.02	0.41
12:L:3:ASN:C	12:L:3:ASN:HD22	2.26	0.41
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.67	0.41
11:Y:175:VAL:HB	11:Y:191:HIS:HB2	2.01	0.41
2:B:69:ASN:HB3	2:B:72:ILE:H	1.84	0.41
6:F:53:LYS:H	6:F:53:LYS:HG2	1.63	0.41
8:H:1:THR:CG2	8:H:3:ILE:HG23	2.50	0.41
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.03	0.41
13:a:4:PRO:HD3	13:a:111:TRP:CE2	2.55	0.41
2:B:63:GLU:HG3	2:B:64:LYS:HG3	2.02	0.41
3:C:70:VAL:HG13	3:C:219:ILE:HD13	2.02	0.41
4:D:5:SER:HB2	5:E:125:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.02	0.41
3:Q:29:THR:HB	3:Q:45:GLU:HG3	2.03	0.41
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.19	0.41
1:A:115:ALA:HB1	1:A:154:GLY:O	2.20	0.41
9:I:15:THR:HG22	9:I:20:VAL:HG12	2.02	0.41
10:J:118:GLN:HG2	10:J:133:HIS:CE1	2.54	0.41
3:Q:45:GLU:HA	3:Q:207:ASN:O	2.21	0.41
5:S:1:PHE:C	5:S:1:PHE:CD1	2.96	0.41
6:T:36:ILE:HD13	6:T:192:ALA:HB2	2.01	0.41
8:V:104:ASP:C	8:V:106:THR:H	2.28	0.41
8:V:152:ILE:HD11	8:V:177:VAL:HG21	2.01	0.41
4:D:60:VAL:HG23	4:D:68:CYS:HB3	2.03	0.41
6:F:122:TYR:HB2	6:F:125:VAL:HG22	2.03	0.41
10:J:103:LEU:CD2	10:J:118:GLN:HG3	2.51	0.41
11:K:4:LEU:HD22	11:K:4:LEU:C	2.46	0.41
12:L:100:LYS:HE2	12:L:105:TYR:CE2	2.56	0.41
8:V:191:LEU:C	8:V:193:PRO:HD3	2.45	0.41
3:C:158:SER:HB3	3:C:177:TYR:CE1	2.55	0.41
6:F:34:ILE:HD11	6:F:45:ALA:HB3	2.02	0.41
11:K:47:GLY:O	15:K:301:OV2:H15	2.20	0.41
13:M:230:THR:HG22	8:V:77:VAL:HB	2.03	0.41
4:R:38:VAL:HG23	4:R:145:TYR:HB3	2.03	0.41
1:A:38:LYS:HG3	1:A:43:VAL:HG22	2.03	0.41
10:J:103:LEU:HD21	10:J:118:GLN:HG3	2.03	0.41
8:V:113:ILE:HG12	8:V:119:THR:HG22	2.02	0.41
2:B:180:LYS:O	2:B:183:MET:HG3	2.20	0.41
6:F:74:TYR:CE1	6:F:81:GLY:HA3	2.56	0.41
8:H:18:THR:HB	8:H:30:ASN:HA	2.03	0.41
12:L:50:ILE:HG12	12:L:86:ILE:HD12	2.03	0.41
13:M:48:ASN:HD22	13:M:48:ASN:H	1.67	0.41
14:N:175:MET:HB2	14:N:186:LEU:HB2	2.02	0.41
6:T:123:ASN:HD22	6:T:123:ASN:C	2.29	0.41
8:V:3:ILE:HD11	8:V:127:LEU:HB2	2.03	0.41
8:V:168:GLY:O	15:V:301:OV2:H25	2.21	0.41
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.02	0.41
13:a:48:ASN:H	13:a:48:ASN:HD22	1.67	0.41
14:b:168:SER:HB3	15:b:301:OV2:H28	2.03	0.41
4:D:104:LEU:HD13	4:D:104:LEU:C	2.46	0.41
5:E:12:PHE:HB2	6:F:19:GLN:HE22	1.86	0.41
9:I:189:ILE:HD13	9:I:194:VAL:HG13	2.03	0.41
13:M:26:ASN:HA	13:M:39:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.02	0.41
5:S:6:ASP:HB2	5:S:23:TYR:HE2	1.86	0.41
12:Z:1:GLN:HG2	13:a:1:THR:HG21	2.03	0.41
14:b:49:ALA:HB2	15:b:301:OV2:H19	2.03	0.41
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.56	0.40
3:Q:235:GLU:HA	3:Q:238:LYS:HE2	2.03	0.40
6:T:8:ASN:HB3	6:T:123:ASN:HA	2.03	0.40
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.40
9:W:14:MET:HB2	9:W:166:ILE:HD12	2.03	0.40
6:F:50:ILE:HD11	6:F:209:GLU:HB2	2.03	0.40
6:F:91:GLU:HG3	6:F:111:ARG:HH11	1.85	0.40
8:H:113:ILE:HG12	8:H:119:THR:HG22	2.03	0.40
13:M:83:ALA:O	13:M:84:GLU:HB2	2.22	0.40
14:N:55:ILE:HD11	14:N:93:LEU:HD13	2.02	0.40
4:R:227:LYS:O	4:R:231:LEU:HD12	2.21	0.40
13:a:179:ASN:HD22	13:a:182:ARG:HH11	1.67	0.40
3:C:186:VAL:O	3:C:190:VAL:HG23	2.21	0.40
4:R:36:GLU:HB2	4:R:185:LEU:HB2	2.03	0.40
9:W:137:VAL:HG11	9:W:145:LEU:HB3	2.04	0.40
2:B:49:ARG:HG2	2:B:63:GLU:OE2	2.21	0.40
5:S:8:ASP:OD1	5:S:8:ASP:C	2.62	0.40
1:A:82:TYR:O	1:A:86:VAL:HG23	2.21	0.40
7:G:119:TYR:CE1	7:G:125:MET:HE2	2.57	0.40
5:S:206:THR:H	5:S:209:ASN:HD22	1.70	0.40
13:a:139:SER:HB3	13:a:141:THR:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	247/249 (99%)	240 (97%)	5 (2%)	2 (1%)	16 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	247/249 (99%)	240 (97%)	7 (3%)	0	100	100
2	B	242/244 (99%)	228 (94%)	12 (5%)	2 (1%)	16	44
2	P	242/244 (99%)	228 (94%)	12 (5%)	2 (1%)	16	44
3	C	239/241 (99%)	231 (97%)	7 (3%)	1 (0%)	30	60
3	Q	239/241 (99%)	230 (96%)	7 (3%)	2 (1%)	16	44
4	D	240/242 (99%)	233 (97%)	6 (2%)	1 (0%)	30	60
4	R	240/242 (99%)	222 (92%)	17 (7%)	1 (0%)	30	60
5	E	231/233 (99%)	219 (95%)	12 (5%)	0	100	100
5	S	231/233 (99%)	217 (94%)	13 (6%)	1 (0%)	30	60
6	F	242/244 (99%)	229 (95%)	10 (4%)	3 (1%)	10	34
6	T	242/244 (99%)	230 (95%)	11 (4%)	1 (0%)	30	60
7	G	241/243 (99%)	231 (96%)	9 (4%)	1 (0%)	30	60
7	U	241/243 (99%)	236 (98%)	4 (2%)	1 (0%)	30	60
8	H	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
8	V	220/222 (99%)	207 (94%)	9 (4%)	4 (2%)	6	23
9	I	202/204 (99%)	190 (94%)	11 (5%)	1 (0%)	24	55
9	W	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
10	J	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	24	55
10	X	196/198 (99%)	186 (95%)	10 (5%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
12	L	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
12	Z	220/222 (99%)	209 (95%)	11 (5%)	0	100	100
13	M	231/233 (99%)	219 (95%)	10 (4%)	2 (1%)	14	41
13	a	231/233 (99%)	225 (97%)	5 (2%)	1 (0%)	30	60
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	182 (94%)	12 (6%)	0	100	100
All	All	6310/6366 (99%)	6037 (96%)	246 (4%)	27 (0%)	30	60

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	123	GLU

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Mol	Chain	Res	Type
5	S	7	GLY
8	V	148	LYS
4	R	2	ARG
8	V	171	SER
2	B	52	THR
3	C	203	THR
7	G	2	GLY
9	I	39	PHE
13	M	83	ALA
2	P	50	LYS
2	P	219	ALA
6	T	97	LYS
8	V	221	CYS
1	A	3	ASP
1	A	166	LYS
6	F	67	ASP
6	F	204	LYS
3	Q	206	LYS
7	U	2	GLY
2	B	219	ALA
3	Q	207	ASN
13	M	229	GLY
8	V	105	PRO
6	F	229	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	208/208 (100%)	200 (96%)	8 (4%)	29	64
1	O	208/208 (100%)	197 (95%)	11 (5%)	20	52
2	B	203/203 (100%)	187 (92%)	16 (8%)	11	35
2	P	203/203 (100%)	189 (93%)	14 (7%)	14	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	213/213 (100%)	193 (91%)	20 (9%)	8	27
3	Q	213/213 (100%)	199 (93%)	14 (7%)	15	43
4	D	198/198 (100%)	189 (96%)	9 (4%)	24	58
4	R	198/198 (100%)	185 (93%)	13 (7%)	15	43
5	E	192/192 (100%)	180 (94%)	12 (6%)	16	45
5	S	192/192 (100%)	179 (93%)	13 (7%)	14	42
6	F	201/201 (100%)	184 (92%)	17 (8%)	10	31
6	T	201/201 (100%)	186 (92%)	15 (8%)	12	37
7	G	207/207 (100%)	197 (95%)	10 (5%)	23	56
7	U	207/207 (100%)	196 (95%)	11 (5%)	20	52
8	H	181/181 (100%)	177 (98%)	4 (2%)	45	78
8	V	181/181 (100%)	172 (95%)	9 (5%)	22	54
9	I	172/172 (100%)	167 (97%)	5 (3%)	37	73
9	W	172/172 (100%)	163 (95%)	9 (5%)	21	53
10	J	175/175 (100%)	166 (95%)	9 (5%)	21	54
10	X	175/175 (100%)	167 (95%)	8 (5%)	24	58
11	K	169/169 (100%)	159 (94%)	10 (6%)	18	48
11	Y	169/169 (100%)	162 (96%)	7 (4%)	27	62
12	L	185/185 (100%)	182 (98%)	3 (2%)	55	83
12	Z	185/185 (100%)	177 (96%)	8 (4%)	26	60
13	M	199/199 (100%)	188 (94%)	11 (6%)	19	51
13	a	199/199 (100%)	190 (96%)	9 (4%)	24	58
14	N	162/162 (100%)	157 (97%)	5 (3%)	35	70
14	b	162/162 (100%)	155 (96%)	7 (4%)	26	60
All	All	5330/5330 (100%)	5043 (95%)	287 (5%)	20	51

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	122	THR
1	A	157	PHE
1	A	178	ARG
1	A	184	GLU

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Mol	Chain	Res	Type
1	A	197	LYS
1	A	209	ILE
1	A	250	LEU
2	B	49	ARG
2	B	51	VAL
2	B	52	THR
2	B	53	SER
2	B	54	THR
2	B	55	LEU
2	B	56	LEU
2	B	58	GLN
2	B	60	THR
2	B	122	THR
2	B	149	THR
2	B	184	LYS
2	B	191	LEU
2	B	212	PHE
2	B	230	LYS
2	B	237	ILE
3	C	4	ARG
3	C	15	ILE
3	C	19	GLU
3	C	29	THR
3	C	49	THR
3	C	51	LYS
3	C	55	THR
3	C	61	LYS
3	C	102	VAL
3	C	129	VAL
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	171	GLU
3	C	185	THR
3	C	201	VAL
3	C	203	THR
3	C	213	VAL
3	C	228	ASN
3	C	241	GLN
4	D	5	SER
4	D	20	LEU
4	D	44	LYS

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Mol	Chain	Res	Type
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	195	ILE
4	D	214	ILE
4	D	235	LEU
5	E	9	THR
5	E	10	VAL
5	E	29	LYS
5	E	71	LEU
5	E	95	SER
5	E	104	VAL
5	E	133	ILE
5	E	188	LEU
5	E	198	GLN
5	E	205	LEU
5	E	227	GLU
5	E	231	LYS
6	F	14	ASP
6	F	31	THR
6	F	34	ILE
6	F	39	ASN
6	F	51	THR
6	F	65	VAL
6	F	68	ARG
6	F	123	ASN
6	F	130	VAL
6	F	132	THR
6	F	166	GLN
6	F	172	LEU
6	F	181	GLU
6	F	186	ARG
6	F	203	ASN
6	F	228	LYS
6	F	243	ILE
7	G	83	ASN
7	G	115	LEU
7	G	120	THR
7	G	162	THR
7	G	166	GLN
7	G	182	ILE
7	G	201	MET

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Mol	Chain	Res	Type
7	G	207	THR
7	G	221	LYS
7	G	235	ARG
8	H	25	ILE
8	H	34	LEU
8	H	56	THR
8	H	68	LEU
9	I	1	SER
9	I	37	ASN
9	I	81	ILE
9	I	171	LEU
9	I	182	TRP
10	J	7	ILE
10	J	35	THR
10	J	36	ARG
10	J	92	ILE
10	J	110	LYS
10	J	126	VAL
10	J	127	GLU
10	J	136	SER
10	J	143	LEU
11	K	4	LEU
11	K	65	LEU
11	K	69	ARG
11	K	73	ARG
11	K	84	SER
11	K	87	VAL
11	K	99	THR
11	K	107	LYS
11	K	181	THR
11	K	195	GLU
12	L	42	LYS
12	L	109	THR
12	L	172	LEU
13	M	3	GLN
13	M	5	ILE
13	M	48	ASN
13	M	49	THR
13	M	69	ASP
13	M	70	LEU
13	M	104	ARG
13	M	127	LEU

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Mol	Chain	Res	Type
13	M	139	SER
13	M	161	ARG
13	M	170	VAL
14	N	2	SER
14	N	80	SER
14	N	83	LYS
14	N	105	LYS
14	N	119	VAL
1	O	2	THR
1	O	4	ARG
1	O	6	SER
1	O	30	GLN
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
1	O	178	ARG
1	O	184	GLU
1	O	197	LYS
1	O	250	LEU
2	P	54	THR
2	P	55	LEU
2	P	58	GLN
2	P	60	THR
2	P	62	THR
2	P	65	LEU
2	P	74	VAL
2	P	122	THR
2	P	149	THR
2	P	155	ASN
2	P	184	LYS
2	P	191	LEU
2	P	200	THR
2	P	206	THR
3	Q	4	ARG
3	Q	15	ILE
3	Q	19	GLU
3	Q	53	GLN
3	Q	55	THR
3	Q	61	LYS
3	Q	107	LEU
3	Q	147	GLN
3	Q	153	ILE

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Mol	Chain	Res	Type
3	Q	160	GLN
3	Q	169	VAL
3	Q	185	THR
3	Q	213	VAL
3	Q	228	ASN
4	R	4	VAL
4	R	20	LEU
4	R	44	LYS
4	R	51	LEU
4	R	99	ILE
4	R	102	GLU
4	R	122	GLU
4	R	124	ARG
4	R	176	LEU
4	R	191	LEU
4	R	193	LEU
4	R	204	LEU
4	R	214	ILE
5	S	2	ARG
5	S	9	THR
5	S	15	THR
5	S	71	LEU
5	S	92	ASN
5	S	95	SER
5	S	99	ASN
5	S	190	LYS
5	S	196	ILE
5	S	198	GLN
5	S	211	SER
5	S	222	THR
5	S	231	LYS
6	T	31	THR
6	T	32	THR
6	T	39	ASN
6	T	68	ARG
6	T	123	ASN
6	T	130	VAL
6	T	140	ASN
6	T	148	GLU
6	T	166	GLN
6	T	172	LEU
6	T	181	GLU

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Mol	Chain	Res	Type
6	T	203	ASN
6	T	207	ASP
6	T	221	ASN
6	T	228	LYS
7	U	83	ASN
7	U	115	LEU
7	U	120	THR
7	U	169	ILE
7	U	171	THR
7	U	182	ILE
7	U	201	MET
7	U	207	THR
7	U	221	LYS
7	U	235	ARG
7	U	236	LEU
8	V	20	SER
8	V	25	ILE
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	84	LYS
8	V	153	LYS
8	V	187	LEU
8	V	214	LYS
9	W	1	SER
9	W	28	LEU
9	W	37	ASN
9	W	52	ILE
9	W	61	THR
9	W	81	ILE
9	W	138	SER
9	W	171	LEU
9	W	185	VAL
10	X	2	ASP
10	X	35	THR
10	X	36	ARG
10	X	92	ILE
10	X	110	LYS
10	X	136	SER
10	X	174	MET
10	X	183	ILE
11	Y	4	LEU

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Mol	Chain	Res	Type
11	Y	9	GLN
11	Y	69	ARG
11	Y	87	VAL
11	Y	147	ASP
11	Y	209	ASN
11	Y	211	ILE
12	Z	13	LEU
12	Z	49	ASN
12	Z	109	THR
12	Z	130	SER
12	Z	132	GLU
12	Z	150	LEU
12	Z	165	ASN
12	Z	173	LYS
13	a	3	GLN
13	a	12	ILE
13	a	48	ASN
13	a	69	ASP
13	a	70	LEU
13	a	104	ARG
13	a	159	VAL
13	a	170	VAL
13	a	213	GLN
14	b	36	ARG
14	b	83	LYS
14	b	105	LYS
14	b	115	LEU
14	b	119	VAL
14	b	149	GLU
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (179) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	143	ASN
2	B	20	GLN
2	B	69	ASN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN

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Mol	Chain	Res	Type
2	B	232	GLN
3	C	17	GLN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	228	ASN
3	C	241	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	198	GLN
4	D	225	ASN
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	198	GLN
6	F	19	GLN
6	F	39	ASN
6	F	83	HIS
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	203	ASN
7	G	28	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	167	GLN
7	G	175	ASN
7	G	176	HIS
7	G	212	ASN
7	G	231	ASN
8	H	30	ASN

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Mol	Chain	Res	Type
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	88	GLN
9	I	156	ASN
10	J	10	GLN
10	J	55	GLN
10	J	63	ASN
10	J	86	GLN
10	J	146	HIS
10	J	147	HIS
10	J	191	GLN
11	K	9	GLN
11	K	85	ASN
11	K	143	ASN
11	K	176	ASN
11	K	190	ASN
11	K	209	ASN
12	L	1	GLN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	79	HIS
12	L	195	HIS
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	171	GLN
13	M	179	ASN
13	M	194	ASN
13	M	211	ASN
13	M	213	GLN
14	N	60	GLN
14	N	69	GLN
14	N	141	ASN
14	N	161	GLN
1	O	94	HIS
1	O	119	GLN
1	O	123	GLN
2	P	20	GLN
2	P	69	ASN

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Mol	Chain	Res	Type
2	P	93	HIS
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	146	GLN
2	P	232	GLN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	236	GLN
3	Q	241	GLN
4	R	15	GLN
4	R	91	HIS
4	R	146	GLN
4	R	160	ASN
4	R	180	HIS
4	R	198	GLN
4	R	217	GLN
4	R	225	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	184	ASN
5	S	198	GLN
5	S	209	ASN
6	T	19	GLN
6	T	39	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	178	HIS
6	T	224	HIS
7	U	28	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN

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Mol	Chain	Res	Type
7	U	121	GLN
7	U	175	ASN
7	U	186	ASN
8	V	30	ASN
8	V	66	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
8	V	194	ASN
9	W	71	ASN
9	W	88	GLN
10	X	55	GLN
10	X	63	ASN
10	X	118	GLN
10	X	146	HIS
10	X	147	HIS
10	X	191	GLN
10	X	198	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	190	ASN
11	Y	208	ASN
11	Y	209	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	80	ASN
12	Z	153	GLN
12	Z	159	GLN
12	Z	165	ASN
12	Z	195	HIS
13	a	18	ASN
13	a	48	ASN
13	a	62	HIS
13	a	102	GLN
13	a	149	HIS
13	a	171	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN

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Mol	Chain	Res	Type
14	b	38	HIS
14	b	69	GLN
14	b	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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	$\# Z > 2$
15	OV2	K	301	11	36,36,36	0.43	0	44,47,47	1.37	2 (4%)
15	OV2	H	301	8	36,36,36	0.44	0	44,47,47	1.19	2 (4%)
15	OV2	b	301	14	36,36,36	0.41	0	44,47,47	1.31	3 (6%)
15	OV2	V	301	8	36,36,36	0.39	0	44,47,47	1.08	3 (6%)
15	OV2	N	301	14	36,36,36	0.46	0	44,47,47	1.29	4 (9%)
15	OV2	Y	301	11	36,36,36	0.44	0	44,47,47	1.41	3 (6%)

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
15	OV2	K	301	11	-	20/52/52/52	-
15	OV2	H	301	8	-	13/52/52/52	-
15	OV2	b	301	14	-	14/52/52/52	-
15	OV2	V	301	8	-	19/52/52/52	-
15	OV2	N	301	14	-	14/52/52/52	-
15	OV2	Y	301	11	-	22/52/52/52	-

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	301	OV2	C25-C16-N4	-7.47	100.61	110.20
15	K	301	OV2	C25-C16-N4	-6.09	102.39	110.20
15	H	301	OV2	C25-C16-N4	-6.03	102.46	110.20
15	N	301	OV2	C25-C16-N4	-5.91	102.62	110.20
15	b	301	OV2	C25-C16-N4	-5.30	103.39	110.20
15	V	301	OV2	C25-C16-C17	-4.07	105.66	112.18
15	K	301	OV2	C12-C13-C14	-3.35	108.97	113.39
15	V	301	OV2	C26-C25-C16	3.31	122.22	115.54
15	N	301	OV2	C6-N1-C5	3.18	128.08	121.80
15	b	301	OV2	C12-C13-C14	-2.94	109.52	113.39
15	V	301	OV2	C25-C16-N4	2.86	113.87	110.20
15	H	301	OV2	C12-C13-C14	-2.54	110.05	113.39
15	b	301	OV2	C6-N1-C5	2.49	126.72	121.80
15	Y	301	OV2	C7-C6-N1	-2.40	105.63	111.44
15	Y	301	OV2	C12-C13-C14	-2.18	110.52	113.39
15	N	301	OV2	C23-C22-C24	-2.14	107.04	109.76
15	N	301	OV2	C4-C5-N1	2.04	119.46	115.86

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	H	301	OV2	C13-C14-N3-C30
15	H	301	OV2	C13-C14-N3-C31
15	H	301	OV2	O8-C14-N3-C30
15	H	301	OV2	O8-C14-N3-C31
15	H	301	OV2	C17-C16-C25-C26

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Mol	Chain	Res	Type	Atoms
15	H	301	OV2	C16-C17-C22-C24
15	H	301	OV2	C16-C17-C22-C23
15	H	301	OV2	C17-C22-C24-O7
15	H	301	OV2	C23-C22-C24-O7
15	K	301	OV2	C13-C14-N3-C30
15	K	301	OV2	C13-C14-N3-C31
15	K	301	OV2	O8-C14-N3-C30
15	K	301	OV2	O8-C14-N3-C31
15	K	301	OV2	N4-C16-C25-C26
15	K	301	OV2	C17-C16-C25-C26
15	K	301	OV2	C16-C17-C22-C24
15	K	301	OV2	C16-C17-C22-C23
15	N	301	OV2	C17-C16-C25-C26
15	N	301	OV2	C16-C17-C22-C24
15	N	301	OV2	C16-C17-C22-C23
15	V	301	OV2	C13-C14-N3-C30
15	V	301	OV2	C13-C14-N3-C31
15	V	301	OV2	O8-C14-N3-C30
15	V	301	OV2	O8-C14-N3-C31
15	V	301	OV2	C25-C16-C17-O4
15	V	301	OV2	C25-C16-C17-C22
15	V	301	OV2	C16-C17-C22-C24
15	V	301	OV2	C16-C17-C22-C23
15	V	301	OV2	C23-C22-C24-O7
15	Y	301	OV2	C13-C14-N3-C30
15	Y	301	OV2	C13-C14-N3-C31
15	Y	301	OV2	O8-C14-N3-C30
15	Y	301	OV2	O8-C14-N3-C31
15	Y	301	OV2	C17-C16-C25-C26
15	Y	301	OV2	C16-C17-C22-C24
15	Y	301	OV2	C16-C17-C22-C23
15	b	301	OV2	C17-C16-C25-C26
15	b	301	OV2	C16-C17-C22-C24
15	b	301	OV2	C16-C17-C22-C23
15	K	301	OV2	N1-C6-C7-C9
15	K	301	OV2	C10-C6-C7-C9
15	K	301	OV2	C2-C1-C4-C5
15	K	301	OV2	C10-C6-C7-C8
15	K	301	OV2	N1-C6-C7-C8
15	N	301	OV2	C4-C5-N1-C6
15	Y	301	OV2	C10-C6-C7-C9
15	N	301	OV2	O1-C5-N1-C6

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Mol	Chain	Res	Type	Atoms
15	H	301	OV2	C11-C12-C13-C14
15	Y	301	OV2	C11-C12-C13-C14
15	N	301	OV2	O8-C14-N3-C31
15	N	301	OV2	C13-C14-N3-C31
15	V	301	OV2	C11-C12-C13-C14
15	Y	301	OV2	C10-C6-C7-C8
15	b	301	OV2	C7-C6-N1-C5
15	V	301	OV2	C2-C1-C4-C5
15	V	301	OV2	N2-C11-C12-C13
15	V	301	OV2	O4-C17-C22-C24
15	K	301	OV2	C4-C1-C2-C3
15	K	301	OV2	C11-C12-C13-C14
15	Y	301	OV2	N1-C6-C7-C9
15	b	301	OV2	C2-C1-C4-C5
15	b	301	OV2	C4-C1-C2-C3
15	Y	301	OV2	C2-C1-C4-C5
15	N	301	OV2	O8-C14-N3-C30
15	Y	301	OV2	N1-C6-C7-C8
15	H	301	OV2	O4-C17-C22-C24
15	H	301	OV2	O4-C17-C22-C23
15	K	301	OV2	O4-C17-C22-C24
15	K	301	OV2	O4-C17-C22-C23
15	N	301	OV2	O4-C17-C22-C24
15	N	301	OV2	O4-C17-C22-C23
15	V	301	OV2	O4-C17-C22-C23
15	Y	301	OV2	O4-C17-C22-C24
15	Y	301	OV2	O4-C17-C22-C23
15	b	301	OV2	O4-C17-C22-C23
15	K	301	OV2	C1-C2-C3-C29
15	V	301	OV2	C1-C2-C3-C29
15	N	301	OV2	C13-C14-N3-C30
15	b	301	OV2	C1-C2-C3-C29
15	N	301	OV2	C1-C2-C3-C29
15	H	301	OV2	N4-C16-C25-C26
15	N	301	OV2	N4-C16-C25-C26
15	Y	301	OV2	N4-C16-C25-C26
15	b	301	OV2	N4-C16-C25-C26
15	N	301	OV2	C2-C1-C4-C5
15	b	301	OV2	C11-C12-C13-C14
15	V	301	OV2	C17-C22-C24-O7
15	Y	301	OV2	C1-C2-C3-C29
15	Y	301	OV2	C4-C1-C2-C3

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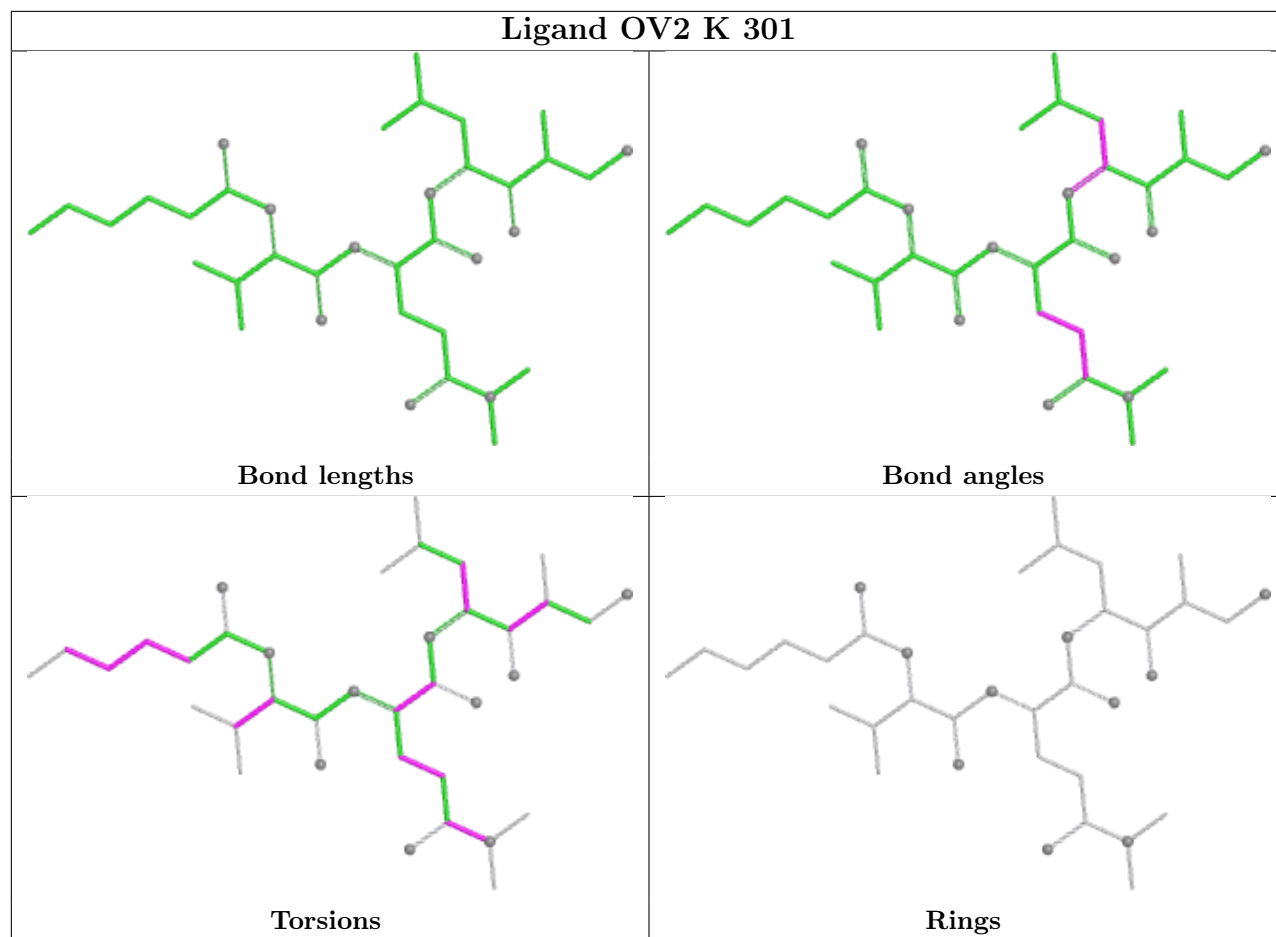
Mol	Chain	Res	Type	Atoms
15	b	301	OV2	O4-C17-C22-C24
15	V	301	OV2	N4-C16-C17-C22
15	Y	301	OV2	N2-C11-C15-O3
15	b	301	OV2	O2-C10-C6-N1
15	Y	301	OV2	N2-C11-C15-N4
15	K	301	OV2	N2-C11-C15-O3
15	b	301	OV2	N2-C10-C6-N1
15	Y	301	OV2	C12-C11-C15-O3
15	V	301	OV2	N4-C16-C17-O4
15	V	301	OV2	C4-C1-C2-C3
15	b	301	OV2	N2-C11-C15-O3
15	K	301	OV2	N2-C11-C15-N4
15	Y	301	OV2	C12-C11-C15-N4

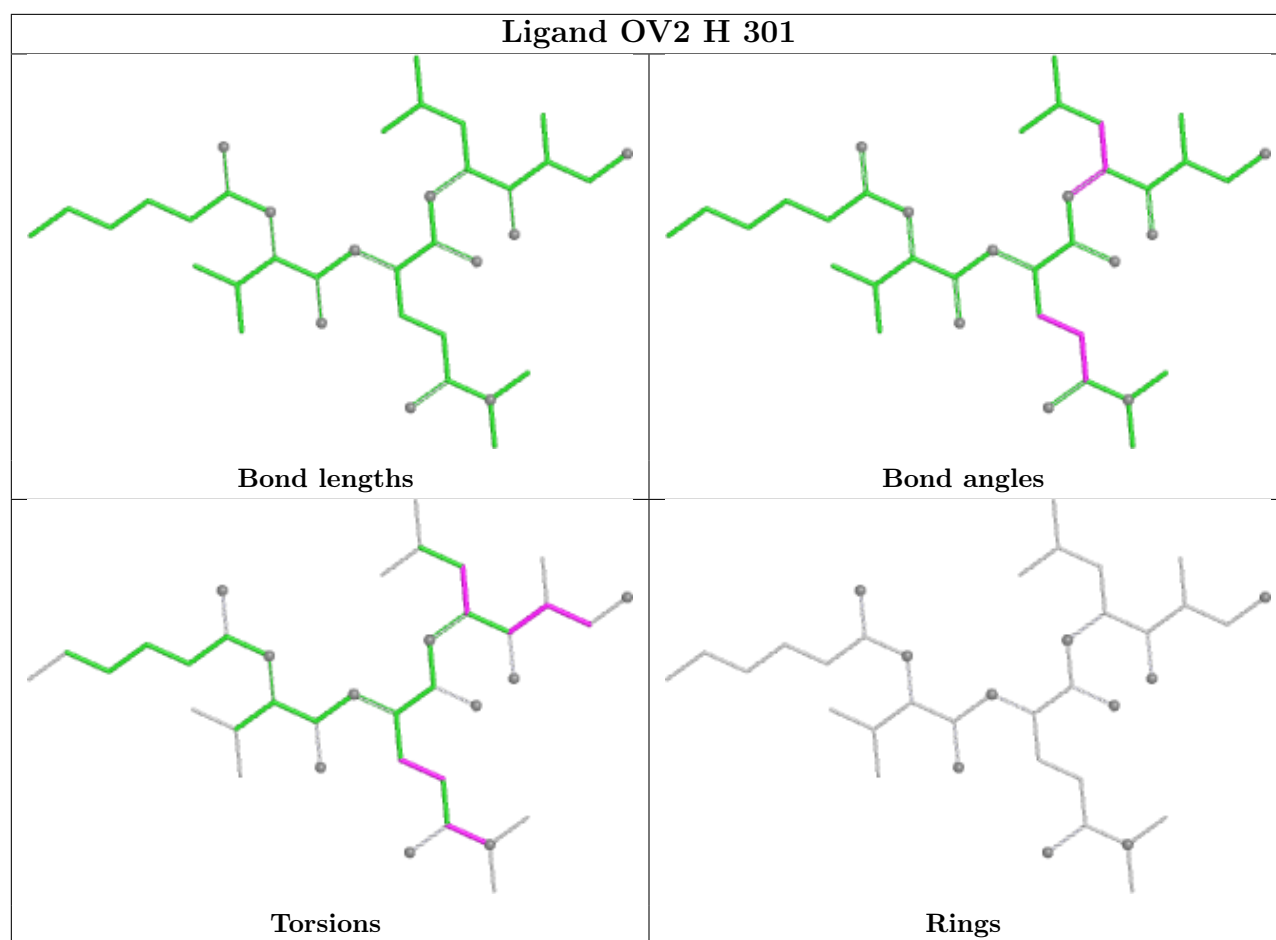
There are no ring outliers.

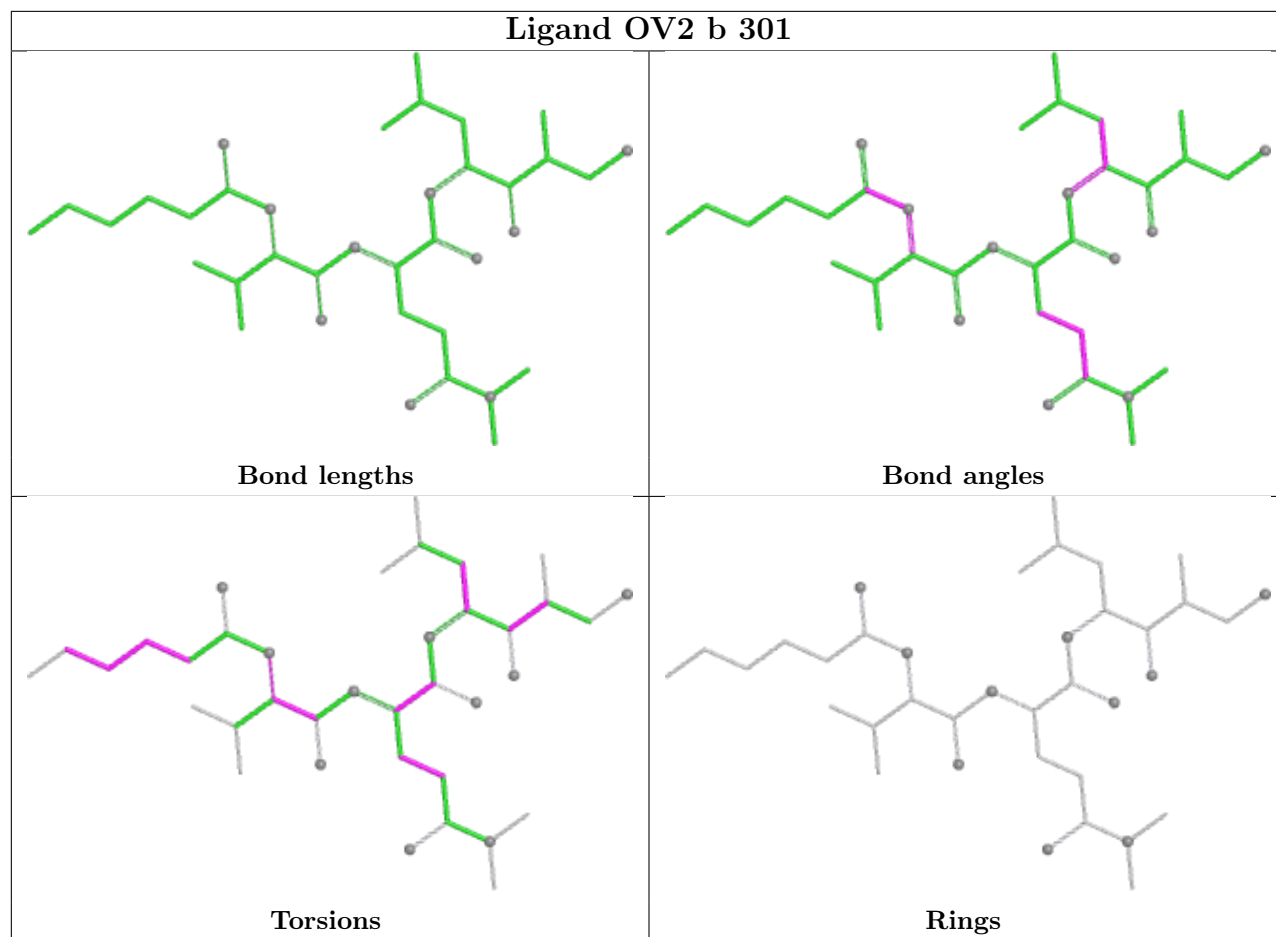
5 monomers are involved in 13 short contacts:

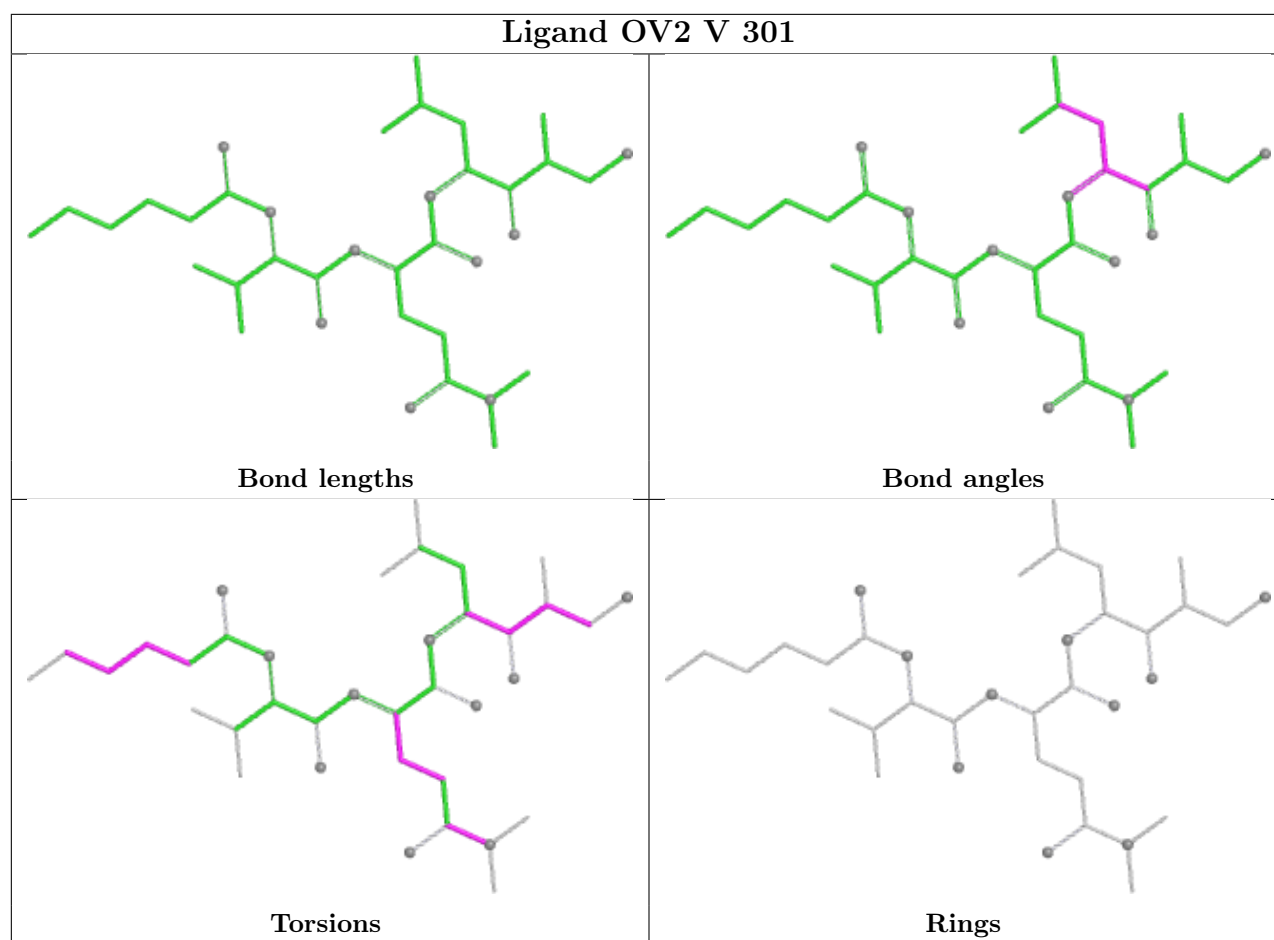
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	K	301	OV2	3	0
15	H	301	OV2	2	0
15	b	301	OV2	2	0
15	V	301	OV2	5	0
15	Y	301	OV2	1	0

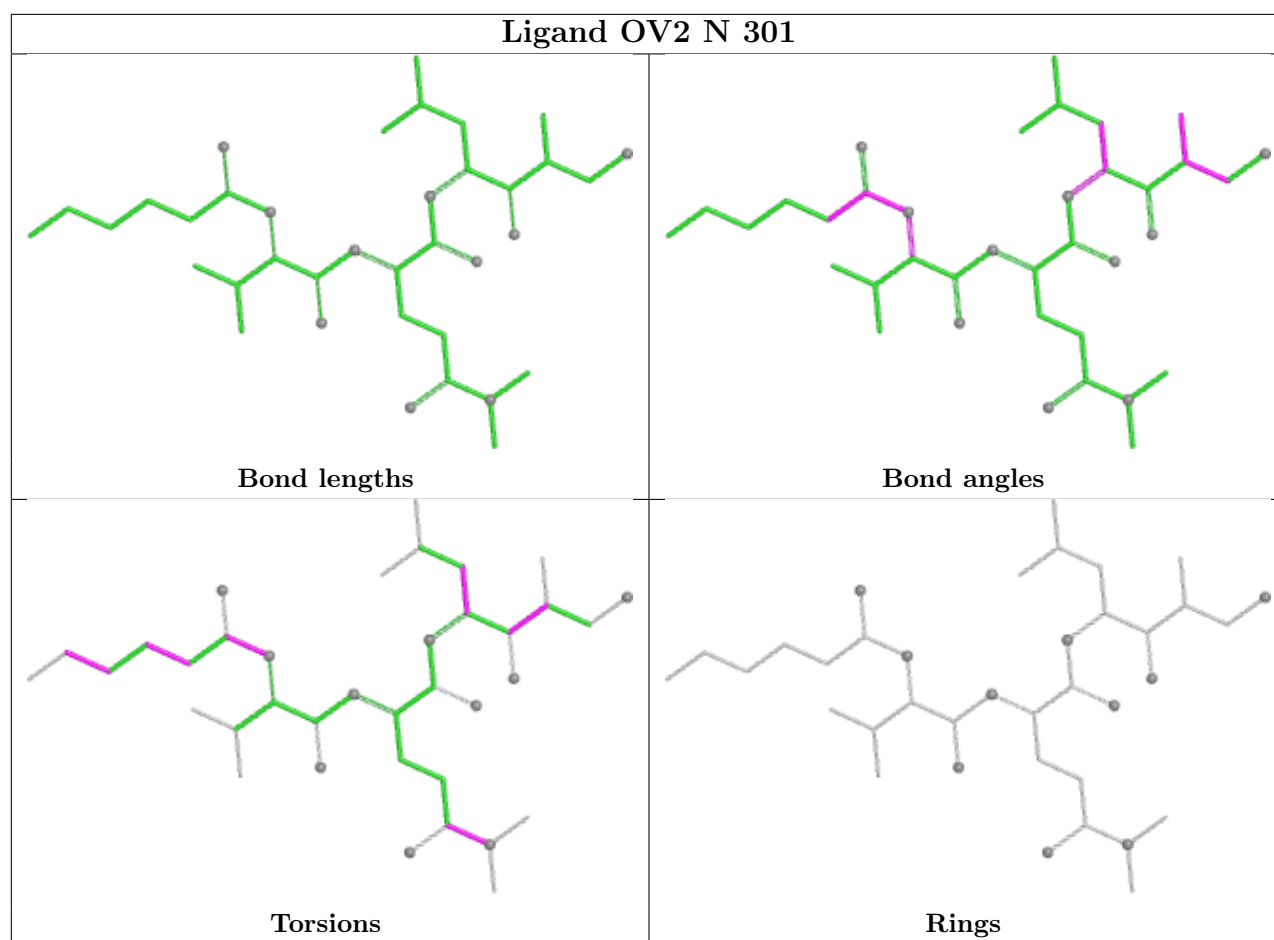
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

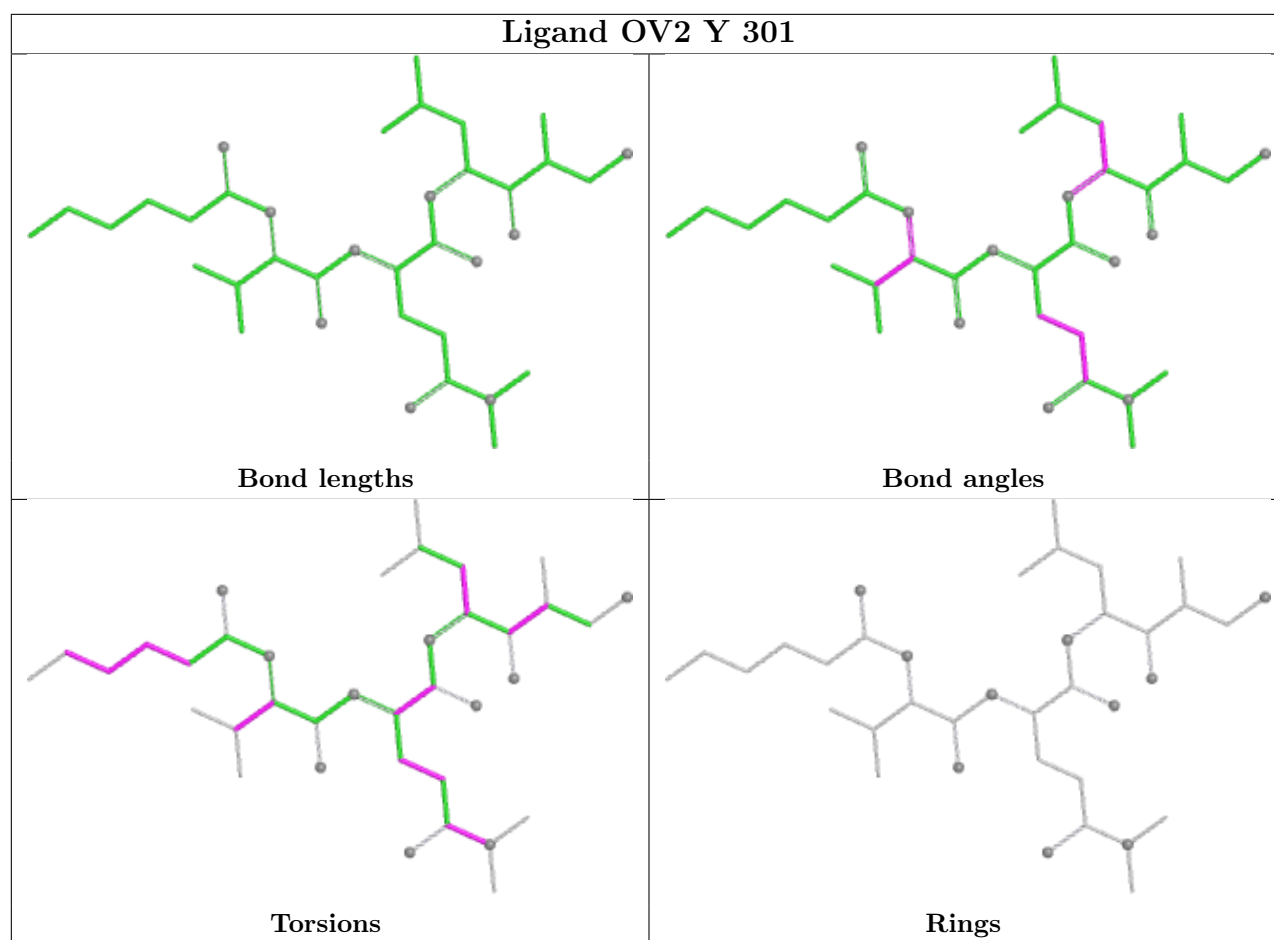












5.7 Other polymers [i](#)

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	249/249 (100%)	-0.04	1 (0%) 88 84	54, 72, 100, 117	0
1	O	249/249 (100%)	-0.05	2 (0%) 82 75	56, 74, 104, 122	0
2	B	244/244 (100%)	0.25	9 (3%) 45 36	51, 78, 119, 137	0
2	P	244/244 (100%)	0.10	9 (3%) 45 36	55, 75, 107, 121	0
3	C	241/241 (100%)	0.13	12 (4%) 34 26	48, 73, 115, 147	0
3	Q	241/241 (100%)	0.19	10 (4%) 41 33	62, 91, 132, 168	0
4	D	242/242 (100%)	0.06	7 (2%) 53 43	54, 74, 101, 122	0
4	R	242/242 (100%)	0.31	12 (4%) 34 26	63, 84, 116, 145	0
5	E	233/233 (100%)	0.29	2 (0%) 81 74	63, 86, 122, 132	0
5	S	233/233 (100%)	0.25	4 (1%) 69 60	53, 87, 119, 129	0
6	F	244/244 (100%)	0.18	1 (0%) 88 84	60, 84, 116, 144	0
6	T	244/244 (100%)	0.02	2 (0%) 82 75	59, 79, 111, 134	0
7	G	243/243 (100%)	0.02	1 (0%) 88 84	58, 78, 105, 126	0
7	U	243/243 (100%)	-0.06	2 (0%) 82 75	57, 73, 100, 118	0
8	H	222/222 (100%)	-0.20	0 100 100	49, 67, 88, 96	0
8	V	222/222 (100%)	0.04	2 (0%) 81 74	50, 66, 90, 120	0
9	I	204/204 (100%)	-0.13	0 100 100	46, 65, 92, 99	0
9	W	204/204 (100%)	-0.26	0 100 100	44, 60, 84, 91	0
10	J	198/198 (100%)	0.04	4 (2%) 65 56	46, 66, 94, 119	0
10	X	198/198 (100%)	-0.20	3 (1%) 72 63	50, 64, 84, 104	0
11	K	212/212 (100%)	-0.33	1 (0%) 87 82	43, 62, 85, 92	0
11	Y	212/212 (100%)	-0.17	1 (0%) 87 82	53, 67, 92, 103	0
12	L	222/222 (100%)	-0.14	1 (0%) 87 82	49, 65, 87, 91	0
12	Z	222/222 (100%)	-0.17	1 (0%) 87 82	48, 67, 91, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/233 (100%)	-0.01	4 (1%) 69 60	53, 72, 99, 116	0
13	a	233/233 (100%)	-0.29	1 (0%) 88 84	44, 66, 87, 99	0
14	N	196/196 (100%)	-0.26	0 100 100	53, 64, 87, 93	0
14	b	196/196 (100%)	-0.23	0 100 100	51, 63, 87, 93	0
All	All	6366/6366 (100%)	-0.01	92 (1%) 73 64	43, 72, 109, 168	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	50	LEU	7.3
2	B	1	GLY	5.1
4	D	119	ALA	5.0
4	R	120	SER	4.8
2	P	1	GLY	4.8
4	R	119	ALA	4.8
13	M	233	ILE	4.8
3	Q	49	THR	4.6
4	R	121	GLY	4.5
4	D	120	SER	4.3
10	J	197	ALA	4.3
2	P	51	VAL	4.2
3	C	50	LEU	4.2
2	B	244	THR	4.2
2	B	219	ALA	4.1
4	D	118	GLY	4.1
10	X	197	ALA	3.9
5	E	1	PHE	3.8
2	P	60	THR	3.8
3	Q	205	ALA	3.6
4	R	118	GLY	3.4
7	U	1	ALA	3.3
5	S	1	PHE	3.3
4	D	121	GLY	3.3
3	C	49	THR	3.3
10	X	1	MET	3.2
5	E	16	GLY	3.2
10	J	1	MET	3.1
3	Q	52	LEU	3.1
13	a	1	THR	3.1
3	C	206	LYS	3.1
4	D	125	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
13	M	1	THR	3.1
6	F	202	ASP	3.0
4	R	113	LEU	3.0
2	P	244	THR	3.0
7	G	1	ALA	2.9
1	O	2	THR	2.9
3	C	205	ALA	2.8
11	K	211	ILE	2.8
12	L	108	HIS	2.8
10	J	174	MET	2.7
5	S	6	ASP	2.7
3	C	59	PRO	2.7
3	C	52	LEU	2.7
6	T	1	GLY	2.7
4	R	46	ALA	2.7
4	R	4	VAL	2.6
3	Q	59	PRO	2.6
11	Y	211	ILE	2.6
10	X	198	GLN	2.6
8	V	222	ASP	2.5
2	B	243	ILE	2.5
3	Q	204	GLY	2.5
6	T	2	THR	2.5
4	R	124	ARG	2.4
4	R	242	GLU	2.4
3	Q	51	LYS	2.4
4	D	124	ARG	2.4
3	Q	55	THR	2.4
7	U	243	ASP	2.4
3	Q	58	THR	2.4
4	R	125	LEU	2.4
13	M	232	LYS	2.3
2	P	219	ALA	2.3
3	C	51	LYS	2.3
2	P	62	THR	2.3
3	C	60	SER	2.3
13	M	229	GLY	2.3
8	V	219	ASN	2.2
4	R	112	ALA	2.2
2	P	2	SER	2.2
2	P	61	SER	2.2
10	J	25	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	Q	48	SER	2.2
2	P	220	ASN	2.2
2	B	60	THR	2.2
1	A	201	GLU	2.2
3	C	241	GLN	2.1
4	R	94	TYR	2.1
2	B	7	SER	2.1
3	C	57	ILE	2.1
2	B	5	TYR	2.1
5	S	207	VAL	2.1
1	O	62	SER	2.0
2	B	61	SER	2.0
5	S	204	SER	2.0
12	Z	172	LEU	2.0
2	B	54	THR	2.0
3	C	203	THR	2.0
3	C	58	THR	2.0
4	D	155	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	OV2	N	301	37/37	0.91	0.14	54,59,65,66	0
15	OV2	b	301	37/37	0.91	0.13	53,57,61,61	0
15	OV2	H	301	37/37	0.93	0.12	55,60,62,63	0
15	OV2	V	301	37/37	0.93	0.13	54,58,61,61	0
15	OV2	K	301	37/37	0.93	0.11	51,53,60,61	0

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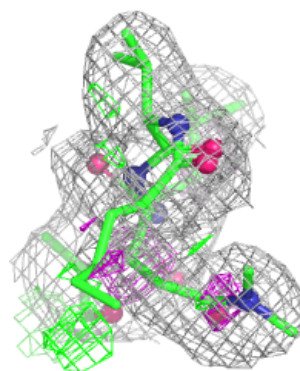
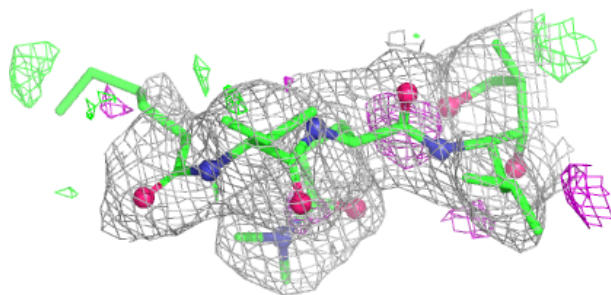
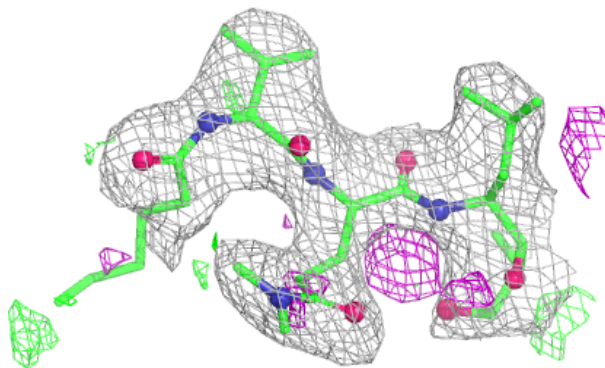
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	OV2	Y	301	37/37	0.94	0.11	55,57,63,64	0

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.

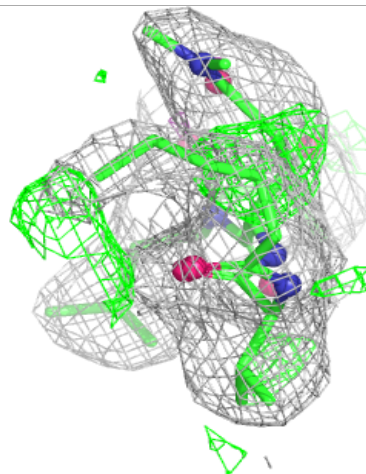
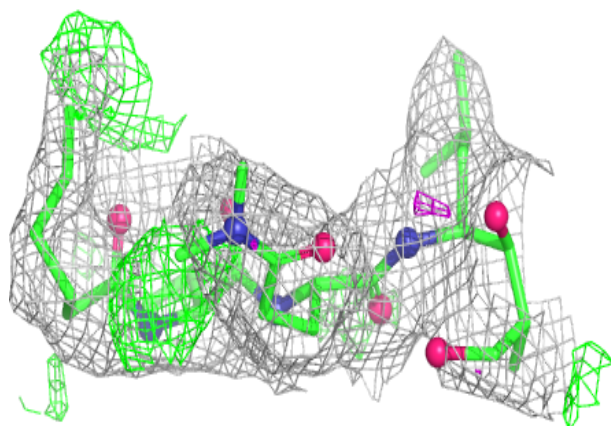
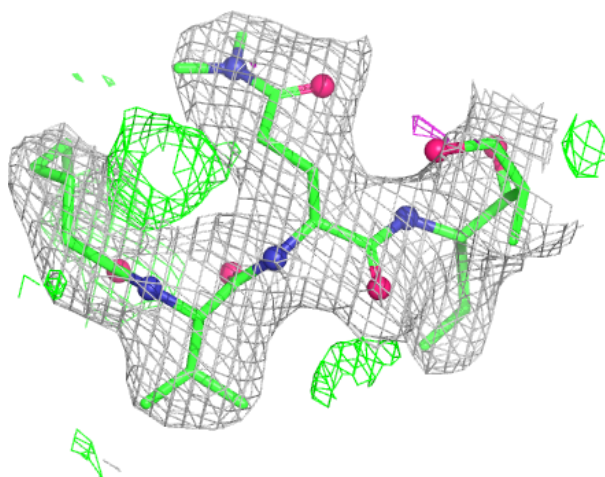
Electron density around OV2 N 301:

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



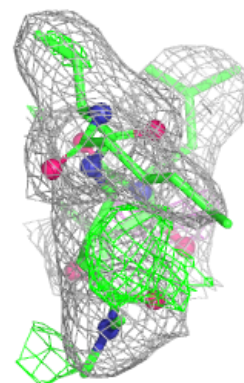
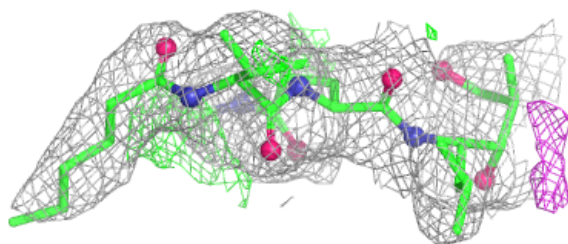
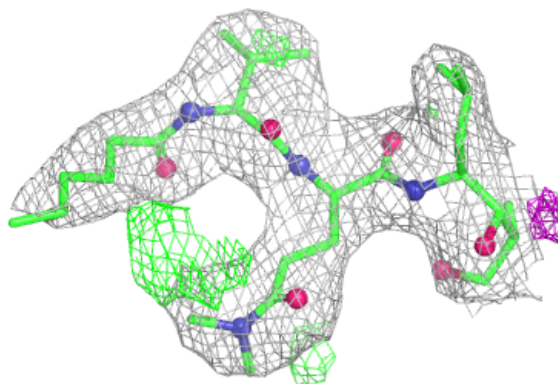
Electron density around OV2 b 301:

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

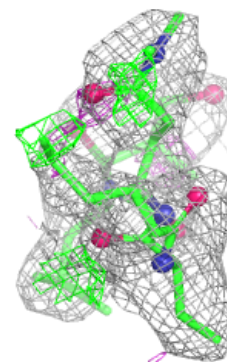
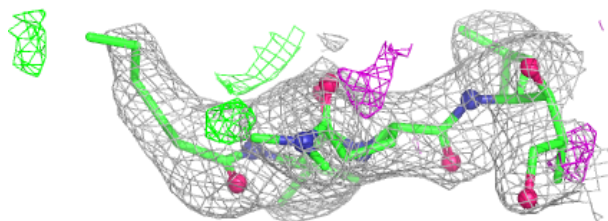
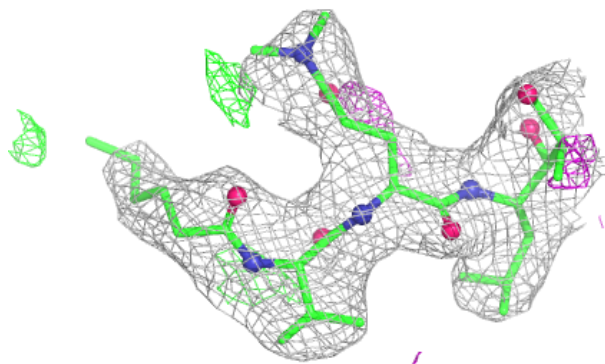


Electron density around OV2 H 301:

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

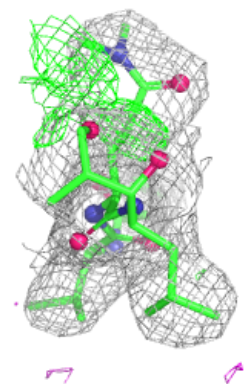
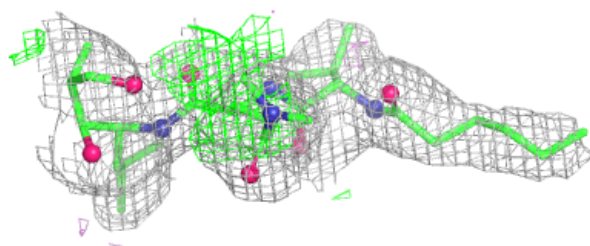
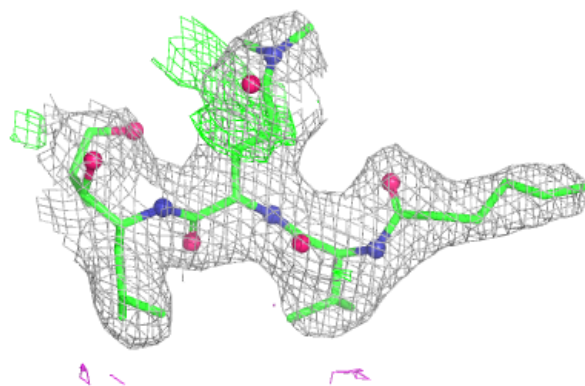
**Electron density around OV2 V 301:**

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

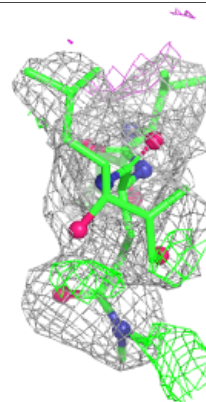
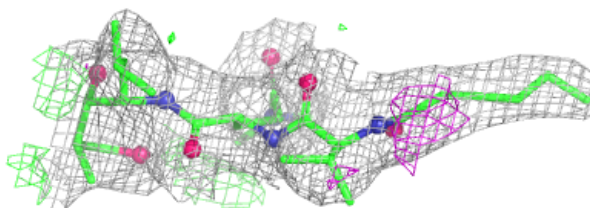
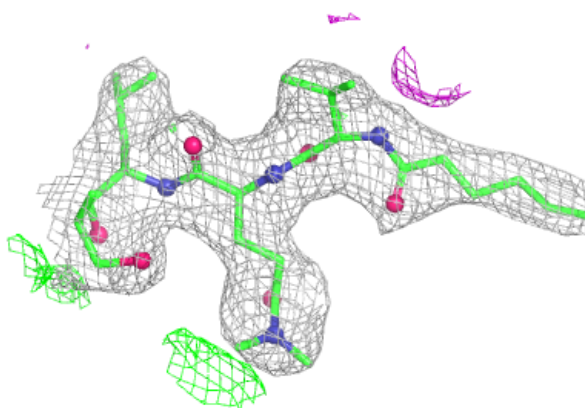


Electron density around OV2 K 301:

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

**Electron density around OV2 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.