



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:39 AM UTC

PDB ID : 7AWE / pdb_00007awe
Title : HUMAN IMMUNOPROTEASOME 20S PARTICLE IN COMPLEX WITH [(1R)-2-(1-benzofuran-3-yl)-1-{[(1S,2R,4R)-7-oxabicyclo[2.2.1]heptan-2-yl]formamido}ethyl]boronic acid
Authors : Musil, D.; Klein, M.
Deposited on : 2020-11-06
Resolution : 2.29 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

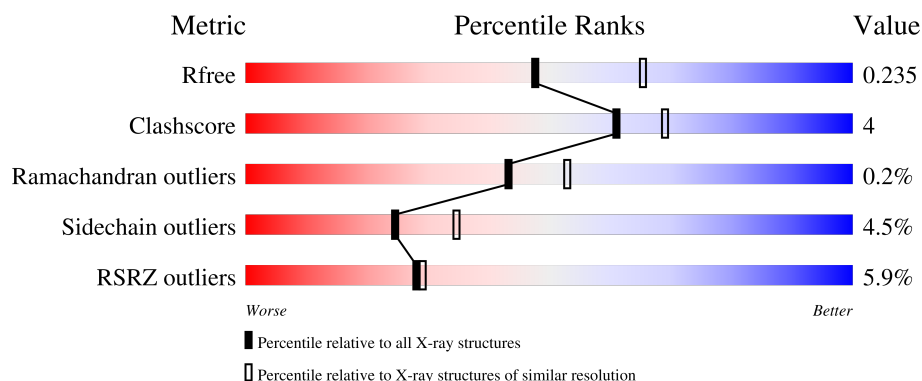
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	242	9% 86% 12% ..
1	O	242	8% 86% 12% .
2	B	229	11% 87% 12% .
2	P	229	3% 89% 9% .

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Mol	Chain	Length	Quality of chain
3	C	256	
3	Q	256	
4	D	237	
4	R	237	
5	E	232	
5	S	232	
6	F	236	
6	T	236	
7	G	242	
7	U	242	
8	H	199	
8	V	199	
9	I	223	
9	W	223	
10	J	204	
10	X	204	
11	K	197	
11	Y	197	
12	L	203	
12	Z	203	
13	M	213	
13	a	213	
14	N	214	
14	b	214	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49839 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-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	31	0	0
			1871	1189	310	359	13			
1	O	242	Total	C	N	O	S	30	0	0
			1886	1197	315	361	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	34	0	0
			1787	1144	301	336	6			
2	P	229	Total	C	N	O	S	32	0	0
			1787	1144	301	336	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	243	Total	C	N	O	S	38	0	0
			1912	1210	327	365	10			
3	Q	253	Total	C	N	O	S	4	0	0
			2003	1264	345	384	10			

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	227	Total	C	N	O	S	48	0	0
			1798	1132	318	343	5			
4	R	234	Total	C	N	O	S	54	0	0
			1848	1160	327	356	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	230	Total	C	N	O	S	31	0	0
			1758	1103	291	353	11			
5	S	232	Total	C	N	O	S	58	0	0
			1769	1110	293	355	11			

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	236	Total	C	N	O	S	38	0	0
			1857	1162	334	350	11			
6	T	235	Total	C	N	O	S	12	0	0
			1846	1156	330	349	11			

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	242	Total	C	N	O	S	38	0	0
			1894	1200	323	360	11			
7	U	240	Total	C	N	O	S	25	0	0
			1881	1193	321	356	11			

- Molecule 8 is a protein called Proteasome subunit beta type-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	199	Total	C	N	O	S	3	0	0
			1493	939	254	291	9			
8	V	199	Total	C	N	O	S	7	0	0
			1493	939	254	291	9			

- Molecule 9 is a protein called Proteasome subunit beta type-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	223	Total	C	N	O	S	20	0	0
			1641	1031	290	312	8			
9	W	223	Total	C	N	O	S	16	0	0
			1641	1031	290	312	8			

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	4	0	0
			1591	1013	265	294	19			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	204	Total	C	N	O	S	7	0	0
			1591	1013	265	294	19			

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	196	Total	C	N	O	S	7	0	0
			1571	1006	267	289	9			
11	Y	197	Total	C	N	O	S	14	0	0
			1578	1011	268	290	9			

- Molecule 12 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	203	Total	C	N	O	S	4	0	0
			1576	984	276	301	15			
12	Z	203	Total	C	N	O	S	2	0	0
			1576	984	276	301	15			

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	213	Total	C	N	O	S	10	0	0
			1654	1047	284	313	10			
13	a	213	Total	C	N	O	S	16	0	0
			1654	1047	284	313	10			

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	214	Total	C	N	O	S	7	0	0
			1673	1055	289	317	12			
14	b	214	Total	C	N	O	S	3	0	0
			1673	1055	289	317	12			

- Molecule 15 is SODIUM ION (CCD ID: NA) (formula: Na).

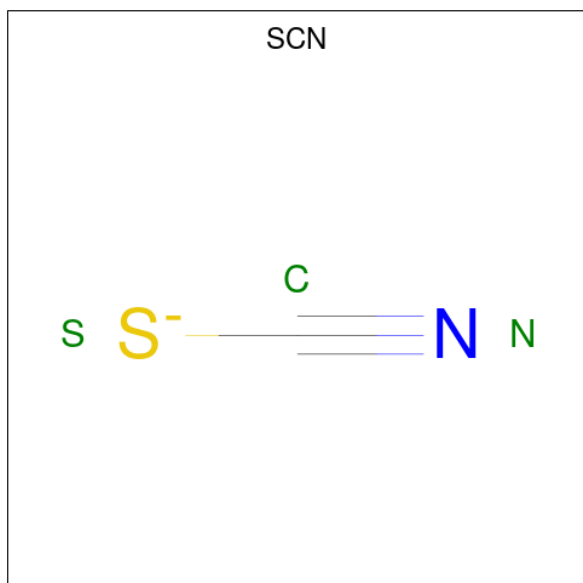
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Na	0	0
			1	1		
15	H	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	I	1	Total	Na	0	0
			1	1		
15	J	2	Total	Na	0	0
			2	2		
15	L	1	Total	Na	0	0
			1	1		
15	M	1	Total	Na	0	0
			1	1		
15	O	1	Total	Na	0	0
			1	1		
15	V	1	Total	Na	0	0
			1	1		
15	W	1	Total	Na	0	0
			1	1		
15	X	1	Total	Na	0	0
			1	1		
15	Z	1	Total	Na	0	0
			1	1		
15	a	1	Total	Na	0	0
			1	1		

- Molecule 16 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



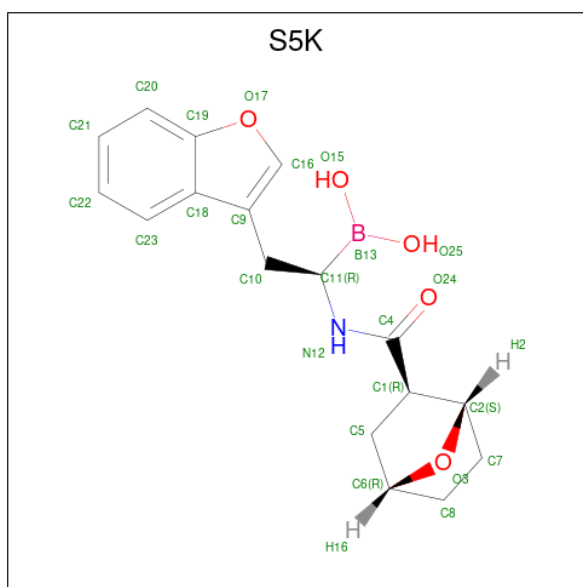
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	F	1	Total	C	N	S	0	0
			3	1	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	K	1	Total	C	N	S	0	0
			3	1	1	1		
16	K	1	Total	C	N	S	0	0
			3	1	1	1		
16	M	1	Total	C	N	S	0	0
			3	1	1	1		
16	M	1	Total	C	N	S	0	0
			3	1	1	1		
16	M	1	Total	C	N	S	0	0
			3	1	1	1		
16	T	1	Total	C	N	S	0	0
			3	1	1	1		
16	U	1	Total	C	N	S	0	0
			3	1	1	1		
16	Z	1	Total	C	N	S	0	0
			3	1	1	1		
16	a	1	Total	C	N	S	0	0
			3	1	1	1		
16	a	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 17 is [(1R)-2-(1-benzofuran-3-yl)-1-{[(1S,2R,4R)-7-oxabicyclo[2.2.1]heptan-2-yl]formamido}ethyl]boronic acid (CCD ID: S5K) (formula: C₁₇H₂₀BNO₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	B	C	N	O	0	0
			24	1	17	1	5		
17	L	1	Total	B	C	N	O	0	0
			24	1	17	1	5		
17	V	1	Total	B	C	N	O	0	0
			24	1	17	1	5		
17	Z	1	Total	B	C	N	O	0	0
			24	1	17	1	5		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	44	Total	O	0	0
			44	44		
18	B	35	Total	O	0	0
			35	35		
18	C	60	Total	O	0	0
			60	60		
18	D	27	Total	O	0	0
			27	27		
18	E	38	Total	O	0	0
			38	38		
18	F	37	Total	O	0	0
			37	37		
18	G	34	Total	O	0	0
			34	34		
18	H	52	Total	O	0	0
			52	52		
18	I	52	Total	O	0	0
			52	52		
18	J	69	Total	O	0	0
			69	69		
18	K	48	Total	O	0	0
			48	48		
18	L	63	Total	O	0	0
			63	63		
18	M	80	Total	O	0	0
			80	80		
18	N	75	Total	O	0	0
			75	75		
18	O	35	Total	O	0	0
			35	35		
18	P	34	Total	O	0	0
			34	34		

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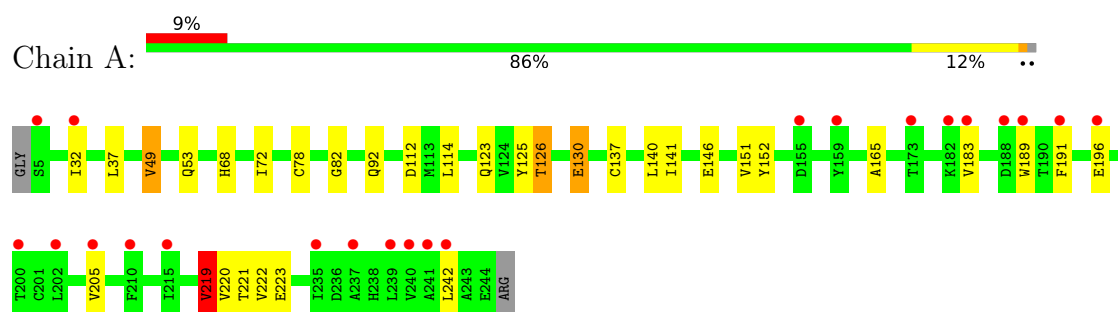
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	Q	40	Total 40	O 40	0	0
18	R	29	Total 29	O 29	0	0
18	S	22	Total 22	O 22	0	0
18	T	58	Total 58	O 58	0	0
18	U	43	Total 43	O 43	0	0
18	V	57	Total 57	O 57	0	0
18	W	52	Total 52	O 52	0	0
18	X	68	Total 68	O 68	0	0
18	Y	42	Total 42	O 42	0	0
18	Z	62	Total 62	O 62	0	0
18	a	67	Total 67	O 67	0	0
18	b	72	Total 72	O 72	0	0

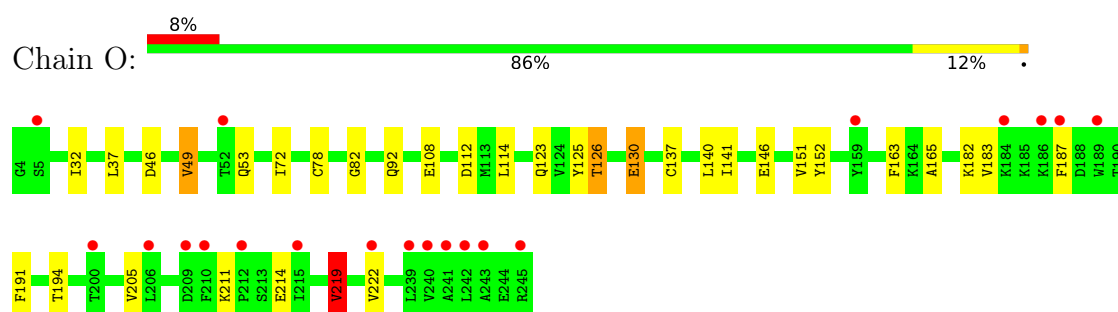
3 Residue-property plots [i](#)

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

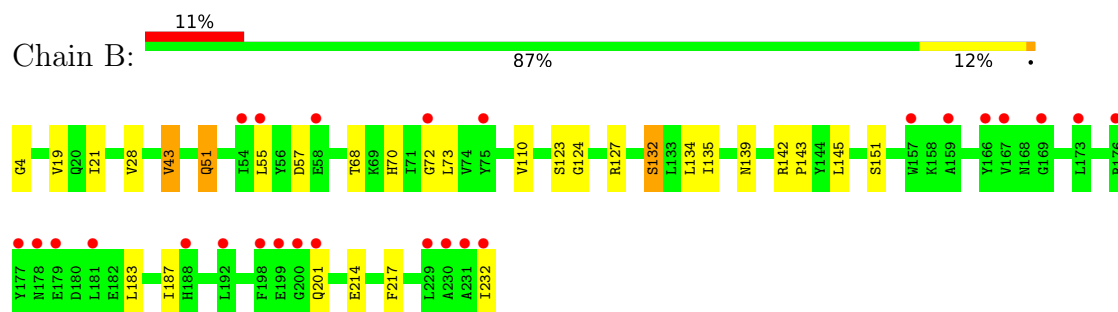
- Molecule 1: Proteasome subunit alpha type-6



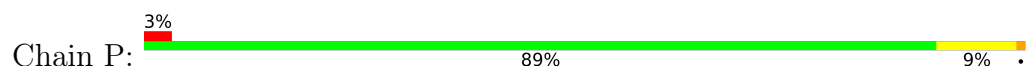
- Molecule 1: Proteasome subunit alpha type-6



- Molecule 2: Proteasome subunit alpha type-2

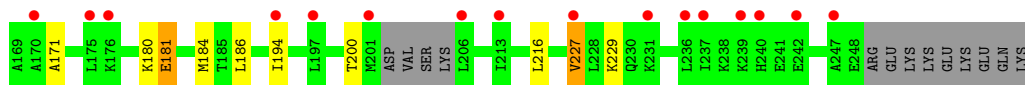
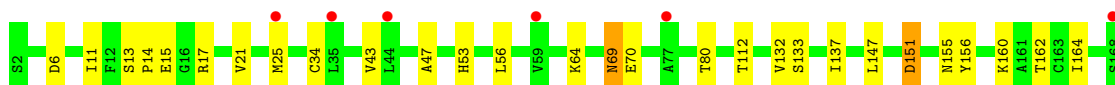
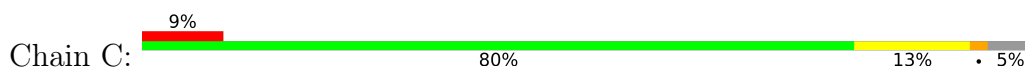


- Molecule 2: Proteasome subunit alpha type-2

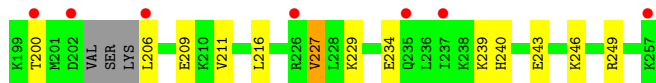
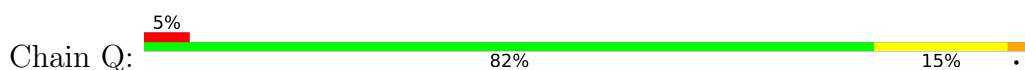




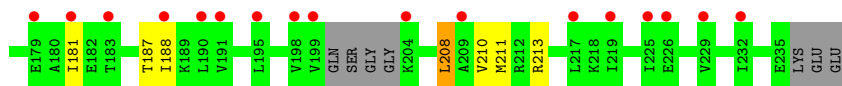
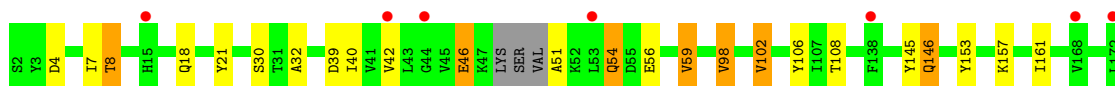
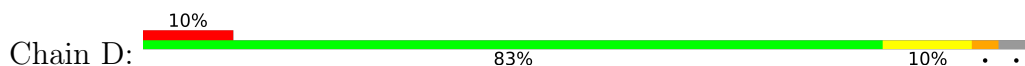
• Molecule 3: Proteasome subunit alpha type-4



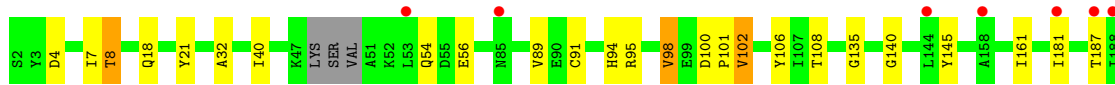
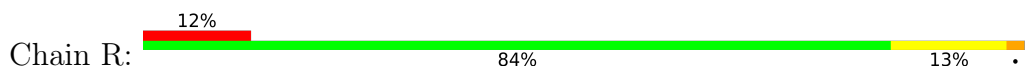
• Molecule 3: Proteasome subunit alpha type-4



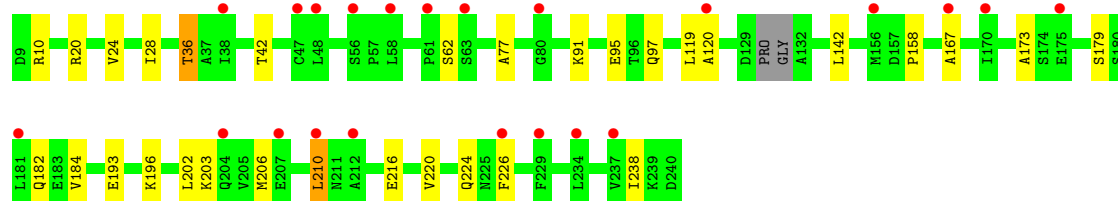
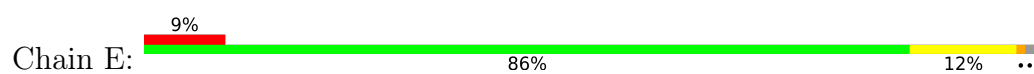
• Molecule 4: Proteasome subunit alpha type-7



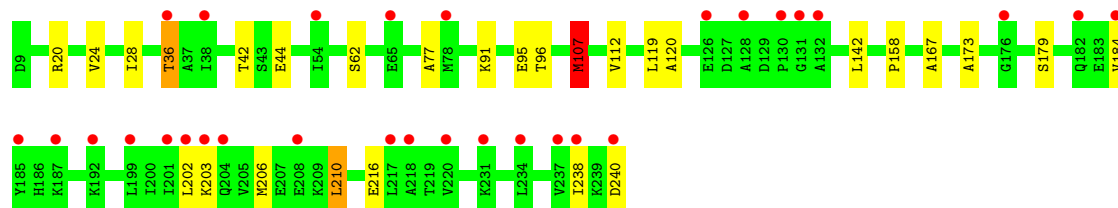
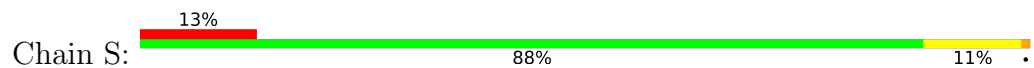
• Molecule 4: Proteasome subunit alpha type-7



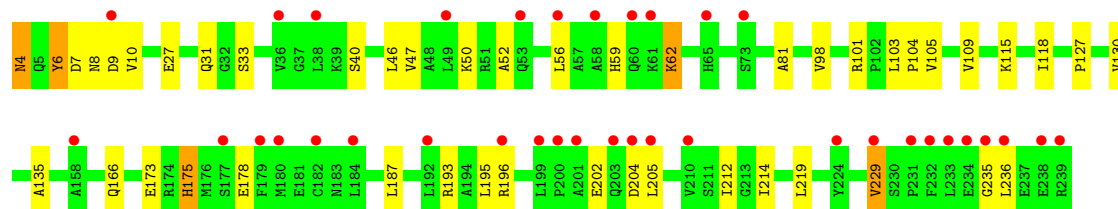
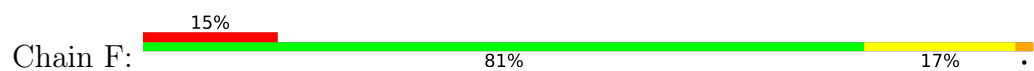
• Molecule 5: Proteasome subunit alpha type-5



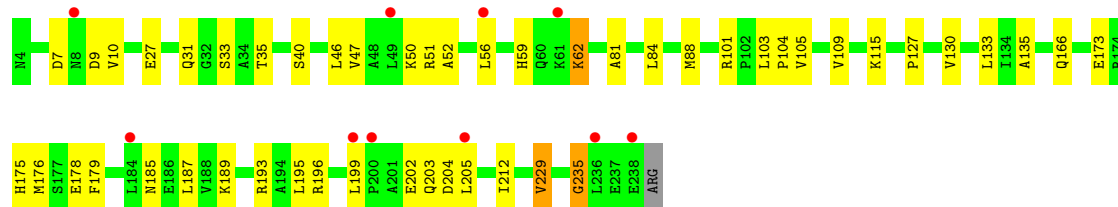
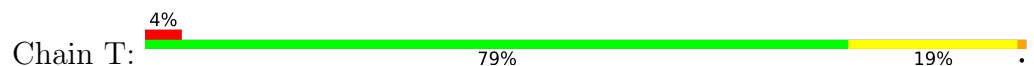
• Molecule 5: Proteasome subunit alpha type-5



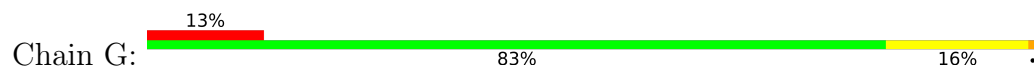
• Molecule 6: Proteasome subunit alpha type-1

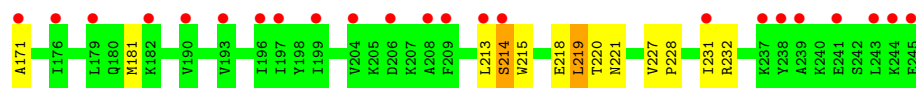


• Molecule 6: Proteasome subunit alpha type-1

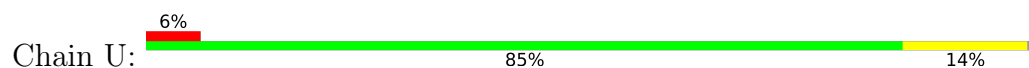


• Molecule 7: Proteasome subunit alpha type-3

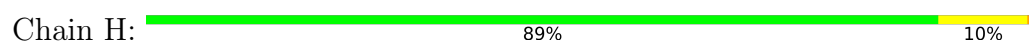




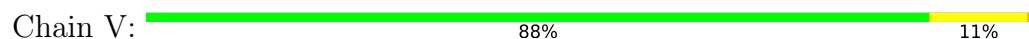
• Molecule 7: Proteasome subunit alpha type-3



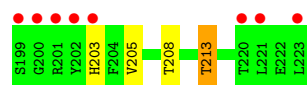
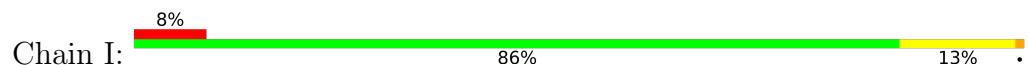
• Molecule 8: Proteasome subunit beta type-9



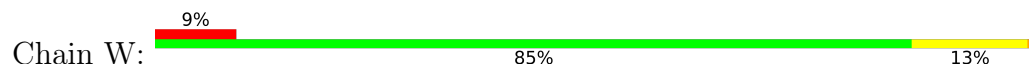
• Molecule 8: Proteasome subunit beta type-9



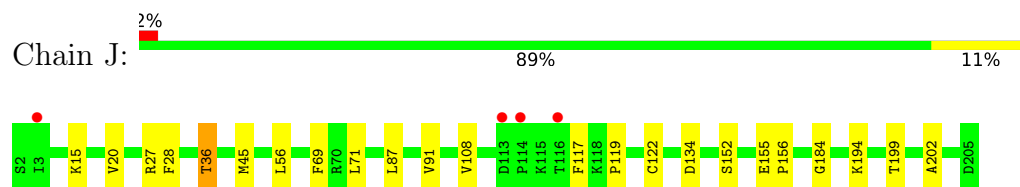
• Molecule 9: Proteasome subunit beta type-10



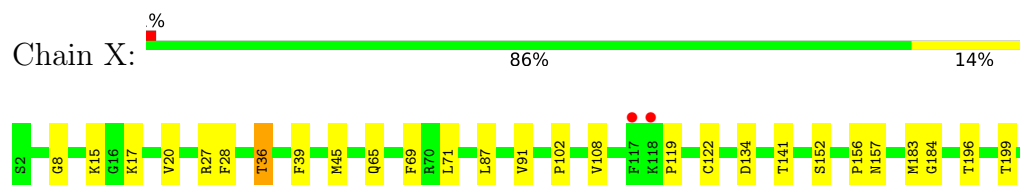
• Molecule 9: Proteasome subunit beta type-10



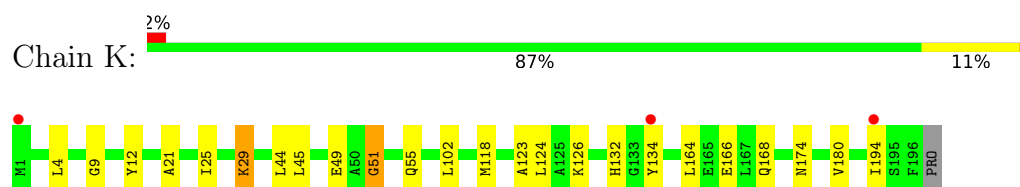
- Molecule 10: Proteasome subunit beta type-3



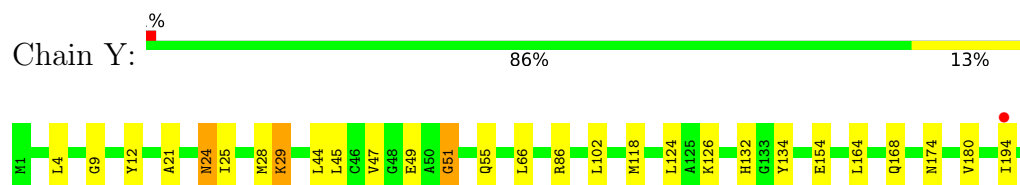
- Molecule 10: Proteasome subunit beta type-3



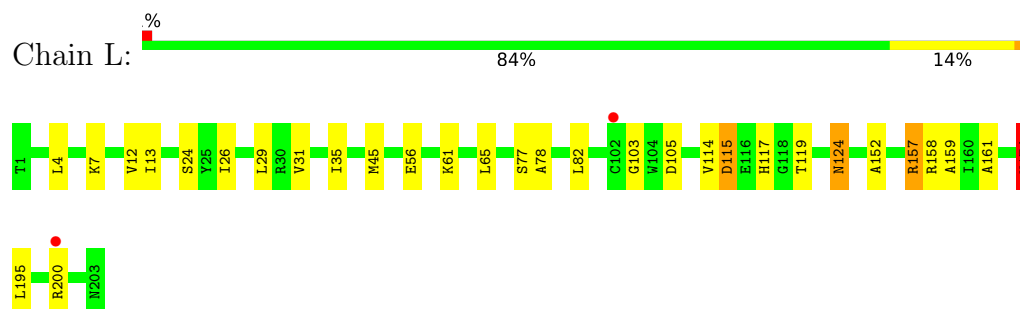
- Molecule 11: Proteasome subunit beta type-2



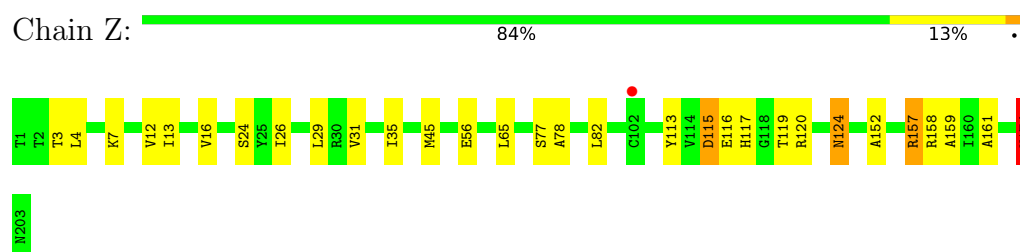
- Molecule 11: Proteasome subunit beta type-2



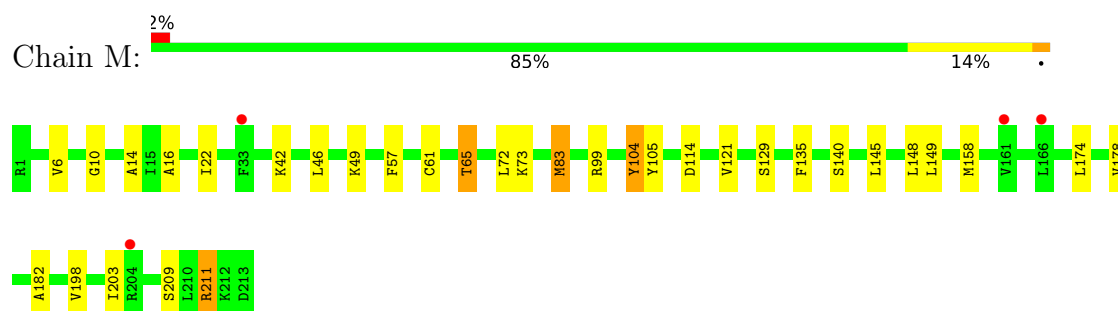
- Molecule 12: Proteasome subunit beta type-8



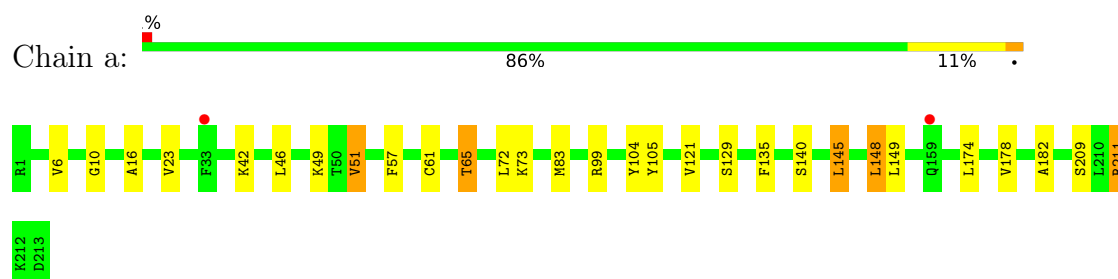
- Molecule 12: Proteasome subunit beta type-8



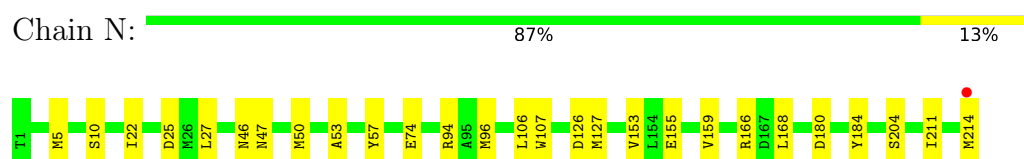
- Molecule 13: Proteasome subunit beta type-1



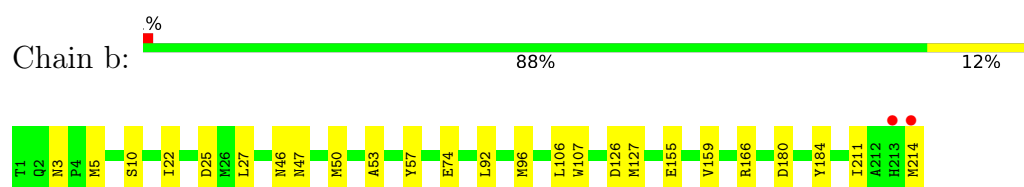
- Molecule 13: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.47Å 206.05Å 162.81Å 90.00° 106.69° 90.00°	Depositor
Resolution (Å)	155.95 – 2.29 155.95 – 2.29	Depositor EDS
% Data completeness (in resolution range)	94.3 (155.95-2.29) 62.4 (155.95-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.7 (18-SEP-2020)	Depositor
R, R_{free}	0.178 , 0.214 0.205 , 0.235	Depositor DCC
R_{free} test set	10251 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	49839	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.02% 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: NA, SCN, S5K

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	0.70	0/1905	1.12	3/2576 (0.1%)
1	O	0.73	0/1920	1.10	4/2595 (0.2%)
2	B	0.72	0/1826	1.11	4/2474 (0.2%)
2	P	0.74	0/1826	1.09	1/2474 (0.0%)
3	C	0.70	0/1941	1.08	5/2614 (0.2%)
3	Q	0.71	0/2032	1.07	5/2731 (0.2%)
4	D	0.69	0/1822	1.04	2/2458 (0.1%)
4	R	0.69	0/1873	1.04	0/2526
5	E	0.73	0/1783	1.08	1/2406 (0.0%)
5	S	0.75	1/1796 (0.1%)	1.07	3/2426 (0.1%)
6	F	0.73	1/1891 (0.1%)	1.15	5/2555 (0.2%)
6	T	0.74	0/1880	1.16	2/2541 (0.1%)
7	G	0.71	0/1929	1.11	0/2597
7	U	0.72	0/1916	1.11	0/2580
8	H	0.77	1/1521 (0.1%)	1.08	1/2062 (0.0%)
8	V	0.76	0/1521	1.11	1/2062 (0.0%)
9	I	0.78	0/1667	1.11	0/2266
9	W	0.77	0/1667	1.12	1/2266 (0.0%)
10	J	0.84	0/1620	1.09	5/2184 (0.2%)
10	X	0.84	1/1620 (0.1%)	1.08	2/2184 (0.1%)
11	K	0.76	0/1603	1.09	5/2168 (0.2%)
11	Y	0.78	0/1611	1.09	5/2180 (0.2%)
12	L	0.81	1/1609 (0.1%)	1.10	2/2170 (0.1%)
12	Z	0.82	2/1609 (0.1%)	1.10	2/2170 (0.1%)
13	M	0.84	1/1684 (0.1%)	1.12	2/2268 (0.1%)
13	a	0.84	1/1684 (0.1%)	1.12	1/2268 (0.0%)
14	N	0.73	0/1706	1.10	6/2309 (0.3%)
14	b	0.74	0/1706	1.08	6/2309 (0.3%)
All	All	0.75	9/49168 (0.0%)	1.10	74/66419 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	Z	45	MET	SD-CE	-9.11	1.56	1.79
12	L	45	MET	SD-CE	-8.69	1.57	1.79
5	S	107	MET	SD-CE	-8.63	1.57	1.79
13	a	83	MET	SD-CE	-6.06	1.64	1.79
13	M	83	MET	SD-CE	-5.87	1.64	1.79
8	H	172	VAL	CA-C	5.50	1.57	1.52
6	F	118	ILE	CA-CB	5.43	1.56	1.54
10	X	183	MET	SD-CE	-5.26	1.66	1.79
12	Z	116	GLU	CA-C	5.12	1.59	1.52

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	69	ASN	CA-CB-CG	9.28	121.88	112.60
3	C	69	ASN	CA-CB-CG	9.26	121.86	112.60
8	H	191	ASN	CA-CB-CG	8.00	120.60	112.60
8	V	191	ASN	CA-CB-CG	7.99	120.59	112.60
11	Y	24	ASN	CA-CB-CG	7.81	120.41	112.60
6	F	204	ASP	CA-CB-CG	7.40	120.00	112.60
1	O	125	TYR	CA-C-N	7.22	131.29	120.31
1	O	125	TYR	C-N-CA	7.22	131.29	120.31
1	A	125	TYR	CA-C-N	7.20	131.25	120.31
1	A	125	TYR	C-N-CA	7.20	131.25	120.31
6	T	204	ASP	CA-CB-CG	7.00	119.61	112.60
3	Q	151	ASP	CA-CB-CG	6.70	119.30	112.60
3	C	151	ASP	CA-CB-CG	6.55	119.15	112.60
9	W	23	ASP	CA-CB-CG	6.47	119.08	112.60
14	N	46	ASN	CA-CB-CG	6.21	118.81	112.60
14	N	180	ASP	CA-CB-CG	6.21	118.81	112.60
14	b	180	ASP	CA-CB-CG	6.19	118.79	112.60
14	b	46	ASN	CA-CB-CG	6.09	118.69	112.60
2	B	142	ARG	N-CA-C	5.92	115.12	108.25
10	J	117	PHE	CA-CB-CG	-5.87	107.93	113.80
5	E	120	ALA	N-CA-C	5.84	117.34	110.97
3	C	6	ASP	CA-C-N	5.79	128.62	120.28
3	C	6	ASP	C-N-CA	5.79	128.62	120.28
10	J	69	PHE	CA-CB-CG	5.70	119.50	113.80
14	b	126	ASP	CA-CB-CG	5.69	118.29	112.60
10	X	102	PRO	N-CA-C	5.67	120.19	111.57
11	K	49	GLU	CA-C-N	5.67	129.32	120.82
11	K	49	GLU	C-N-CA	5.67	129.32	120.82
5	S	120	ALA	N-CA-C	5.63	117.11	110.97
12	Z	124	ASN	CA-CB-CG	5.62	118.22	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	51	GLY	CA-C-N	5.60	128.10	120.54
11	K	51	GLY	C-N-CA	5.60	128.10	120.54
14	N	126	ASP	CA-CB-CG	5.59	118.19	112.60
3	Q	6	ASP	CA-C-N	5.54	128.26	120.28
3	Q	6	ASP	C-N-CA	5.54	128.26	120.28
14	b	106	LEU	N-CA-C	-5.45	98.89	108.20
10	J	56	LEU	CA-C-N	5.42	127.86	120.54
10	J	56	LEU	C-N-CA	5.42	127.86	120.54
2	P	139	ASN	CA-CB-CG	5.41	118.01	112.60
3	Q	227	VAL	N-CA-CB	5.38	117.14	111.00
11	Y	49	GLU	CA-C-N	5.38	128.90	120.82
11	Y	49	GLU	C-N-CA	5.38	128.90	120.82
3	C	227	VAL	N-CA-CB	5.38	116.58	110.72
6	F	175	HIS	CA-C-N	5.37	127.73	120.38
6	F	175	HIS	C-N-CA	5.37	127.73	120.38
14	N	25	ASP	CA-CB-CG	5.36	117.96	112.60
13	a	145	LEU	N-CA-C	5.36	117.20	111.36
14	N	106	LEU	N-CA-C	-5.35	99.05	108.20
11	Y	51	GLY	CA-C-N	5.34	127.76	120.54
11	Y	51	GLY	C-N-CA	5.34	127.76	120.54
6	F	6	TYR	CA-C-N	5.34	131.65	122.09
6	F	6	TYR	C-N-CA	5.34	131.65	122.09
12	Z	174	VAL	CB-CA-C	-5.31	103.70	110.98
10	X	69	PHE	CA-CB-CG	5.30	119.10	113.80
6	T	235	GLY	N-CA-C	5.28	119.53	112.77
13	M	114	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	219	VAL	N-CA-C	5.27	115.95	108.42
1	O	219	VAL	N-CA-C	5.26	115.94	108.42
2	B	124	GLY	N-CA-C	5.25	117.50	111.36
12	L	124	ASN	CA-CB-CG	5.20	117.80	112.60
4	D	59	VAL	N-CA-CB	-5.18	105.21	111.94
11	K	123	ALA	N-CA-C	-5.15	101.31	109.96
12	L	174	VAL	CB-CA-C	-5.13	103.96	110.98
1	O	163	PHE	CA-CB-CG	5.11	118.91	113.80
14	N	53	ALA	N-CA-C	5.10	117.39	108.76
5	S	238	ILE	CA-C-N	5.08	127.34	120.38
5	S	238	ILE	C-N-CA	5.08	127.34	120.38
13	M	104	TYR	N-CA-C	-5.07	101.70	109.76
14	b	25	ASP	CA-CB-CG	5.06	117.66	112.60
10	J	194	LYS	N-CA-C	5.04	115.96	108.60
14	b	53	ALA	N-CA-C	5.03	117.27	108.76
4	D	157	LYS	N-CA-C	-5.01	105.53	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	57	ASP	CA-C-N	5.01	127.24	120.38
2	B	57	ASP	C-N-CA	5.01	127.24	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1871	0	1876	17	0
1	O	1886	0	1892	19	0
2	B	1787	0	1782	14	0
2	P	1787	0	1782	18	0
3	C	1912	0	1928	14	0
3	Q	2003	0	2023	18	0
4	D	1798	0	1820	15	0
4	R	1848	0	1865	18	0
5	E	1758	0	1742	13	0
5	S	1769	0	1753	11	0
6	F	1857	0	1845	24	0
6	T	1846	0	1832	28	0
7	G	1894	0	1877	24	0
7	U	1881	0	1868	15	0
8	H	1493	0	1457	12	0
8	V	1493	0	1457	15	0
9	I	1641	0	1681	16	0
9	W	1641	0	1681	21	0
10	J	1591	0	1608	12	0
10	X	1591	0	1609	14	0
11	K	1571	0	1573	12	0
11	Y	1578	0	1580	14	0
12	L	1576	0	1522	16	0
12	Z	1576	0	1522	15	0
13	M	1654	0	1656	15	0
13	a	1654	0	1656	13	0
14	N	1673	0	1650	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	b	1673	0	1650	10	0
15	A	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	J	2	0	0	0	0
15	L	1	0	0	0	0
15	M	1	0	0	0	0
15	O	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	X	1	0	0	0	0
15	Z	1	0	0	0	0
15	a	1	0	0	0	0
16	F	3	0	0	0	0
16	K	6	0	0	0	0
16	M	9	0	0	0	0
16	T	3	0	0	0	0
16	U	3	0	0	0	0
16	Z	3	0	0	0	0
16	a	6	0	0	0	0
17	H	24	0	0	2	0
17	L	24	0	0	0	0
17	V	24	0	0	3	0
17	Z	24	0	0	0	0
18	A	44	0	0	1	0
18	B	35	0	0	0	0
18	C	60	0	0	0	0
18	D	27	0	0	0	0
18	E	38	0	0	0	0
18	F	37	0	0	0	0
18	G	34	0	0	0	0
18	H	52	0	0	0	0
18	I	52	0	0	0	0
18	J	69	0	0	0	0
18	K	48	0	0	0	0
18	L	63	0	0	2	0
18	M	80	0	0	0	0
18	N	75	0	0	0	0
18	O	35	0	0	0	0
18	P	34	0	0	0	0
18	Q	40	0	0	0	0
18	R	29	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	S	22	0	0	0	0
18	T	58	0	0	0	0
18	U	43	0	0	0	0
18	V	57	0	0	0	0
18	W	52	0	0	0	0
18	X	68	0	0	1	0
18	Y	42	0	0	0	0
18	Z	62	0	0	0	0
18	a	67	0	0	0	0
18	b	72	0	0	0	0
All	All	49839	0	48187	403	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 (403) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:28:PHE:HB3	10:J:36:THR:HG22	1.39	1.05
7:U:34:SER:HB3	7:U:65:ARG:HH12	1.36	0.89
13:a:145:LEU:HD21	13:a:182:ALA:HB2	1.57	0.86
13:M:145:LEU:HD21	13:M:182:ALA:HB2	1.57	0.85
10:J:45:MET:HE3	10:J:71:LEU:HD22	1.58	0.84
10:X:45:MET:HE3	10:X:71:LEU:HD22	1.60	0.82
14:N:107:TRP:CE2	14:N:127:MET:HE1	2.16	0.80
14:b:107:TRP:CE2	14:b:127:MET:HE1	2.19	0.78
6:T:185:ASN:HD21	6:T:189:LYS:HZ2	1.33	0.77
6:T:189:LYS:HE2	6:T:235:GLY:HA3	1.68	0.76
6:T:185:ASN:HD21	6:T:189:LYS:NZ	1.84	0.74
10:J:28:PHE:CB	10:J:36:THR:HG22	2.17	0.74
7:U:34:SER:HB3	7:U:65:ARG:NH1	2.03	0.73
13:M:211:ARG:HG3	9:W:196:VAL:HG21	1.72	0.72
4:R:98:VAL:HG22	12:Z:78:ALA:HB1	1.71	0.72
5:S:107:MET:HE3	5:S:112:VAL:HG22	1.70	0.71
4:R:135:GLY:HA2	4:R:211:MET:HE3	1.73	0.71
8:V:20:VAL:HG22	17:V:901:S5K:C16	2.21	0.71
10:J:28:PHE:HB3	10:J:36:THR:CG2	2.19	0.70
5:E:167:ALA:HB3	6:F:56:LEU:HD13	1.73	0.70
8:H:20:VAL:HG22	17:H:901:S5K:O17	1.92	0.69
3:Q:171:ALA:HB2	3:Q:200:THR:HG21	1.76	0.66
12:Z:115:ASP:HB2	12:Z:119:THR:HB	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:115:ASP:HB2	12:L:119:THR:HB	1.78	0.65
6:T:50:LYS:HB3	6:T:59:HIS:HB3	1.77	0.65
3:C:171:ALA:HB2	3:C:200:THR:HG21	1.78	0.65
4:R:8:THR:HB	4:R:18:GLN:HB2	1.79	0.65
4:D:8:THR:HB	4:D:18:GLN:HB2	1.80	0.64
1:A:196:GLU:HB2	1:A:242:LEU:HD11	1.79	0.64
9:W:63:MET:HE3	9:W:74:PRO:HB3	1.79	0.64
7:G:38:GLY:HA3	7:G:136:MET:HE1	1.79	0.63
7:G:136:MET:HE3	7:G:163:CYS:HB3	1.81	0.63
7:U:228:PRO:HG2	7:U:231:ILE:HD12	1.81	0.63
6:T:189:LYS:HB3	6:T:193:ARG:HH21	1.64	0.62
7:U:108:LEU:HD13	7:U:139:SER:HB2	1.81	0.62
8:V:20:VAL:HG22	17:V:901:S5K:O17	2.00	0.62
7:G:49:VAL:CG1	7:G:65:ARG:HE	2.13	0.62
5:S:28:ILE:HD13	5:S:158:PRO:HD2	1.81	0.62
10:X:36:THR:HG21	18:X:425:HOH:O	1.98	0.62
11:K:118:MET:HE2	11:K:124:LEU:HD13	1.80	0.62
8:V:28:ASN:ND2	9:W:120:SER:OG	2.32	0.62
5:E:28:ILE:HD13	5:E:158:PRO:HD2	1.82	0.62
4:R:181:ILE:HA	4:R:187:THR:HG22	1.81	0.62
4:D:181:ILE:HA	4:D:187:THR:HG22	1.81	0.61
6:F:52:ALA:HB2	6:F:59:HIS:ND1	2.16	0.61
7:G:49:VAL:HG11	7:G:65:ARG:HE	1.65	0.61
9:I:63:MET:HE3	9:I:74:PRO:HB3	1.82	0.61
5:S:42:THR:HG22	5:S:44:GLU:H	1.64	0.61
6:F:175:HIS:HD2	6:F:178:GLU:OE2	1.84	0.61
7:G:108:LEU:HD13	7:G:139:SER:HB2	1.82	0.60
6:F:52:ALA:HB2	6:F:59:HIS:CE1	2.36	0.60
1:O:37:LEU:HD22	1:O:53:GLN:HB2	1.83	0.60
13:a:99:ARG:HG3	13:a:104:TYR:CE2	2.37	0.60
6:T:175:HIS:HD2	6:T:178:GLU:OE2	1.84	0.59
6:T:189:LYS:CE	6:T:235:GLY:HA3	2.31	0.59
3:C:15:GLU:HB2	3:C:17:ARG:HG3	1.85	0.59
11:Y:21:ALA:HB3	11:Y:29:LYS:HB2	1.83	0.59
1:A:37:LEU:HD22	1:A:53:GLN:HB2	1.84	0.59
13:M:99:ARG:HG3	13:M:104:TYR:CE2	2.37	0.59
11:Y:118:MET:HE2	11:Y:124:LEU:HD13	1.83	0.59
2:P:68:THR:HG23	2:P:70:HIS:ND1	2.17	0.59
9:W:13:ILE:HG22	9:W:155:LEU:HD22	1.85	0.58
6:F:47:VAL:HG12	6:F:195:LEU:HD22	1.85	0.58
9:I:41:ILE:HG21	9:I:79:VAL:HG11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:4:ASN:HD22	6:F:6:TYR:H	1.51	0.58
6:T:47:VAL:HG12	6:T:195:LEU:HD22	1.86	0.58
4:D:98:VAL:HG22	12:L:78:ALA:HB1	1.85	0.58
7:U:215:TRP:CD2	7:U:227:VAL:HG22	2.39	0.58
8:V:97:HIS:HE1	8:V:114:THR:H	1.52	0.57
11:K:21:ALA:HB3	11:K:29:LYS:HB2	1.85	0.57
7:G:215:TRP:CD2	7:G:227:VAL:HG22	2.39	0.56
5:S:167:ALA:HB3	6:T:56:LEU:HD13	1.86	0.56
2:P:68:THR:CG2	2:P:70:HIS:CE1	2.88	0.56
6:F:193:ARG:HD3	6:F:236:LEU:HD23	1.88	0.56
12:Z:174:VAL:HG22	12:Z:192:VAL:HG23	1.88	0.56
2:P:68:THR:HG21	2:P:70:HIS:CE1	2.41	0.56
4:D:39:ASP:HA	4:D:213:ARG:HE	1.70	0.56
1:O:32:ILE:HD13	1:O:137:CYS:HB2	1.88	0.55
10:X:15:LYS:HE3	10:X:134:ASP:HA	1.89	0.55
12:L:174:VAL:HG22	12:L:192:VAL:HG23	1.89	0.55
5:E:24:VAL:O	5:E:28:ILE:HG12	2.07	0.55
13:a:61:CYS:O	13:a:65:THR:HB	2.07	0.55
6:F:50:LYS:HB3	6:F:59:HIS:HB3	1.87	0.55
6:F:175:HIS:CD2	6:F:178:GLU:OE2	2.60	0.55
9:I:13:ILE:HG22	9:I:155:LEU:HD22	1.89	0.55
1:O:130:GLU:HG2	2:P:4:GLY:HA2	1.89	0.55
13:M:61:CYS:O	13:M:65:THR:HB	2.07	0.55
6:T:175:HIS:CD2	6:T:178:GLU:OE2	2.60	0.55
12:Z:7:LYS:HB2	12:Z:124:ASN:HB2	1.88	0.55
10:J:15:LYS:HE3	10:J:134:ASP:HA	1.90	0.54
12:L:7:LYS:HB2	12:L:124:ASN:HB2	1.88	0.54
1:A:141:ILE:HD12	1:A:220:VAL:HG22	1.90	0.54
5:S:24:VAL:O	5:S:28:ILE:HG12	2.07	0.54
1:A:130:GLU:HG2	2:B:4:GLY:HA2	1.89	0.54
1:A:165:ALA:HB3	2:B:55:LEU:HD22	1.88	0.54
7:G:213:LEU:HD12	7:G:232:ARG:HG2	1.88	0.54
7:G:136:MET:HE2	7:G:148:LEU:HD11	1.88	0.54
9:W:149:GLU:CD	9:W:149:GLU:H	2.15	0.54
18:L:1052:HOH:O	10:X:204:MET:HG3	2.07	0.54
1:O:165:ALA:HB3	2:P:55:LEU:HD22	1.89	0.54
7:U:213:LEU:HD12	7:U:232:ARG:HG2	1.89	0.53
1:A:32:ILE:HD13	1:A:137:CYS:HB2	1.90	0.53
9:I:143:GLN:O	9:I:146:MET:HG3	2.08	0.53
9:W:216:VAL:HG22	10:X:196:THR:HG23	1.89	0.53
9:W:143:GLN:O	9:W:146:MET:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:54:LEU:HB2	7:G:58:TYR:HE2	1.73	0.53
8:H:66:HIS:CE1	8:H:70:LEU:HD22	2.44	0.53
3:C:34:CYS:HB3	3:C:164:ILE:HG13	1.91	0.53
12:L:105:ASP:HB2	18:L:1040:HOH:O	2.09	0.53
4:R:140:GLY:O	4:R:213:ARG:NH1	2.42	0.53
1:A:68:HIS:HD2	18:A:406:HOH:O	1.92	0.52
7:G:12:SER:HB3	7:G:125:TYR:HA	1.91	0.52
9:I:213:THR:HB	10:J:199:THR:OG1	2.09	0.52
3:Q:34:CYS:HB3	3:Q:164:ILE:HG13	1.92	0.52
7:U:12:SER:HB3	7:U:125:TYR:HA	1.91	0.52
1:A:126:THR:HG22	2:B:127:ARG:HH21	1.75	0.52
2:P:110:VAL:HG22	2:P:135:ILE:HD13	1.90	0.52
2:B:110:VAL:HG22	2:B:135:ILE:HD13	1.90	0.52
5:E:193:GLU:HA	5:E:196:LYS:HG2	1.91	0.52
13:M:16:ALA:HB2	13:M:121:VAL:HG23	1.91	0.52
4:D:51:ALA:HB3	4:D:54:GLN:HG3	1.91	0.52
3:Q:239:LYS:O	3:Q:243:GLU:HG2	2.09	0.52
1:O:211:LYS:HB2	1:O:214:GLU:HG3	1.91	0.52
13:a:16:ALA:HB2	13:a:121:VAL:HG23	1.92	0.52
10:J:184:GLY:HA2	10:J:202:ALA:HB3	1.92	0.52
1:O:46:ASP:HB2	1:O:222:VAL:HG12	1.91	0.52
9:W:163:ILE:HG23	9:W:170:GLY:HA2	1.92	0.52
1:A:72:ILE:HG21	1:A:114:LEU:HD21	1.91	0.51
14:N:107:TRP:CD2	14:N:127:MET:HE1	2.44	0.51
11:K:134:TYR:HB3	11:Y:25:ILE:HD13	1.92	0.51
2:P:106:THR:H	2:P:139:ASN:ND2	2.08	0.51
9:I:205:VAL:O	9:I:208:THR:HG23	2.11	0.51
1:O:72:ILE:HG21	1:O:114:LEU:HD21	1.92	0.51
5:S:202:LEU:HG	5:S:206:MET:HE2	1.91	0.51
8:V:48:SER:HA	17:V:901:S5K:C7	2.41	0.51
1:A:191:PHE:HE1	1:A:219:VAL:HG21	1.76	0.51
1:O:126:THR:HG22	2:P:127:ARG:HH21	1.76	0.51
1:O:32:ILE:HA	1:O:82:GLY:HA2	1.92	0.51
4:R:40:ILE:HD11	4:R:210:VAL:HB	1.93	0.51
8:V:118:MET:HE3	14:b:57:TYR:HD2	1.75	0.51
9:W:213:THR:HB	10:X:199:THR:OG1	2.11	0.51
4:D:108:THR:HG21	4:D:145:TYR:HB3	1.93	0.51
8:H:30:VAL:HG11	14:b:211:ILE:HG13	1.92	0.51
5:E:202:LEU:HG	5:E:206:MET:HE2	1.91	0.50
5:E:220:VAL:HG22	5:E:226:PHE:HA	1.93	0.50
14:b:107:TRP:NE1	14:b:127:MET:HE1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:205:VAL:O	9:W:208:THR:HG23	2.11	0.50
14:N:107:TRP:NE1	14:N:127:MET:HE1	2.25	0.50
3:Q:160:LYS:HZ3	3:Q:181:GLU:HG2	1.77	0.50
4:R:95:ARG:HH21	4:R:101:PRO:HB3	1.76	0.50
12:Z:157:ARG:HG3	12:Z:195:LEU:HD13	1.93	0.50
2:B:68:THR:HG23	2:B:70:HIS:ND1	2.26	0.50
7:G:38:GLY:CA	7:G:136:MET:HE1	2.41	0.50
1:A:32:ILE:HA	1:A:82:GLY:HA2	1.92	0.50
5:E:91:LYS:HD2	5:E:119:LEU:HD11	1.94	0.50
7:G:228:PRO:HG2	7:G:231:ILE:HD12	1.94	0.50
4:D:40:ILE:HD11	4:D:210:VAL:HB	1.94	0.50
9:I:163:ILE:HG23	9:I:170:GLY:HA2	1.94	0.50
7:U:168:ALA:HB1	7:U:171:ALA:HB3	1.94	0.50
7:G:168:ALA:HB1	7:G:171:ALA:HB3	1.94	0.49
14:b:107:TRP:CD2	14:b:127:MET:HE1	2.47	0.49
4:R:199:VAL:HG11	4:R:205:ASN:HB2	1.95	0.49
6:F:81:ALA:HB2	6:F:130:VAL:HG21	1.93	0.49
4:R:91:CYS:O	4:R:95:ARG:HG3	2.12	0.49
7:U:201:HIS:HE1	7:U:206:ASP:O	1.96	0.49
8:H:20:VAL:HG22	17:H:901:S5K:C16	2.42	0.49
4:R:108:THR:HG21	4:R:145:TYR:HB3	1.95	0.48
11:K:44:LEU:HD11	11:K:102:LEU:HD13	1.94	0.48
12:L:157:ARG:HG3	12:L:195:LEU:HD13	1.95	0.48
6:T:81:ALA:HB2	6:T:130:VAL:HG21	1.94	0.48
1:O:49:VAL:HG12	1:O:194:THR:HG22	1.95	0.48
2:B:43:VAL:HG22	2:B:143:PRO:HB2	1.94	0.48
8:V:152:ARG:HG2	8:V:175:LEU:HD13	1.94	0.48
6:T:185:ASN:ND2	6:T:189:LYS:NZ	2.58	0.48
6:F:212:ILE:HD12	6:F:229:VAL:HG22	1.95	0.48
7:U:19:ARG:HH21	7:U:21:PHE:HE1	1.60	0.48
7:G:70:ASP:OD2	7:G:72:HIS:HE1	1.95	0.48
4:R:102:VAL:HG22	4:R:106:TYR:CD2	2.48	0.48
5:S:91:LYS:HD2	5:S:119:LEU:HD11	1.95	0.48
1:O:123:GLN:O	1:O:126:THR:HB	2.14	0.48
10:X:184:GLY:HA2	10:X:202:ALA:HB3	1.96	0.48
8:H:75:LEU:HA	8:H:104:ASP:OD1	2.13	0.48
10:X:28:PHE:HB3	10:X:36:THR:HG22	1.96	0.48
11:Y:44:LEU:HD11	11:Y:102:LEU:HD13	1.95	0.48
3:C:160:LYS:HZ3	3:C:181:GLU:HG2	1.79	0.48
1:O:49:VAL:HB	1:O:219:VAL:HG23	1.95	0.47
2:P:106:THR:H	2:P:139:ASN:HD21	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:4:LEU:HB2	11:Y:132:HIS:HB2	1.95	0.47
1:A:78:CYS:HB3	1:A:140:LEU:HD23	1.96	0.47
8:H:152:ARG:HG2	8:H:175:LEU:HD13	1.95	0.47
13:M:46:LEU:HB3	13:M:72:LEU:HD11	1.96	0.47
11:K:4:LEU:HB2	11:K:132:HIS:HB2	1.96	0.47
1:O:191:PHE:HE1	1:O:219:VAL:HG21	1.79	0.47
4:R:94:HIS:CG	4:R:102:VAL:HG23	2.48	0.47
6:T:33:SER:HB3	6:T:51:ARG:HG3	1.95	0.47
13:a:57:PHE:HB3	13:a:105:TYR:HB3	1.97	0.47
7:G:136:MET:CE	7:G:163:CYS:HB3	2.43	0.47
9:I:196:VAL:HG21	13:a:211:ARG:HG3	1.95	0.47
6:T:212:ILE:HD12	6:T:229:VAL:HG22	1.96	0.47
6:F:105:VAL:O	6:F:109:VAL:HG23	2.15	0.47
8:H:132:THR:HG22	8:V:132:THR:HG22	1.97	0.47
12:Z:161:ALA:HA	12:Z:192:VAL:HG22	1.96	0.47
14:b:22:ILE:HG23	14:b:50:MET:HE3	1.96	0.47
9:W:9:GLN:HB2	9:W:146:MET:O	2.14	0.47
11:Y:9:GLY:HA3	11:Y:12:TYR:CE1	2.49	0.47
1:A:221:THR:HG22	1:A:223:GLU:H	1.80	0.47
12:L:161:ALA:HA	12:L:192:VAL:HG22	1.96	0.47
13:M:57:PHE:HB3	13:M:105:TYR:HB3	1.97	0.47
14:N:22:ILE:HG23	14:N:50:MET:HE3	1.95	0.47
9:W:109:GLN:HG2	9:W:121:ARG:HE	1.80	0.47
14:b:211:ILE:HA	14:b:214:MET:HE3	1.96	0.47
3:Q:47:ALA:HB1	3:Q:64:LYS:HE2	1.97	0.47
6:T:176:MET:HA	6:T:179:PHE:CD2	2.49	0.47
7:U:70:ASP:OD2	7:U:72:HIS:HE1	1.97	0.47
1:A:123:GLN:O	1:A:126:THR:HB	2.15	0.47
6:F:4:ASN:ND2	6:F:6:TYR:H	2.13	0.47
9:I:109:GLN:HG2	9:I:121:ARG:HE	1.79	0.47
14:N:211:ILE:HA	14:N:214:MET:HE3	1.96	0.47
6:F:10:VAL:HG11	6:F:127:PRO:HD3	1.96	0.47
13:M:145:LEU:HD22	13:M:178:VAL:HB	1.97	0.47
13:a:46:LEU:HB3	13:a:72:LEU:HD11	1.97	0.47
8:H:118:MET:HE3	14:N:57:TYR:HD2	1.80	0.46
9:I:9:GLN:HB2	9:I:146:MET:O	2.15	0.46
14:N:27:LEU:HD22	14:N:184:TYR:HB2	1.97	0.46
11:K:9:GLY:HA3	11:K:12:TYR:CE1	2.50	0.46
2:P:134:LEU:HD22	2:P:145:LEU:HD11	1.96	0.46
8:V:114:THR:HA	8:V:118:MET:O	2.15	0.46
14:b:27:LEU:HD22	14:b:184:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:ALA:HB1	3:C:64:LYS:HE2	1.97	0.46
8:V:66:HIS:CE1	8:V:70:LEU:HD11	2.50	0.46
12:L:26:ILE:HG21	12:L:29:LEU:HD23	1.97	0.46
1:O:49:VAL:CG1	1:O:194:THR:HG22	2.45	0.46
1:O:78:CYS:HB3	1:O:140:LEU:HD23	1.97	0.46
6:T:105:VAL:O	6:T:109:VAL:HG23	2.16	0.46
5:E:182:GLN:HA	6:F:56:LEU:HD11	1.96	0.46
13:a:145:LEU:HD22	13:a:178:VAL:HB	1.98	0.46
14:N:153:VAL:HG21	14:N:168:LEU:HD13	1.98	0.46
5:S:96:THR:HA	5:S:107:MET:HE2	1.96	0.46
12:Z:26:ILE:HG21	12:Z:29:LEU:HD23	1.97	0.46
3:C:53:HIS:HB3	3:C:56:LEU:HG	1.97	0.46
1:A:49:VAL:HB	1:A:219:VAL:HG23	1.97	0.46
6:T:10:VAL:HG11	6:T:127:PRO:HD3	1.96	0.46
7:U:151:ILE:HA	7:U:156:VAL:O	2.16	0.46
11:K:166:GLU:OE1	11:K:166:GLU:HA	2.16	0.46
7:U:30:VAL:HG11	7:U:134:SER:HB2	1.99	0.46
11:Y:4:LEU:HD22	11:Y:45:LEU:HB3	1.97	0.46
11:K:4:LEU:HD22	11:K:45:LEU:HB3	1.97	0.45
8:V:15:GLY:HA2	8:V:174:TYR:O	2.16	0.45
2:B:21:ILE:HG21	2:B:151:SER:HB3	1.98	0.45
7:G:75:MET:HA	7:G:136:MET:O	2.17	0.45
1:A:112:ASP:HB3	1:A:152:TYR:CZ	2.52	0.45
3:Q:11:ILE:HG22	4:R:7:ILE:HG23	1.99	0.45
5:E:203:LYS:HB2	5:E:210:LEU:HD23	1.98	0.45
2:P:106:THR:OG1	2:P:139:ASN:ND2	2.50	0.45
5:S:203:LYS:HB2	5:S:210:LEU:HD23	1.98	0.45
11:Y:24:ASN:CG	11:Y:25:ILE:H	2.25	0.45
2:B:134:LEU:HD22	2:B:145:LEU:HD11	1.97	0.45
7:G:151:ILE:HA	7:G:156:VAL:O	2.17	0.45
3:C:11:ILE:HG22	4:D:7:ILE:HG23	1.99	0.45
9:I:59:VAL:HG21	9:I:83:LEU:HG	1.99	0.45
10:J:87:LEU:O	10:J:91:VAL:HG23	2.17	0.45
11:K:180:VAL:HG21	11:K:194:ILE:HG12	1.98	0.45
10:X:87:LEU:O	10:X:91:VAL:HG23	2.17	0.45
8:H:188:ILE:HG22	8:H:193:LEU:HD23	1.99	0.44
3:Q:137:ILE:HD12	3:Q:216:LEU:HB2	1.98	0.44
11:Y:180:VAL:HG21	11:Y:194:ILE:HG12	1.98	0.44
6:T:46:LEU:HG	6:T:135:ALA:HB2	1.99	0.44
6:T:50:LYS:CB	6:T:59:HIS:HB3	2.44	0.44
8:V:75:LEU:HD21	8:V:106:ARG:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:GLY:HA2	8:H:174:TYR:O	2.17	0.44
2:P:21:ILE:HG21	2:P:151:SER:HB3	1.99	0.44
9:W:6:LEU:HD13	9:W:138:LEU:HD22	1.99	0.44
4:D:102:VAL:HG22	4:D:106:TYR:CD2	2.53	0.44
6:F:46:LEU:HG	6:F:135:ALA:HB2	1.99	0.44
7:G:47:PHE:HB2	7:G:214:SER:HB2	1.99	0.44
2:B:68:THR:CG2	2:B:70:HIS:CE1	3.01	0.44
2:B:68:THR:HG21	2:B:70:HIS:CE1	2.53	0.44
11:Y:164:LEU:O	11:Y:168:GLN:HG2	2.18	0.44
9:I:6:LEU:HD13	9:I:138:LEU:HD22	2.00	0.44
1:O:182:LYS:HG3	1:O:187:PHE:HE2	1.83	0.44
3:Q:17:ARG:NH2	3:Q:19:TYR:HE1	2.15	0.44
6:F:196:ARG:HB2	6:F:205:LEU:HD11	2.00	0.44
8:V:75:LEU:HA	8:V:104:ASP:OD1	2.17	0.44
14:b:96:MET:HE3	14:b:127:MET:HA	2.00	0.44
2:P:28:VAL:HG11	2:P:132:SER:HB2	2.00	0.44
10:X:28:PHE:HB2	10:X:39:PHE:HB2	2.00	0.44
2:B:28:VAL:HG11	2:B:132:SER:HB2	2.00	0.44
9:I:67:ALA:HB2	9:I:74:PRO:HG3	2.00	0.44
6:T:27:GLU:O	6:T:31:GLN:HG2	2.18	0.44
6:T:52:ALA:HB2	6:T:59:HIS:CE1	2.53	0.44
6:T:196:ARG:HB2	6:T:205:LEU:HD11	2.00	0.44
9:W:7:VAL:HG22	9:W:12:VAL:HG12	2.00	0.44
7:G:30:VAL:HG11	7:G:134:SER:HB2	2.00	0.43
9:W:59:VAL:HG21	9:W:83:LEU:HG	1.99	0.43
7:G:165:ILE:HG22	7:G:169:ARG:HH21	1.83	0.43
11:K:51:GLY:HA3	12:L:117:HIS:O	2.17	0.43
9:I:7:VAL:HG22	9:I:12:VAL:HG12	2.01	0.43
14:N:96:MET:HE3	14:N:127:MET:HA	2.00	0.43
4:R:98:VAL:HG22	12:Z:78:ALA:CB	2.45	0.43
8:V:188:ILE:HG22	8:V:193:LEU:HD23	2.00	0.43
2:B:51:GLN:HE21	2:B:51:GLN:HA	1.83	0.43
4:R:89:VAL:HG22	11:Y:66:LEU:HD21	2.00	0.43
13:a:23:VAL:HG21	13:a:51:VAL:HG22	2.01	0.43
6:F:27:GLU:O	6:F:31:GLN:HG2	2.18	0.43
3:Q:14:PRO:HA	4:R:21:TYR:CD1	2.54	0.43
3:Q:195:LYS:HA	3:Q:240:HIS:CE1	2.53	0.43
1:A:141:ILE:HG22	1:A:151:VAL:HG22	2.01	0.43
11:K:164:LEU:O	11:K:168:GLN:HG2	2.19	0.43
2:P:58:GLU:CD	2:P:58:GLU:H	2.26	0.43
2:P:68:THR:HG21	2:P:70:HIS:HE1	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:VAL:O	3:C:25:MET:HG2	2.18	0.43
7:G:108:LEU:HD22	7:G:147:GLN:HB3	2.00	0.43
1:O:112:ASP:HB3	1:O:152:TYR:CZ	2.54	0.43
3:Q:246:LYS:HA	3:Q:249:ARG:HD2	2.00	0.43
4:R:212:ARG:HB2	4:R:215:GLN:HB2	2.01	0.43
5:S:77:ALA:HB3	5:S:142:LEU:HB2	2.00	0.43
11:Y:51:GLY:HA3	12:Z:117:HIS:O	2.18	0.43
3:C:147:LEU:HD21	3:C:162:THR:HG22	2.01	0.42
10:J:152:SER:CB	13:a:148:LEU:HD13	2.49	0.42
3:C:14:PRO:HA	4:D:21:TYR:CD1	2.54	0.42
3:C:137:ILE:HD12	3:C:216:LEU:HB2	2.00	0.42
5:E:97:GLN:HB3	12:L:61:LYS:HG3	2.01	0.42
6:F:214:ILE:HG22	6:F:219:LEU:HD23	2.01	0.42
13:M:158:MET:CE	9:W:204:PHE:HE1	2.32	0.42
7:U:47:PHE:HB2	7:U:214:SER:HB2	2.00	0.42
6:F:40:SER:HB3	6:F:187:LEU:HD22	2.01	0.42
5:E:36:THR:HG21	5:E:173:ALA:HB3	2.01	0.42
1:O:141:ILE:HG22	1:O:151:VAL:HG22	2.02	0.42
4:R:32:ALA:HB3	4:R:161:ILE:HG13	2.01	0.42
6:T:84:LEU:O	6:T:88:MET:HG3	2.19	0.42
7:G:38:GLY:HA3	7:G:136:MET:CE	2.48	0.42
10:J:152:SER:HB2	13:a:148:LEU:HD13	2.02	0.42
10:X:17:LYS:HB2	10:X:157:ASN:HB3	2.00	0.42
4:D:32:ALA:HB3	4:D:161:ILE:HG13	2.01	0.42
13:a:135:PHE:CD2	13:a:149:LEU:HB3	2.55	0.42
12:L:4:LEU:CD2	12:L:159:ALA:HB3	2.49	0.42
3:Q:147:LEU:HD21	3:Q:162:THR:HG22	2.02	0.42
3:Q:198:ASN:HA	3:Q:206:LEU:HD13	2.01	0.42
3:Q:209:GLU:H	3:Q:209:GLU:HG3	1.75	0.42
6:T:33:SER:OG	6:T:62:LYS:HE3	2.20	0.42
6:T:40:SER:HB3	6:T:187:LEU:HD22	2.02	0.42
9:W:15:GLY:HA3	9:W:155:LEU:HD21	2.02	0.42
2:P:72:GLY:HA3	2:P:217:PHE:CE1	2.55	0.42
9:W:63:MET:CE	9:W:74:PRO:HB3	2.46	0.42
12:Z:115:ASP:HB3	12:Z:117:HIS:H	1.85	0.42
9:W:13:ILE:HG12	9:W:177:VAL:HG22	2.02	0.42
9:W:67:ALA:HB2	9:W:74:PRO:HG3	2.02	0.42
7:G:19:ARG:HH21	7:G:21:PHE:HE1	1.60	0.41
3:C:160:LYS:NZ	3:C:181:GLU:HG2	2.35	0.41
12:L:13:ILE:HG13	12:L:152:ALA:HB1	2.02	0.41
14:N:211:ILE:HG13	8:V:30:VAL:HG11	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:180:LYS:O	3:Q:184:MET:HG2	2.20	0.41
6:T:199:LEU:HD22	6:T:203:GLN:HG3	2.02	0.41
7:U:34:SER:OG	7:U:50:GLU:O	2.30	0.41
4:D:42:VAL:HG22	4:D:210:VAL:HG12	2.01	0.41
5:E:10:ARG:HB3	6:F:8:ASN:ND2	2.35	0.41
13:M:10:GLY:HA3	13:M:42:LYS:HE3	2.01	0.41
4:D:146:GLN:O	4:D:153:TYR:HA	2.20	0.41
12:L:103:GLY:HA2	12:L:179:MET:HE3	2.02	0.41
13:M:158:MET:HE2	9:W:204:PHE:CE1	2.55	0.41
12:Z:4:LEU:CD2	12:Z:159:ALA:HB3	2.50	0.41
12:L:114:VAL:HA	12:L:119:THR:O	2.21	0.41
12:Z:13:ILE:HG13	12:Z:152:ALA:HB1	2.02	0.41
12:Z:113:TYR:O	12:Z:120:ARG:HA	2.21	0.41
4:D:188:ILE:HG23	4:D:208:LEU:HD21	2.02	0.41
5:E:77:ALA:HB3	5:E:142:LEU:HB2	2.02	0.41
7:G:219:LEU:HD13	7:G:220:THR:HG23	2.02	0.41
13:M:135:PHE:CD2	13:M:149:LEU:HB3	2.55	0.41
6:T:103:LEU:HD12	6:T:104:PRO:HD2	2.01	0.41
12:Z:3:THR:HG22	12:Z:16:VAL:HG12	2.01	0.41
13:a:10:GLY:HA3	13:a:42:LYS:HE3	2.02	0.41
2:B:183:LEU:O	2:B:187:ILE:HG13	2.20	0.41
3:C:112:THR:HG22	3:C:156:TYR:CE1	2.56	0.41
6:F:98:VAL:HA	14:N:94:ARG:HG3	2.02	0.41
8:H:80:ALA:HB1	8:H:119:LEU:HD11	2.02	0.41
12:L:115:ASP:HB3	12:L:117:HIS:H	1.85	0.41
3:Q:21:VAL:O	3:Q:25:MET:HG2	2.20	0.41
5:S:36:THR:HG21	5:S:173:ALA:HB3	2.02	0.41
2:B:72:GLY:HA3	2:B:217:PHE:CE1	2.55	0.41
6:F:33:SER:OG	6:F:62:LYS:HE3	2.20	0.41
8:H:82:VAL:O	8:H:86:ILE:HG13	2.21	0.41
12:L:35:ILE:HG21	12:L:56:GLU:HB3	2.02	0.41
10:X:8:GLY:HA2	10:X:141:THR:HG21	2.02	0.41
10:X:65:GLN:OE1	11:Y:86:ARG:NH2	2.54	0.41
12:Z:35:ILE:HG21	12:Z:56:GLU:HB3	2.02	0.41
14:b:92:LEU:O	14:b:96:MET:HG2	2.20	0.41
3:C:180:LYS:O	3:C:184:MET:HG2	2.21	0.41
13:M:14:ALA:HA	13:M:22:ILE:O	2.21	0.41
1:O:191:PHE:CE1	1:O:219:VAL:HG21	2.56	0.41
3:Q:45:LEU:HD13	3:Q:75:SER:HB2	2.03	0.41
13:M:83:MET:HE2	13:M:83:MET:HB3	1.99	0.40
6:F:103:LEU:HD12	6:F:104:PRO:HD2	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:112:GLY:O	9:I:119:TYR:HA	2.22	0.40
2:P:43:VAL:HG22	2:P:143:PRO:HB2	2.03	0.40
2:P:162:MET:HE3	2:P:162:MET:HB2	1.96	0.40
6:T:35:THR:HG23	6:T:133:LEU:HD12	2.03	0.40
13:M:198:VAL:HG22	13:M:203:ILE:HG12	2.04	0.40
3:Q:13:SER:HB2	3:Q:19:TYR:CE2	2.57	0.40
4:D:30:SER:HB3	4:D:46:GLU:HG3	2.04	0.40
10:J:20:VAL:HG13	10:J:119:PRO:HB3	2.04	0.40
9:I:203:HIS:CE1	10:J:155:GLU:OE2	2.75	0.40
11:K:25:ILE:HD13	11:Y:134:TYR:HB3	2.03	0.40
10:X:20:VAL:HG13	10:X:119:PRO:HB3	2.04	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	238/242 (98%)	237 (100%)	0	1 (0%)	30	36
1	O	240/242 (99%)	237 (99%)	3 (1%)	0	100	100
2	B	227/229 (99%)	217 (96%)	10 (4%)	0	100	100
2	P	227/229 (99%)	222 (98%)	5 (2%)	0	100	100
3	C	239/256 (93%)	235 (98%)	4 (2%)	0	100	100
3	Q	249/256 (97%)	244 (98%)	5 (2%)	0	100	100
4	D	221/237 (93%)	217 (98%)	4 (2%)	0	100	100
4	R	230/237 (97%)	226 (98%)	3 (1%)	1 (0%)	30	36
5	E	226/232 (97%)	219 (97%)	7 (3%)	0	100	100
5	S	230/232 (99%)	226 (98%)	4 (2%)	0	100	100
6	F	234/236 (99%)	228 (97%)	5 (2%)	1 (0%)	30	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	T	233/236 (99%)	227 (97%)	6 (3%)	0	100	100
7	G	240/242 (99%)	233 (97%)	7 (3%)	0	100	100
7	U	238/242 (98%)	231 (97%)	6 (2%)	1 (0%)	30	36
8	H	197/199 (99%)	191 (97%)	6 (3%)	0	100	100
8	V	197/199 (99%)	191 (97%)	6 (3%)	0	100	100
9	I	221/223 (99%)	214 (97%)	6 (3%)	1 (0%)	24	29
9	W	221/223 (99%)	214 (97%)	6 (3%)	1 (0%)	24	29
10	J	202/204 (99%)	195 (96%)	6 (3%)	1 (0%)	24	29
10	X	202/204 (99%)	196 (97%)	5 (2%)	1 (0%)	24	29
11	K	194/197 (98%)	188 (97%)	5 (3%)	1 (0%)	24	29
11	Y	195/197 (99%)	189 (97%)	5 (3%)	1 (0%)	24	29
12	L	201/203 (99%)	197 (98%)	4 (2%)	0	100	100
12	Z	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
13	M	211/213 (99%)	208 (99%)	3 (1%)	0	100	100
13	a	211/213 (99%)	208 (99%)	3 (1%)	0	100	100
14	N	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
14	b	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
All	All	6149/6254 (98%)	5994 (98%)	145 (2%)	10 (0%)	43	53

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	U	207	LYS
1	A	189	TRP
11	K	174	ASN
4	R	213	ARG
11	Y	174	ASN
10	X	156	PRO
9	I	195	PRO
10	J	156	PRO
9	W	195	PRO
6	F	235	GLY

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	205/206 (100%)	196 (96%)	9 (4%)	25	35
1	O	206/206 (100%)	197 (96%)	9 (4%)	25	35
2	B	188/188 (100%)	178 (95%)	10 (5%)	20	28
2	P	188/188 (100%)	180 (96%)	8 (4%)	26	36
3	C	203/216 (94%)	189 (93%)	14 (7%)	14	18
3	Q	213/216 (99%)	201 (94%)	12 (6%)	19	25
4	D	193/201 (96%)	182 (94%)	11 (6%)	18	25
4	R	198/201 (98%)	188 (95%)	10 (5%)	21	29
5	E	193/194 (100%)	182 (94%)	11 (6%)	18	25
5	S	194/194 (100%)	184 (95%)	10 (5%)	21	28
6	F	202/202 (100%)	192 (95%)	10 (5%)	22	30
6	T	201/202 (100%)	192 (96%)	9 (4%)	24	35
7	G	199/199 (100%)	191 (96%)	8 (4%)	28	40
7	U	198/199 (100%)	190 (96%)	8 (4%)	28	40
8	H	153/153 (100%)	151 (99%)	2 (1%)	61	76
8	V	153/153 (100%)	149 (97%)	4 (3%)	40	56
9	I	175/175 (100%)	170 (97%)	5 (3%)	37	52
9	W	175/175 (100%)	169 (97%)	6 (3%)	32	46
10	J	173/173 (100%)	169 (98%)	4 (2%)	44	60
10	X	173/173 (100%)	168 (97%)	5 (3%)	37	52
11	K	167/168 (99%)	164 (98%)	3 (2%)	51	68
11	Y	168/168 (100%)	162 (96%)	6 (4%)	31	44
12	L	165/165 (100%)	153 (93%)	12 (7%)	13	16
12	Z	165/165 (100%)	154 (93%)	11 (7%)	15	19
13	M	178/178 (100%)	168 (94%)	10 (6%)	19	25
13	a	178/178 (100%)	167 (94%)	11 (6%)	16	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	177/177 (100%)	169 (96%)	8 (4%)	24	35
14	b	177/177 (100%)	169 (96%)	8 (4%)	24	35
All	All	5158/5190 (99%)	4924 (96%)	234 (4%)	24	35

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	VAL
1	A	92	GLN
1	A	126	THR
1	A	130	GLU
1	A	146	GLU
1	A	183	VAL
1	A	205	VAL
1	A	219	VAL
1	A	222	VAL
2	B	19	VAL
2	B	43	VAL
2	B	51	GLN
2	B	73	LEU
2	B	123	SER
2	B	132	SER
2	B	139	ASN
2	B	201	GLN
2	B	214	GLU
2	B	232	ILE
3	C	13	SER
3	C	43	VAL
3	C	69	ASN
3	C	70	GLU
3	C	80	THR
3	C	132	VAL
3	C	133	SER
3	C	151	ASP
3	C	155	ASN
3	C	181	GLU
3	C	186	LEU
3	C	194	ILE
3	C	227	VAL
3	C	229	LYS
4	D	4	ASP

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Mol	Chain	Res	Type
4	D	8	THR
4	D	46	GLU
4	D	54	GLN
4	D	56	GLU
4	D	59	VAL
4	D	98	VAL
4	D	102	VAL
4	D	146	GLN
4	D	208	LEU
4	D	211	MET
5	E	20	ARG
5	E	36	THR
5	E	42	THR
5	E	62	SER
5	E	95	GLU
5	E	179	SER
5	E	184	VAL
5	E	210	LEU
5	E	216	GLU
5	E	224	GLN
5	E	238	ILE
6	F	4	ASN
6	F	7	ASP
6	F	9	ASP
6	F	62	LYS
6	F	101	ARG
6	F	115	LYS
6	F	166	GLN
6	F	173	GLU
6	F	202	GLU
6	F	229	VAL
7	G	53	VAL
7	G	69	VAL
7	G	147	GLN
7	G	181	MET
7	G	214	SER
7	G	218	GLU
7	G	219	LEU
7	G	221	ASN
8	H	176	VAL
8	H	191	ASN
9	I	73	GLU

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Mol	Chain	Res	Type
9	I	79	VAL
9	I	149	GLU
9	I	193	THR
9	I	213	THR
10	J	27	ARG
10	J	36	THR
10	J	108	VAL
10	J	122	CYS
11	K	29	LYS
11	K	55	GLN
11	K	126	LYS
12	L	12	VAL
12	L	24	SER
12	L	31	VAL
12	L	65	LEU
12	L	77	SER
12	L	82	LEU
12	L	115	ASP
12	L	157	ARG
12	L	158	ARG
12	L	174	VAL
12	L	192	VAL
12	L	200	ARG
13	M	6	VAL
13	M	49	LYS
13	M	65	THR
13	M	73	LYS
13	M	129	SER
13	M	140	SER
13	M	148	LEU
13	M	174	LEU
13	M	209	SER
13	M	211	ARG
14	N	5	MET
14	N	10	SER
14	N	47	ASN
14	N	74	GLU
14	N	155	GLU
14	N	159	VAL
14	N	166	ARG
14	N	204	SER
1	O	49	VAL

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Mol	Chain	Res	Type
1	O	92	GLN
1	O	108	GLU
1	O	126	THR
1	O	130	GLU
1	O	146	GLU
1	O	183	VAL
1	O	205	VAL
1	O	219	VAL
2	P	19	VAL
2	P	43	VAL
2	P	51	GLN
2	P	58	GLU
2	P	73	LEU
2	P	123	SER
2	P	132	SER
2	P	139	ASN
3	Q	13	SER
3	Q	69	ASN
3	Q	70	GLU
3	Q	80	THR
3	Q	132	VAL
3	Q	133	SER
3	Q	151	ASP
3	Q	181	GLU
3	Q	211	VAL
3	Q	227	VAL
3	Q	229	LYS
3	Q	234	GLU
4	R	4	ASP
4	R	8	THR
4	R	54	GLN
4	R	56	GLU
4	R	98	VAL
4	R	100	ASP
4	R	102	VAL
4	R	206	ILE
4	R	208	LEU
4	R	233	GLU
5	S	20	ARG
5	S	36	THR
5	S	62	SER
5	S	95	GLU

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Mol	Chain	Res	Type
5	S	107	MET
5	S	179	SER
5	S	184	VAL
5	S	210	LEU
5	S	216	GLU
5	S	240	ASP
6	T	7	ASP
6	T	9	ASP
6	T	62	LYS
6	T	101	ARG
6	T	115	LYS
6	T	166	GLN
6	T	173	GLU
6	T	202	GLU
6	T	229	VAL
7	U	28	LYS
7	U	53	VAL
7	U	69	VAL
7	U	181	MET
7	U	205	LYS
7	U	214	SER
7	U	218	GLU
7	U	219	LEU
8	V	71	GLU
8	V	176	VAL
8	V	183	VAL
8	V	191	ASN
9	W	73	GLU
9	W	79	VAL
9	W	120	SER
9	W	149	GLU
9	W	193	THR
9	W	213	THR
10	X	27	ARG
10	X	36	THR
10	X	108	VAL
10	X	122	CYS
10	X	152	SER
11	Y	28	MET
11	Y	29	LYS
11	Y	47	VAL
11	Y	55	GLN

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Mol	Chain	Res	Type
11	Y	126	LYS
11	Y	154	GLU
12	Z	12	VAL
12	Z	24	SER
12	Z	31	VAL
12	Z	65	LEU
12	Z	77	SER
12	Z	82	LEU
12	Z	115	ASP
12	Z	157	ARG
12	Z	158	ARG
12	Z	174	VAL
12	Z	192	VAL
13	a	6	VAL
13	a	49	LYS
13	a	51	VAL
13	a	65	THR
13	a	73	LYS
13	a	129	SER
13	a	140	SER
13	a	148	LEU
13	a	174	LEU
13	a	209	SER
13	a	211	ARG
14	b	3	ASN
14	b	5	MET
14	b	10	SER
14	b	47	ASN
14	b	74	GLU
14	b	155	GLU
14	b	159	VAL
14	b	166	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	51	GLN
2	B	87	HIS
2	B	139	ASN
3	C	40	ASN
3	C	109	GLN
4	D	154	HIS

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Mol	Chain	Res	Type
5	E	98	ASN
5	E	155	HIS
5	E	164	GLN
5	E	214	ASN
5	E	221	GLN
6	F	4	ASN
6	F	8	ASN
6	F	68	ASN
6	F	175	HIS
8	H	66	HIS
11	K	24	ASN
11	K	27	GLN
11	K	32	HIS
11	K	174	ASN
12	L	9	GLN
12	L	10	HIS
12	L	124	ASN
12	L	146	ASN
13	M	79	ASN
13	M	108	ASN
13	M	131	GLN
13	M	151	ASN
13	M	152	GLN
14	N	3	ASN
1	O	75	ASN
1	O	147	GLN
1	O	172	GLN
1	O	238	HIS
2	P	87	HIS
2	P	139	ASN
3	Q	40	ASN
3	Q	240	HIS
4	R	146	GLN
4	R	154	HIS
5	S	114	GLN
5	S	152	GLN
5	S	155	HIS
5	S	164	GLN
5	S	221	GLN
6	T	4	ASN
6	T	8	ASN
6	T	68	ASN

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Mol	Chain	Res	Type
6	T	146	GLN
6	T	175	HIS
6	T	185	ASN
8	V	66	HIS
8	V	97	HIS
9	W	114	HIS
10	X	33	GLN
10	X	169	GLN
11	Y	27	GLN
11	Y	99	HIS
11	Y	174	ASN
12	Z	9	GLN
12	Z	10	HIS
12	Z	124	ASN
12	Z	146	ASN
13	a	79	ASN
13	a	108	ASN
13	a	131	GLN
13	a	151	ASN
13	a	152	GLN
14	b	213	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 13 are monoatomic - leaving 15 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	SCN	F	301	-	1,2,2	0.64	0	0,1,1	-	-
17	S5K	H	901	8	23,27,27	0.50	0	27,39,39	1.28	3 (11%)
16	SCN	K	201	-	1,2,2	0.29	0	0,1,1	-	-
16	SCN	a	302	-	1,2,2	0.14	0	0,1,1	-	-
17	S5K	L	901	12	23,27,27	0.46	0	27,39,39	1.24	1 (3%)
16	SCN	T	301	-	1,2,2	0.40	0	0,1,1	-	-
16	SCN	a	303	-	1,2,2	0.54	0	0,1,1	-	-
17	S5K	V	901	8	23,27,27	0.46	0	27,39,39	1.20	2 (7%)
17	S5K	Z	901	12	23,27,27	0.49	0	27,39,39	1.19	2 (7%)
16	SCN	M	302	-	1,2,2	0.13	0	0,1,1	-	-
16	SCN	K	202	-	1,2,2	0.60	0	0,1,1	-	-
16	SCN	M	304	-	1,2,2	0.49	0	0,1,1	-	-
16	SCN	M	303	-	1,2,2	0.40	0	0,1,1	-	-
16	SCN	U	301	-	1,2,2	0.07	0	0,1,1	-	-
16	SCN	Z	903	-	1,2,2	0.23	0	0,1,1	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	S5K	H	901	8	-	5/11/33/33	0/5/4/4
17	S5K	Z	901	12	-	4/11/33/33	0/5/4/4
17	S5K	L	901	12	-	6/11/33/33	0/5/4/4
17	S5K	V	901	8	-	6/11/33/33	0/5/4/4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	L	901	S5K	C2-O3-C6	-5.18	96.89	108.95
17	V	901	S5K	C2-O3-C6	-4.95	97.43	108.95
17	H	901	S5K	C2-O3-C6	-4.70	98.01	108.95
17	Z	901	S5K	C2-O3-C6	-4.68	98.06	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	901	S5K	O3-C6-C5	-2.33	102.12	105.07
17	Z	901	S5K	O3-C6-C5	-2.11	102.40	105.07
17	V	901	S5K	O3-C6-C5	-2.08	102.43	105.07
17	H	901	S5K	O3-C2-C7	-2.07	100.84	104.34

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	901	S5K	C9-C10-C11-B13
17	Z	901	S5K	C2-C1-C4-O24
17	Z	901	S5K	C2-C1-C4-N12
17	H	901	S5K	C2-C1-C4-O24
17	L	901	S5K	C2-C1-C4-O24
17	L	901	S5K	C2-C1-C4-N12
17	V	901	S5K	C2-C1-C4-O24
17	H	901	S5K	C2-C1-C4-N12
17	V	901	S5K	C2-C1-C4-N12
17	H	901	S5K	C11-C10-C9-C18
17	V	901	S5K	C5-C1-C4-N12
17	L	901	S5K	C9-C10-C11-B13
17	Z	901	S5K	C11-C10-C9-C16
17	L	901	S5K	C11-C10-C9-C18
17	V	901	S5K	C5-C1-C4-O24
17	L	901	S5K	C11-C10-C9-C16
17	Z	901	S5K	C11-C10-C9-C18
17	V	901	S5K	C11-C10-C9-C18
17	L	901	S5K	C5-C1-C4-O24
17	V	901	S5K	C11-C10-C9-C16
17	H	901	S5K	C11-C10-C9-C16

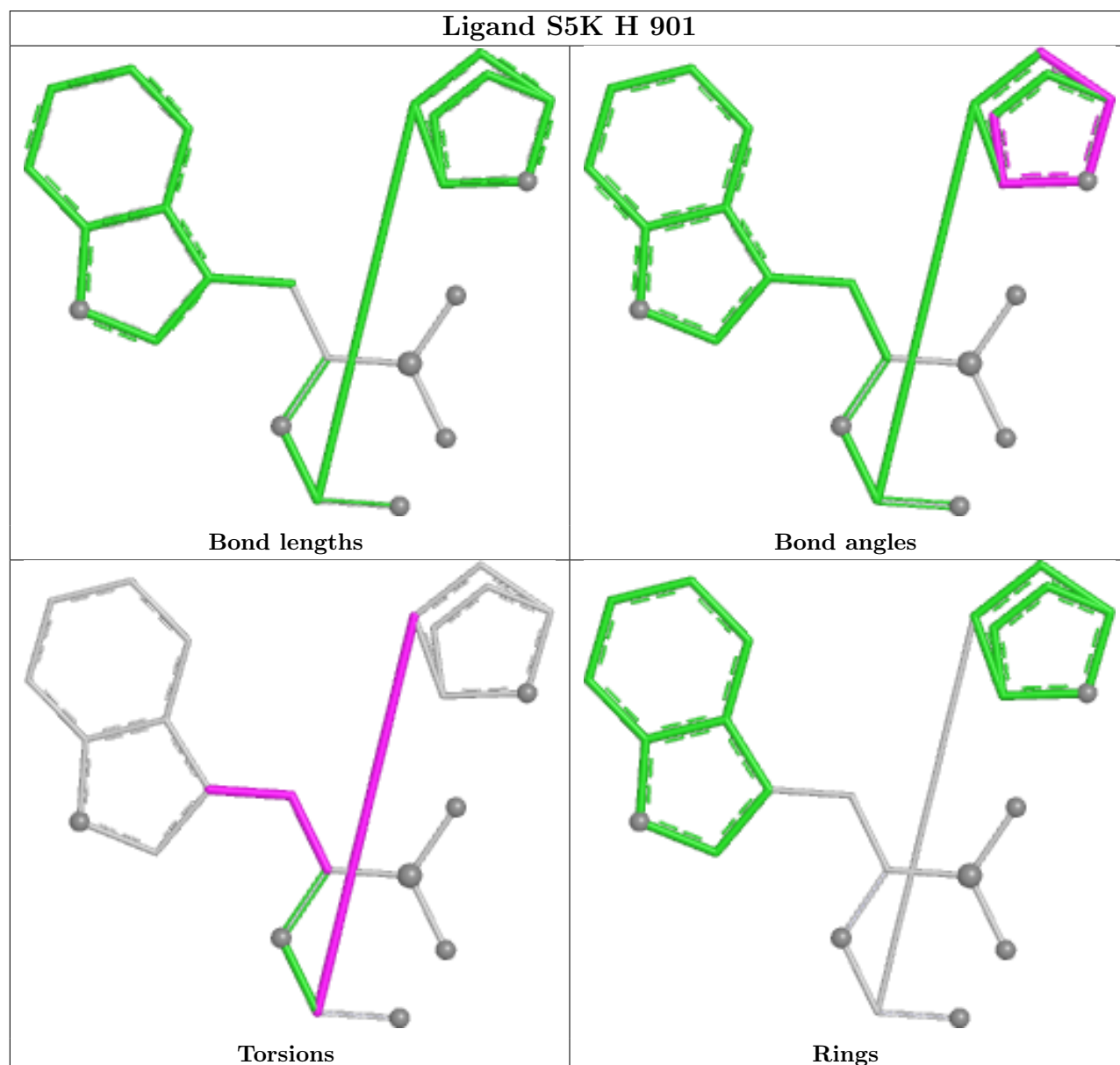
There are no ring outliers.

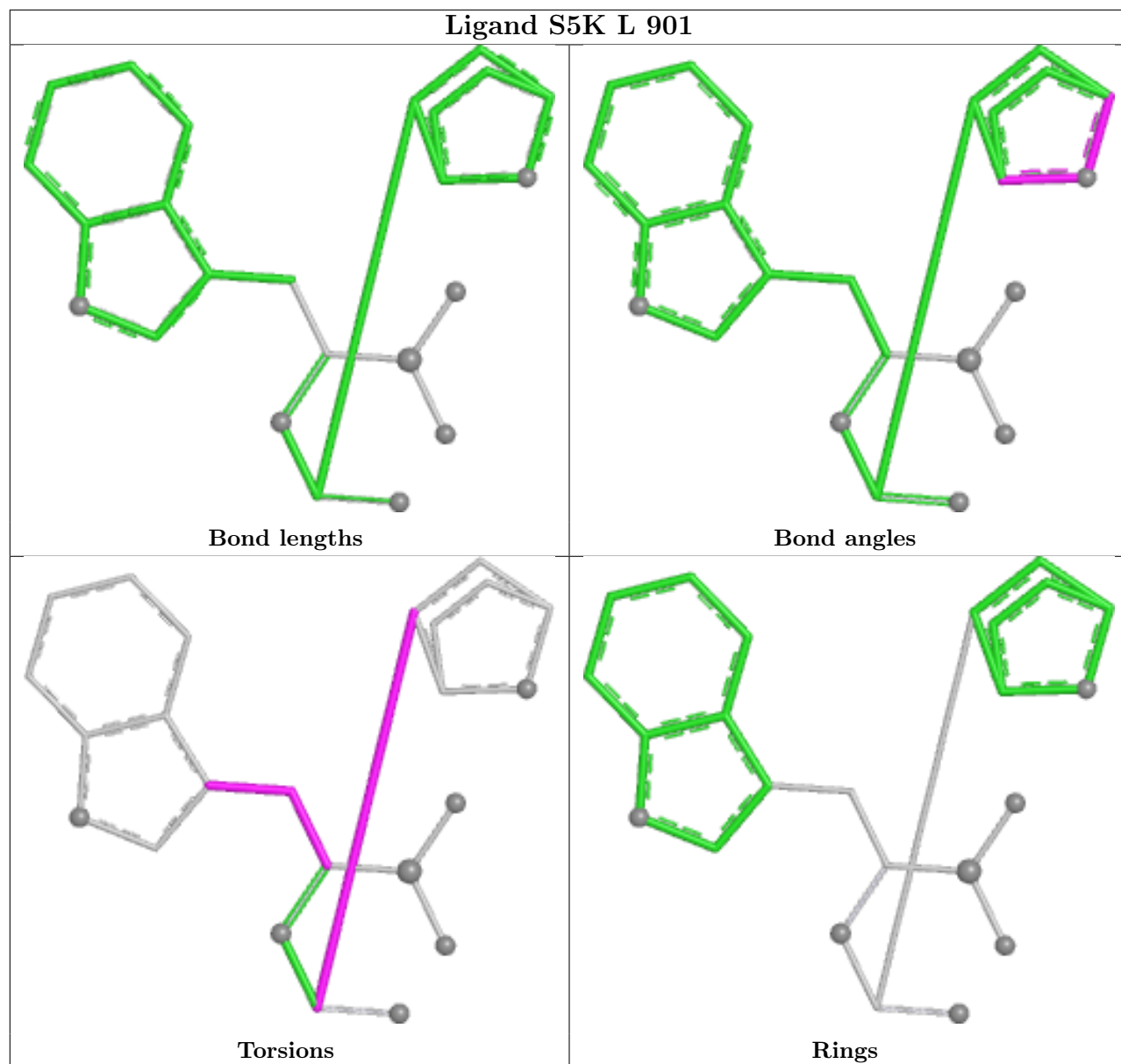
2 monomers are involved in 5 short contacts:

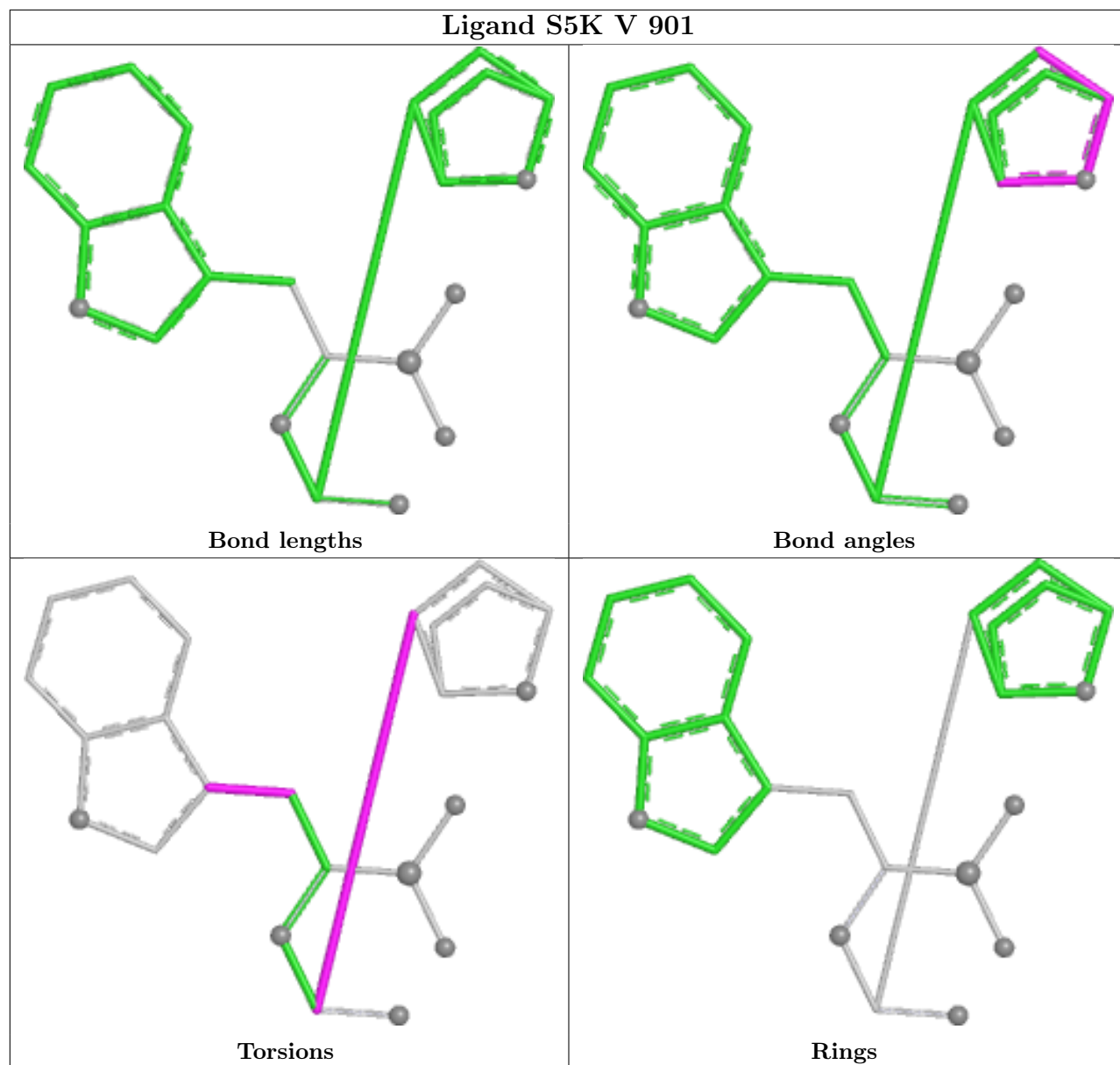
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	901	S5K	2	0
17	V	901	S5K	3	0

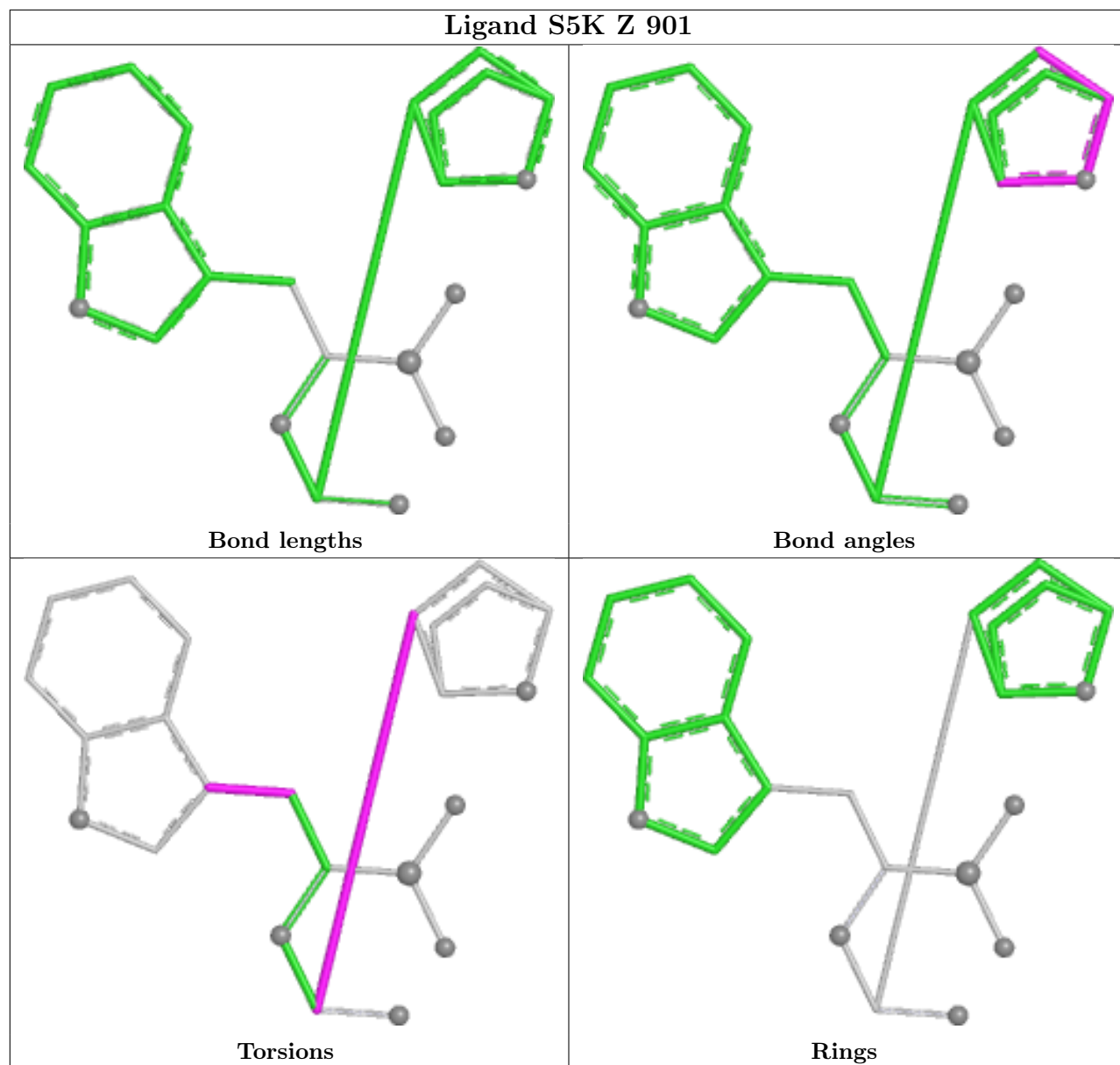
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	240/242 (99%)	1.01	22 (9%)	14 15	43, 68, 104, 129	9 (3%)
1	O	242/242 (100%)	0.76	20 (8%)	17 18	40, 61, 91, 121	9 (3%)
2	B	229/229 (100%)	0.92	26 (11%)	10 10	37, 60, 89, 99	9 (3%)
2	P	229/229 (100%)	0.63	7 (3%)	51 53	31, 58, 85, 97	9 (3%)
3	C	243/256 (94%)	0.89	22 (9%)	15 15	40, 62, 88, 152	13 (5%)
3	Q	253/256 (98%)	0.79	13 (5%)	33 34	40, 65, 134, 192	2 (0%)
4	D	227/237 (95%)	1.04	24 (10%)	11 12	36, 67, 113, 154	13 (5%)
4	R	234/237 (98%)	0.94	28 (11%)	9 9	37, 69, 103, 132	16 (6%)
5	E	230/232 (99%)	1.06	22 (9%)	13 14	38, 67, 98, 129	10 (4%)
5	S	232/232 (100%)	1.00	30 (12%)	7 8	38, 68, 94, 118	17 (7%)
6	F	236/236 (100%)	1.05	36 (15%)	5 5	42, 63, 95, 131	11 (4%)
6	T	235/236 (99%)	0.71	10 (4%)	40 41	43, 60, 95, 119	4 (1%)
7	G	242/242 (100%)	1.07	31 (12%)	7 8	40, 68, 100, 134	12 (4%)
7	U	240/242 (99%)	0.77	14 (5%)	29 30	31, 60, 90, 104	8 (3%)
8	H	199/199 (100%)	0.28	0	100 100	38, 50, 67, 73	1 (0%)
8	V	199/199 (100%)	0.12	0	100 100	33, 47, 66, 76	3 (1%)
9	I	223/223 (100%)	0.57	18 (8%)	18 18	32, 51, 97, 125	6 (2%)
9	W	223/223 (100%)	0.48	19 (8%)	16 17	37, 50, 93, 120	4 (1%)
10	J	204/204 (100%)	0.17	4 (1%)	65 66	32, 45, 66, 86	2 (0%)
10	X	204/204 (100%)	0.01	2 (0%)	79 81	34, 45, 65, 78	3 (1%)
11	K	196/197 (99%)	0.32	3 (1%)	72 73	34, 50, 64, 82	2 (1%)
11	Y	197/197 (100%)	0.22	2 (1%)	79 81	27, 49, 70, 91	3 (1%)
12	L	203/203 (100%)	0.16	2 (0%)	79 81	32, 46, 67, 81	1 (0%)
12	Z	203/203 (100%)	0.10	1 (0%)	87 88	33, 48, 67, 78	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	213/213 (100%)	0.12	4 (1%)	66 68	30, 44, 66, 89	3 (1%)
13	a	213/213 (100%)	0.07	2 (0%)	81 82	29, 44, 65, 89	5 (2%)
14	N	214/214 (100%)	0.16	1 (0%)	87 88	31, 48, 68, 85	2 (0%)
14	b	214/214 (100%)	0.05	2 (0%)	81 82	30, 46, 68, 85	1 (0%)
All	All	6217/6254 (99%)	0.58	365 (5%)	28 29	27, 55, 93, 192	179 (2%)

All (365) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	196	VAL	6.4
6	F	236	LEU	5.2
5	S	240	ASP	5.0
2	P	232	ILE	4.9
1	A	159	TYR	4.7
9	W	196	VAL	4.6
5	S	130	PRO	4.3
9	I	194	GLU	4.2
11	Y	197	PRO	4.1
4	D	199	VAL	4.0
2	B	181	LEU	4.0
7	G	245	GLU	4.0
13	a	33	PHE	4.0
9	I	221	LEU	3.9
9	W	223	LEU	3.9
7	U	6	GLY	3.9
9	I	223	LEU	3.9
13	M	33	PHE	3.9
6	T	236	LEU	3.9
1	O	159	TYR	3.8
9	W	221	LEU	3.8
7	G	199	ILE	3.7
9	I	197	LYS	3.7
3	C	242	GLU	3.6
2	B	232	ILE	3.6
2	B	230	ALA	3.6
4	R	232	ILE	3.6
7	U	41	CYS	3.5
2	B	229	LEU	3.4
4	D	172	LEU	3.4
9	W	202	TYR	3.4
3	C	236	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
7	U	244	LYS	3.4
9	I	202	TYR	3.4
2	B	58	GLU	3.4
7	G	208	ALA	3.3
4	R	234	LYS	3.3
12	L	102	CYS	3.3
3	C	247	ALA	3.2
2	P	181	LEU	3.2
7	G	243	LEU	3.2
6	F	205	LEU	3.2
9	W	195	PRO	3.2
6	F	53	GLN	3.2
6	F	60	GLN	3.2
6	F	203	GLN	3.2
9	W	220	THR	3.2
9	W	192	PRO	3.2
4	R	200	GLN	3.2
1	A	215	ILE	3.2
4	D	232	ILE	3.2
4	R	191	VAL	3.1
4	R	208	LEU	3.1
1	O	209	ASP	3.1
1	A	235	ILE	3.1
7	G	197	ILE	3.1
6	F	235	GLY	3.1
9	W	200	GLY	3.1
6	F	200	PRO	3.1
2	B	179	GLU	3.0
4	R	237	GLU	3.0
5	S	131	GLY	3.0
6	F	233	LEU	3.0
1	O	245	ARG	3.0
9	W	197	LYS	3.0
7	G	6	GLY	3.0
1	A	191	PHE	3.0
5	E	156	MET	3.0
9	W	194	GLU	3.0
10	J	114	PRO	3.0
2	B	54	ILE	3.0
4	D	219	ILE	3.0
7	G	176	ILE	3.0
4	R	238	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	202	LEU	2.9
1	A	240	VAL	2.9
4	D	191	VAL	2.9
9	I	200	GLY	2.9
6	F	238	GLU	2.9
4	D	198	VAL	2.9
5	E	175	GLU	2.9
4	R	198	VAL	2.9
14	N	214	MET	2.9
9	I	184	LYS	2.8
5	E	237	VAL	2.8
1	A	173	THR	2.8
7	G	238	TYR	2.8
5	S	199	LEU	2.8
4	R	181	ILE	2.8
5	E	47	CYS	2.8
9	I	198	ARG	2.8
9	W	199	SER	2.8
2	B	177	TYR	2.8
3	C	175	LEU	2.8
6	F	56	LEU	2.8
6	F	199	LEU	2.8
5	S	220	VAL	2.8
4	R	201	SER	2.8
7	U	242	SER	2.8
4	R	230	ALA	2.8
7	G	53	VAL	2.8
4	R	188	ILE	2.7
5	E	212	ALA	2.7
4	D	15	HIS	2.7
3	C	237	ILE	2.7
3	Q	202	ASP	2.7
7	U	230	ASP	2.7
1	O	242	LEU	2.7
4	D	217	LEU	2.7
1	A	205	VAL	2.7
1	O	200	THR	2.7
2	B	178	ASN	2.7
9	W	23	ASP	2.7
7	G	54	LEU	2.7
5	S	187	LYS	2.7
9	W	198	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
6	F	184	LEU	2.7
6	T	205	LEU	2.7
7	G	241	GLU	2.6
14	b	214	MET	2.6
3	C	206	LEU	2.6
5	S	128	ALA	2.6
4	D	53	LEU	2.6
5	S	182	GLN	2.6
5	S	202	LEU	2.6
5	S	208	GLU	2.6
4	D	229	VAL	2.6
7	G	204	VAL	2.6
9	I	195	PRO	2.6
9	I	199	SER	2.6
5	S	65	GLU	2.6
2	B	75	TYR	2.6
4	R	219	ILE	2.6
3	Q	235	GLN	2.5
5	S	234	LEU	2.5
7	G	169	ARG	2.5
12	L	200	ARG	2.5
3	C	176	LYS	2.5
4	D	204	LYS	2.5
4	D	181	ILE	2.5
5	E	63	SER	2.5
6	F	61	LYS	2.5
6	F	65	HIS	2.5
9	W	203	HIS	2.5
2	B	157	TRP	2.5
2	B	167	VAL	2.5
3	Q	76	VAL	2.5
4	D	225	ILE	2.5
5	S	54	ILE	2.5
7	G	196	ILE	2.5
2	P	194	LEU	2.5
7	G	179	LEU	2.5
5	E	204	GLN	2.5
7	G	142	VAL	2.5
7	G	193	VAL	2.5
4	R	53	LEU	2.5
4	R	217	LEU	2.5
5	E	210	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	201	MET	2.5
5	S	78	MET	2.5
7	U	208	ALA	2.5
7	U	5	THR	2.4
5	E	229	PHE	2.4
7	G	214	SER	2.4
7	G	190	VAL	2.4
1	A	242	LEU	2.4
4	D	195	LEU	2.4
5	E	58	LEU	2.4
6	T	184	LEU	2.4
4	R	204	LYS	2.4
1	A	155	ASP	2.4
1	A	241	ALA	2.4
4	R	158	ALA	2.4
9	W	193	THR	2.4
1	A	210	PHE	2.4
4	D	138	PHE	2.4
5	S	237	VAL	2.4
6	F	179	PHE	2.4
6	T	199	LEU	2.4
9	I	186	LEU	2.4
7	G	58	TYR	2.4
1	A	188	ASP	2.4
2	B	199	GLU	2.4
3	Q	183	GLU	2.4
2	B	231	ALA	2.4
6	F	158	ALA	2.4
1	A	200	THR	2.4
1	O	5	SER	2.4
3	C	35	LEU	2.4
5	E	181	LEU	2.4
6	T	56	LEU	2.4
2	B	188	HIS	2.4
2	B	201	GLN	2.4
1	O	212	PRO	2.4
6	F	231	PRO	2.4
4	D	44	GLY	2.4
4	D	209	ALA	2.4
4	D	183	THR	2.4
2	P	54	ILE	2.4
4	R	195	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
13	M	166	LEU	2.4
9	I	201	ARG	2.4
9	W	201	ARG	2.4
4	R	228	TYR	2.3
1	O	241	ALA	2.3
5	S	132	ALA	2.3
6	F	201	ALA	2.3
3	C	168	SER	2.3
3	C	194	ILE	2.3
5	S	184	VAL	2.3
6	F	232	PHE	2.3
9	I	203	HIS	2.3
1	A	189	TRP	2.3
7	U	238	TYR	2.3
6	F	239	ARG	2.3
1	O	215	ILE	2.3
5	S	201	ILE	2.3
1	O	240	VAL	2.3
6	F	36	VAL	2.3
3	Q	34	CYS	2.3
3	Q	206	LEU	2.3
5	S	217	LEU	2.3
6	F	49	LEU	2.3
3	C	231	LYS	2.3
7	G	206	ASP	2.3
13	M	204	ARG	2.3
4	R	235	GLU	2.3
1	O	187	PHE	2.3
6	T	49	LEU	2.3
6	F	182	CYS	2.3
11	K	1	MET	2.3
5	E	120	ALA	2.3
9	I	193	THR	2.3
10	J	116	THR	2.3
2	P	179	GLU	2.3
3	C	240	HIS	2.3
6	F	177	SER	2.3
6	F	234	GLU	2.3
3	Q	237	ILE	2.3
6	T	61	LYS	2.3
1	O	210	PHE	2.2
5	E	234	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	P	202	MET	2.2
4	R	203	GLY	2.2
4	D	226	GLU	2.2
6	F	58	ALA	2.2
6	F	224	TYR	2.2
5	S	203	LYS	2.2
7	G	237	LYS	2.2
4	D	188	ILE	2.2
1	O	239	LEU	2.2
7	U	190	VAL	2.2
14	b	213	HIS	2.2
3	C	77	ALA	2.2
5	S	192	LYS	2.2
5	S	36	THR	2.2
5	S	38	ILE	2.2
1	A	239	LEU	2.2
2	B	173	LEU	2.2
2	B	198	PHE	2.2
5	E	207	GLU	2.2
5	S	231	LYS	2.2
1	O	243	ALA	2.2
4	R	187	THR	2.2
2	B	166	TYR	2.2
1	A	32	ILE	2.2
10	J	3	ILE	2.2
2	B	176	ARG	2.2
7	U	204	VAL	2.2
9	W	216	VAL	2.2
1	A	196	GLU	2.2
3	C	239	LYS	2.2
3	Q	181	GLU	2.2
5	S	126	GLU	2.2
2	B	200	GLY	2.2
12	Z	102	CYS	2.2
2	B	159	ALA	2.2
4	R	209	ALA	2.2
7	G	62	SER	2.2
7	G	171	ALA	2.2
9	I	220	THR	2.2
1	O	189	TRP	2.1
2	B	55	LEU	2.1
2	B	192	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	170	ILE	2.1
7	G	231	ILE	2.1
1	A	183	VAL	2.1
3	C	227	VAL	2.1
6	F	229	VAL	2.1
9	W	205	VAL	2.1
5	E	226	PHE	2.1
7	G	209	PHE	2.1
10	X	117	PHE	2.1
10	X	118	LYS	2.1
13	a	159	GLN	2.1
3	C	44	LEU	2.1
3	C	213	ILE	2.1
3	Q	25	MET	2.1
7	U	176	ILE	2.1
7	U	196	ILE	2.1
11	Y	194	ILE	2.1
6	F	204	ASP	2.1
3	C	59	VAL	2.1
4	D	42	VAL	2.1
6	F	210	VAL	2.1
3	Q	200	THR	2.1
9	W	188	THR	2.1
1	O	184	LYS	2.1
1	O	206	LEU	2.1
4	D	179	GLU	2.1
3	Q	194	ILE	2.1
4	R	85	ASN	2.1
5	E	38	ILE	2.1
5	E	48	LEU	2.1
5	S	238	ILE	2.1
6	F	38	LEU	2.1
6	T	238	GLU	2.1
10	J	113	ASP	2.1
6	T	200	PRO	2.1
2	B	72	GLY	2.1
2	B	169	GLY	2.1
7	G	4	GLY	2.1
6	F	73	SER	2.1
1	A	237	ALA	2.1
4	R	236	LYS	2.1
5	S	218	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
6	F	180	MET	2.1
3	C	197	LEU	2.1
4	D	190	LEU	2.1
4	R	144	LEU	2.1
5	S	204	GLN	2.1
6	F	9	ASP	2.1
6	T	8	ASN	2.1
13	M	161	VAL	2.1
4	R	202	GLY	2.1
5	E	80	GLY	2.1
5	S	176	GLY	2.1
2	P	176	ARG	2.1
6	F	196	ARG	2.1
7	U	215	TRP	2.1
1	O	186	LYS	2.0
1	O	52	THR	2.0
3	C	25	MET	2.0
3	C	170	ALA	2.0
7	G	213	LEU	2.0
4	R	192	ILE	2.0
5	E	61	PRO	2.0
5	S	185	TYR	2.0
11	K	134	TYR	2.0
1	O	222	VAL	2.0
4	D	168	VAL	2.0
1	A	182	LYS	2.0
3	Q	257	LYS	2.0
7	G	182	LYS	2.0
1	A	5	SER	2.0
5	E	56	SER	2.0
5	E	167	ALA	2.0
7	G	239	ALA	2.0
6	F	192	LEU	2.0
7	U	57	LEU	2.0
9	I	189	LEU	2.0
3	Q	226	ARG	2.0
9	I	187	ARG	2.0
11	K	194	ILE	2.0
7	G	244	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
17	S5K	H	901	24/24	0.72	0.19	61,71,74,74	0
17	S5K	V	901	24/24	0.74	0.20	62,70,72,72	0
15	NA	J	301	1/1	0.85	0.09	44,44,44,44	0
16	SCN	K	202	3/3	0.85	0.16	69,69,69,70	0
15	NA	a	301	1/1	0.87	0.15	61,61,61,61	0
15	NA	H	902	1/1	0.87	0.13	51,51,51,51	0
16	SCN	M	303	3/3	0.88	0.19	60,60,61,62	0
16	SCN	a	303	3/3	0.88	0.20	64,64,65,66	0
16	SCN	Z	903	3/3	0.90	0.14	71,71,72,72	0
15	NA	J	302	1/1	0.90	0.10	55,55,55,55	0
16	SCN	K	201	3/3	0.91	0.12	70,70,70,70	0
16	SCN	F	301	3/3	0.91	0.12	65,65,66,67	0
16	SCN	a	302	3/3	0.91	0.15	69,69,69,69	0
15	NA	M	301	1/1	0.92	0.14	51,51,51,51	0
15	NA	V	902	1/1	0.94	0.11	52,52,52,52	0
16	SCN	M	304	3/3	0.94	0.09	68,68,68,69	0
16	SCN	U	301	3/3	0.94	0.12	69,69,69,69	0
15	NA	X	301	1/1	0.94	0.06	43,43,43,43	0
17	S5K	Z	901	24/24	0.94	0.07	30,35,38,38	0
16	SCN	T	301	3/3	0.95	0.13	78,78,79,79	0
16	SCN	M	302	3/3	0.95	0.12	68,68,68,68	0
17	S5K	L	901	24/24	0.96	0.06	31,34,36,37	0
15	NA	O	301	1/1	0.96	0.05	42,42,42,42	0
15	NA	L	902	1/1	0.96	0.04	34,34,34,34	0
15	NA	A	301	1/1	0.97	0.04	48,48,48,48	0
15	NA	Z	902	1/1	0.97	0.05	38,38,38,38	0
15	NA	W	301	1/1	0.98	0.04	40,40,40,40	0

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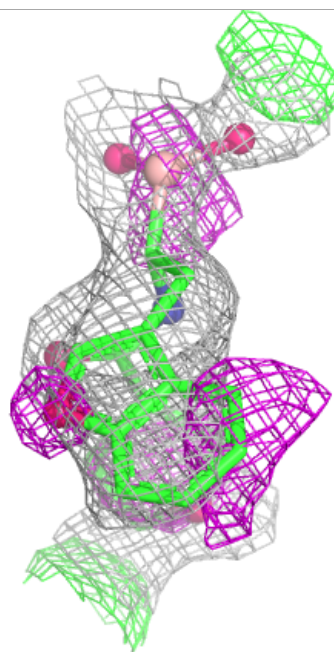
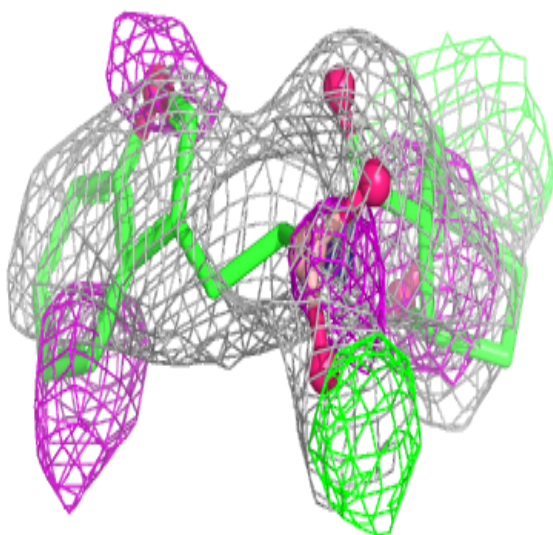
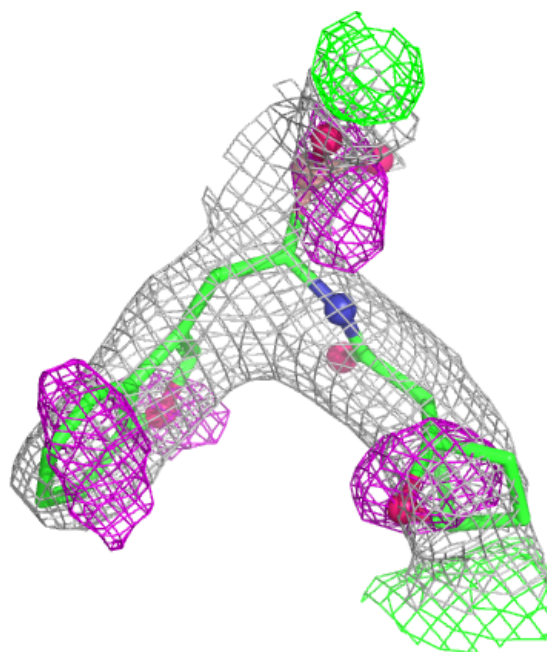
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	NA	I	301	1/1	0.99	0.02	39,39,39,39	0

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.

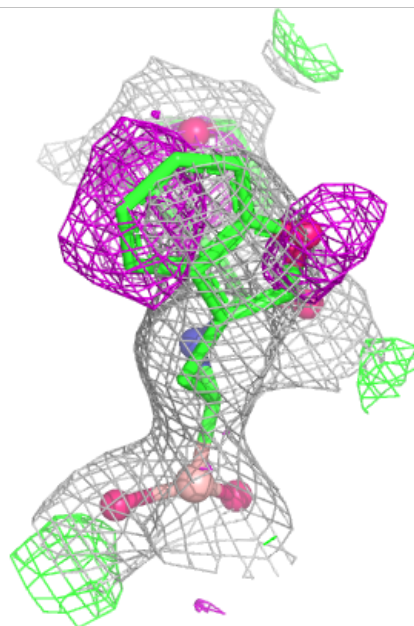
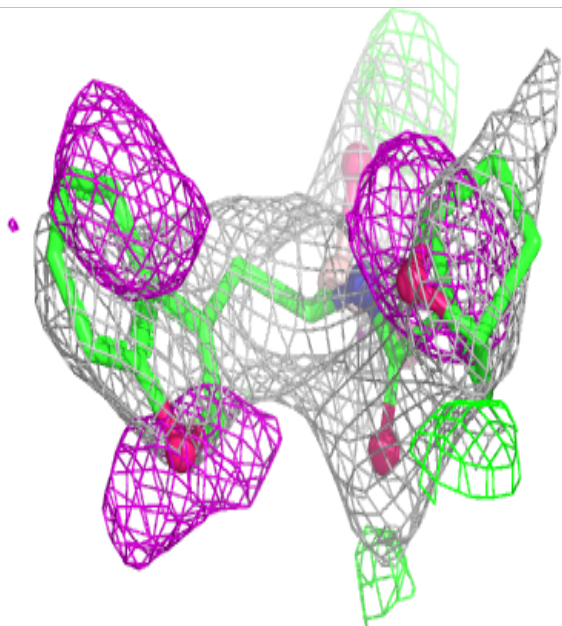
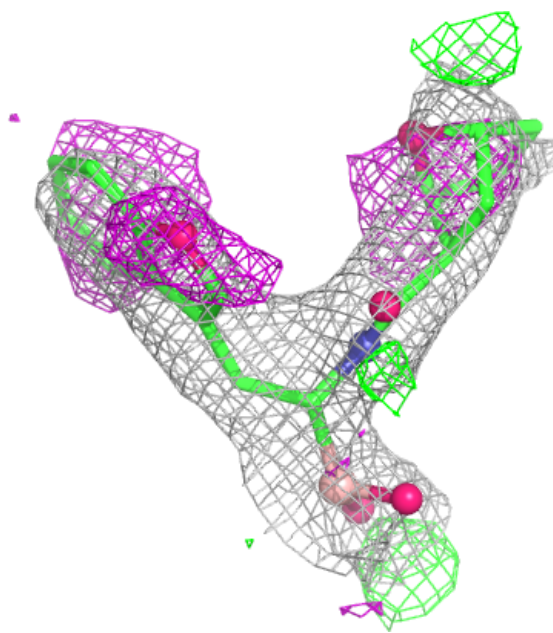
Electron density around S5K H 901:

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



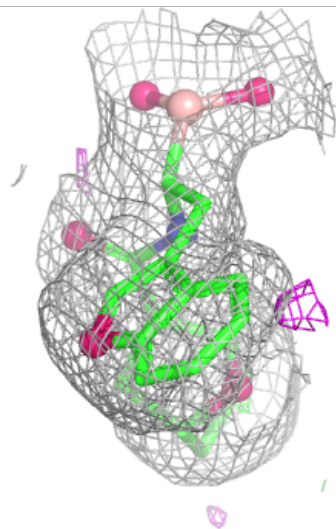
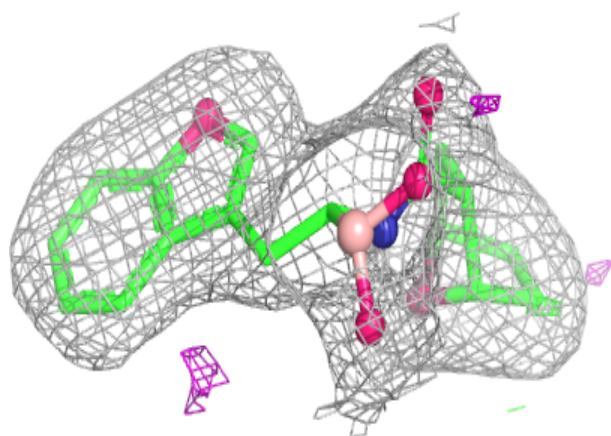
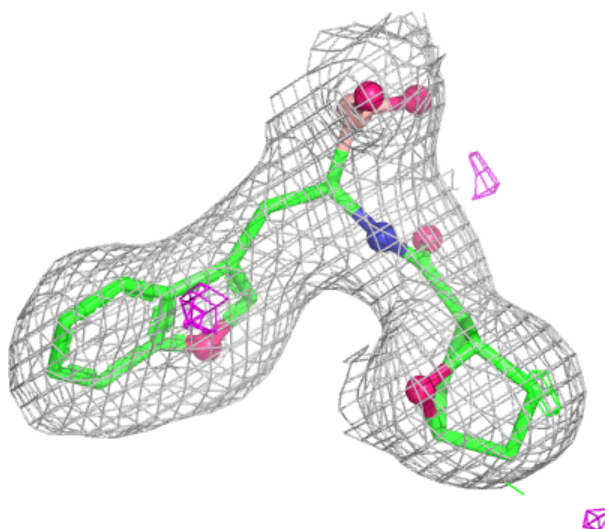
Electron density around S5K V 901:

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



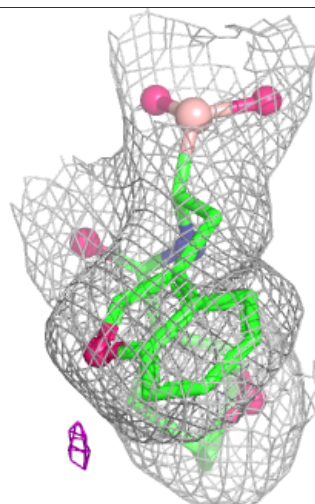
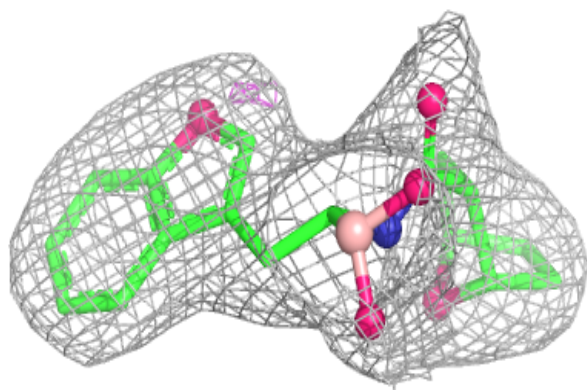
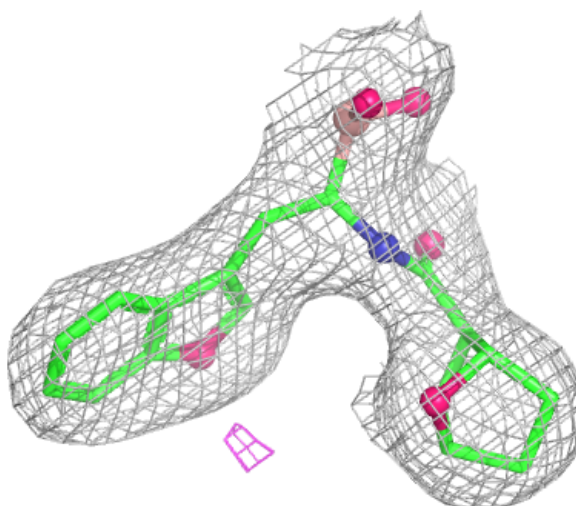
Electron density around S5K Z 901:

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



Electron density around S5K L 901:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.