Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2024 – 12:31 PM EDT

PDB ID	:	6E5B
Title	:	Human Immunoproteasome 20S particle in complex with compound 1
Authors	:	Steinbacher, S.; Augustin, M.; Blaesse, M.; Harris, S.F.
Deposited on	:	2018-07-19
Resolution	:	2.77 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 (i) 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 (i)) were used in the production of this report:

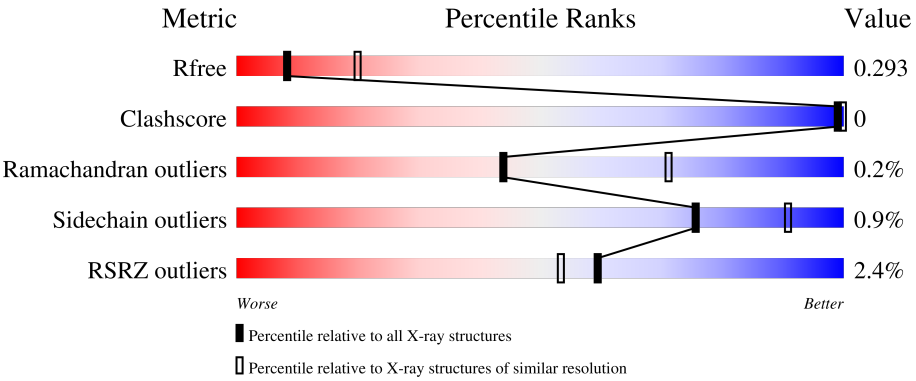
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.77 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}	164625	4924 (2.80-2.76)
Clashscore	180529	5458 (2.80-2.76)
Ramachandran outliers	177936	5386 (2.80-2.76)
Sidechain outliers	177891	5388 (2.80-2.76)
RSRZ outliers	164620	4926 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	234	3% 94%
1	O	234	2% 96%
2	B	261	5% 93% 6%
2	P	261	% 94% 6%
3	C	248	3% 88% 8%

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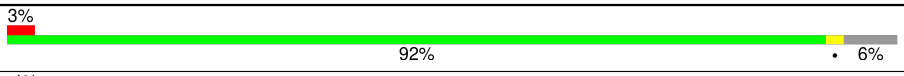
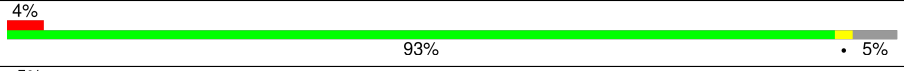
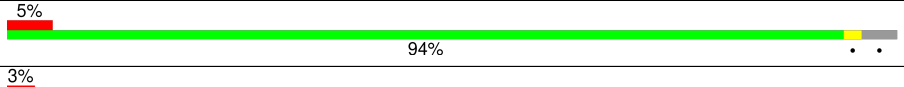
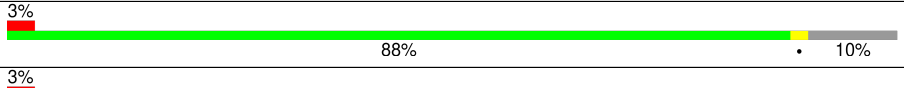
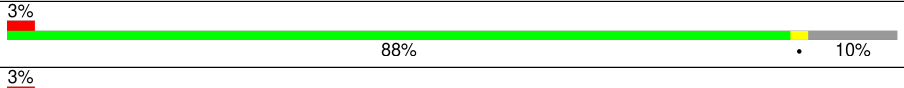
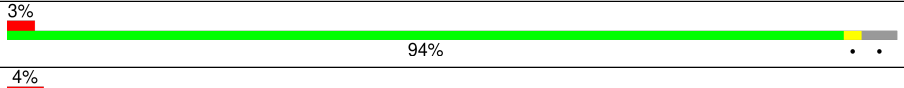
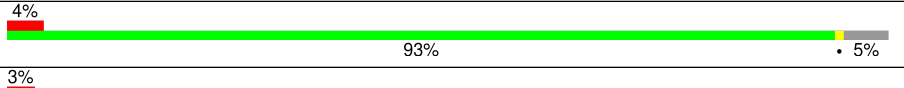
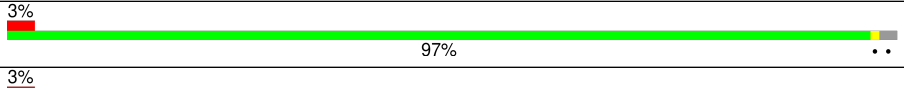
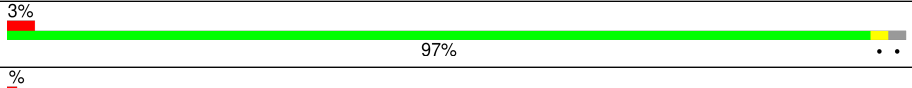
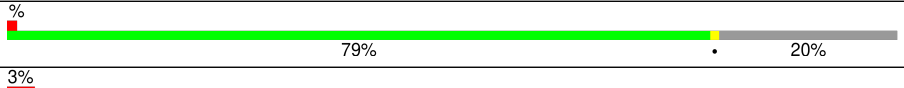
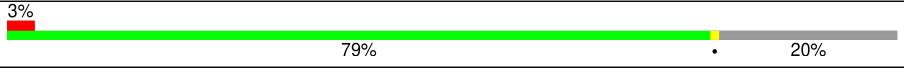
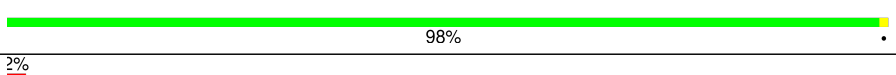
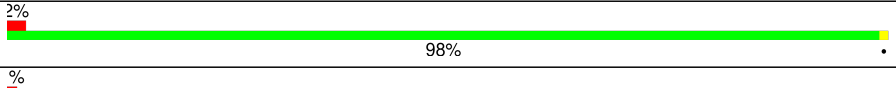
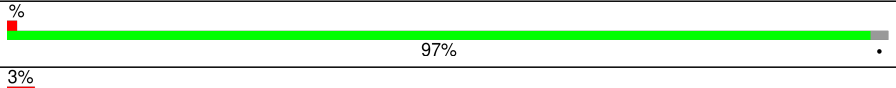
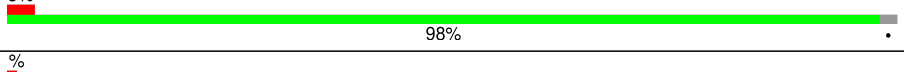
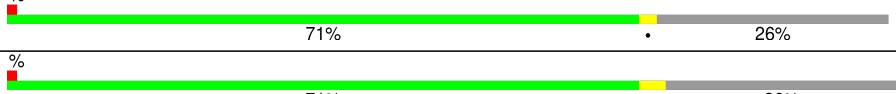
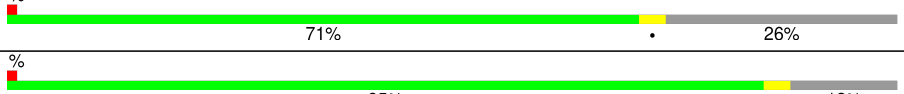
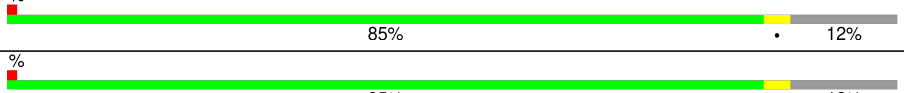
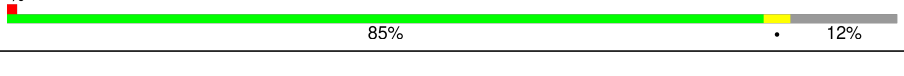
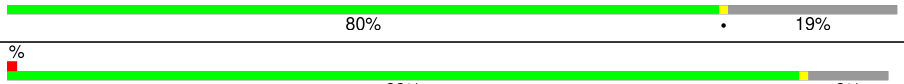
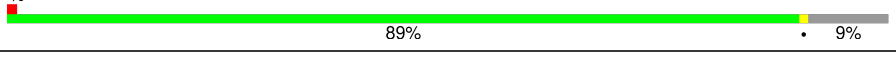
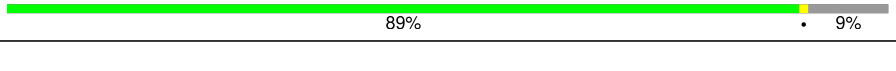
Mol	Chain	Length	Quality of chain
3	Q	248	
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	273	
8	V	273	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	276	
11	Y	276	
12	L	241	
12	Z	241	
13	M	264	
13	a	264	
14	N	219	
14	b	219	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 48431 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	22	0	0
			1787	1144	301	336	6			
1	O	229	Total	C	N	O	S	22	0	0
			1787	1144	301	336	6			

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	245	Total	C	N	O	S	40	0	0
			1932	1221	332	369	10			
2	P	246	Total	C	N	O	S	16	0	0
			1940	1225	333	372	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	227	Total	C	N	O	S	17	0	0
			1798	1132	318	343	5			
3	Q	234	Total	C	N	O	S	23	0	0
			1848	1160	327	356	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	230	Total	C	N	O	S	21	0	0
			1758	1103	291	353	11			
4	R	232	Total	C	N	O	S	12	0	0
			1769	1110	293	355	11			

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	236	Total	C	N	O	S	0	0	0
			1857	1162	334	350	11			
5	S	236	Total	C	N	O	S	6	0	0
			1857	1162	334	350	11			

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	21	0	0
			1911	1209	325	366	11			
6	T	241	Total	C	N	O	S	5	0	0
			1885	1195	322	357	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	13	0	0
			1875	1191	311	360	13			
7	U	242	Total	C	N	O	S	17	0	0
			1886	1197	315	361	13			

- Molecule 8 is a protein called Proteasome subunit beta type-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	218	Total	C	N	O	S	7	0	0
			1601	1004	284	305	8			
8	V	218	Total	C	N	O	S	7	0	0
			1601	1004	284	305	8			

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

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

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	7	0	0
			1571	1006	267	289	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	197	Total	C	N	O	S	13	0	0
			1578	1011	268	290	9			

- Molecule 11 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	203	Total	C	N	O	S	0	0	0
			1576	984	276	301	15			
11	Y	203	Total	C	N	O	S	0	0	0
			1576	984	276	301	15			

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	213	Total	C	N	O	S	6	0	0
			1654	1047	284	313	10			
12	Z	213	Total	C	N	O	S	4	0	0
			1654	1047	284	313	10			

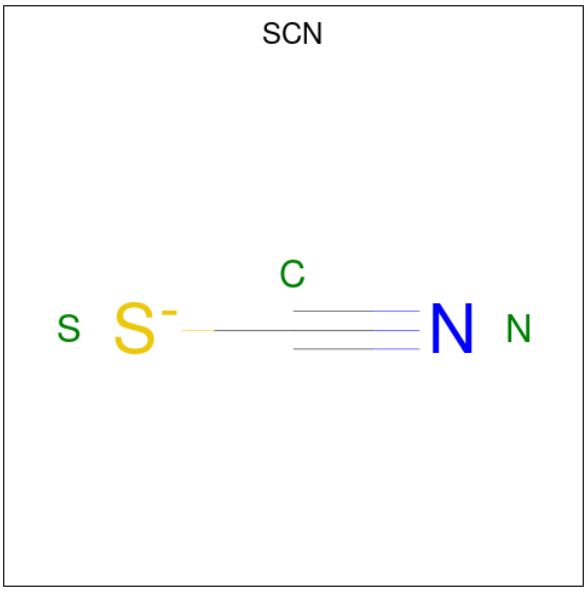
- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	214	Total	C	N	O	S	2	0	0
			1673	1055	289	317	12			
13	a	214	Total	C	N	O	S	0	0	0
			1673	1055	289	317	12			

- Molecule 14 is a protein called Proteasome subunit beta type-9.

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

- Molecule 15 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	E	1	Total C N S 3 1 1 1	0	0
15	L	1	Total C N S 3 1 1 1	0	0
15	Z	1	Total C N S 3 1 1 1	0	0

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Na 1 1	0	0
16	H	1	Total Na 1 1	0	0
16	I	2	Total Na 2 2	0	0
16	K	1	Total Na 1 1	0	0
16	L	2	Total Na 2 2	0	0
16	N	1	Total Na 1 1	0	0
16	U	1	Total Na 1 1	0	0
16	W	1	Total Na 1 1	0	0
16	Z	1	Total Na 1 1	0	0

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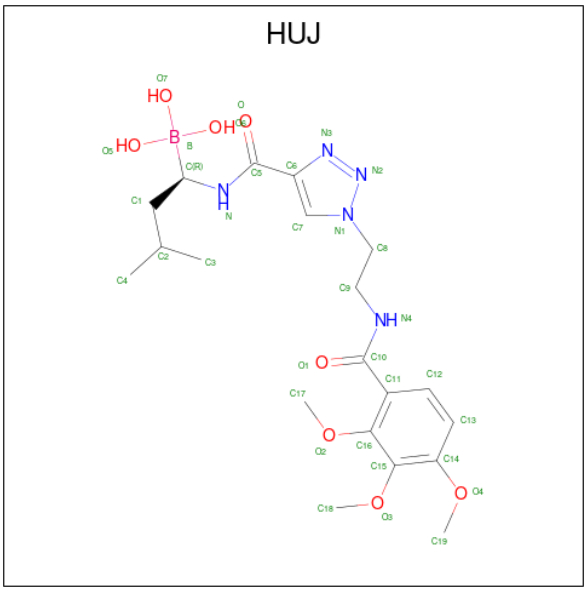
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	b	1	Total Na 1 1	0	0

- Molecule 17 is [(1R)-3-methyl-1-[[1-[2-[(2,3,4-trimethoxyphenyl)carbonylamino]ethyl]-1,2,3-triazol-4-yl]carbonylamino]butyl]-tris(oxidanyl)boron (three-letter code: HUJ) (formula: $C_{20}H_{31}BN_5O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	K	1	Total B C N O 33 1 20 5 7	2	0
17	N	1	Total B C N O 33 1 20 5 7	11	0
17	Y	1	Total B C N O 33 1 20 5 7	2	0
17	b	1	Total B C N O 33 1 20 5 7	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	B	2	Total O 2 2	0	0
18	C	1	Total O 1 1	0	0
18	E	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	F	1	Total O 1 1	0	0
18	H	2	Total O 2 2	0	0
18	I	4	Total O 4 4	0	0
18	J	1	Total O 1 1	0	0
18	K	4	Total O 4 4	0	0
18	L	2	Total O 2 2	0	0
18	M	4	Total O 4 4	0	0
18	N	3	Total O 3 3	0	0
18	O	1	Total O 1 1	0	0
18	P	2	Total O 2 2	0	0
18	Q	1	Total O 1 1	0	0
18	R	4	Total O 4 4	0	0
18	S	4	Total O 4 4	0	0
18	T	2	Total O 2 2	0	0
18	U	1	Total O 1 1	0	0
18	V	5	Total O 5 5	0	0
18	W	3	Total O 3 3	0	0
18	X	3	Total O 3 3	0	0
18	Y	5	Total O 5 5	0	0
18	Z	4	Total O 4 4	0	0
18	a	2	Total O 2 2	0	0

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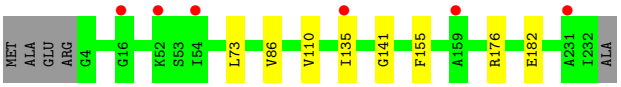
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	b	1	Total O 1 1	0	0

3 Residue-property plots

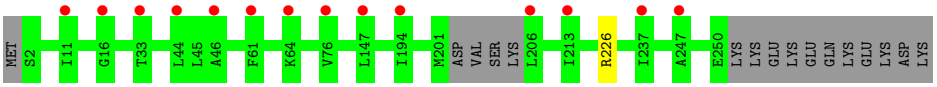
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Proteasome subunit alpha type-2

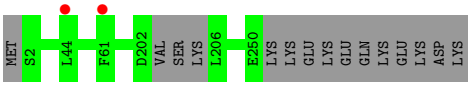


• Molecule 1: Proteasome subunit alpha type-2

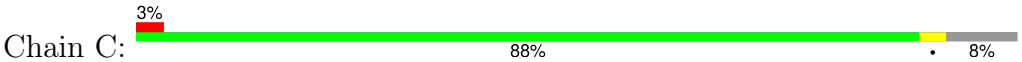
• Molecule 2: Proteasome subunit alpha type-4

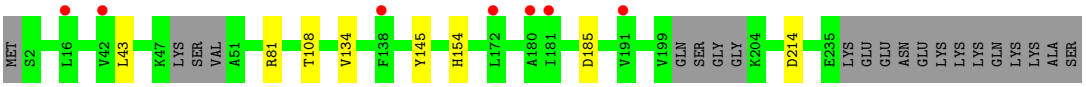


• Molecule 2: Proteasome subunit alpha type-4



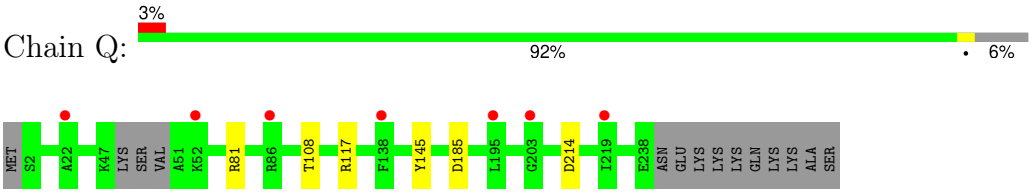
• Molecule 3: Proteasome subunit alpha type-7





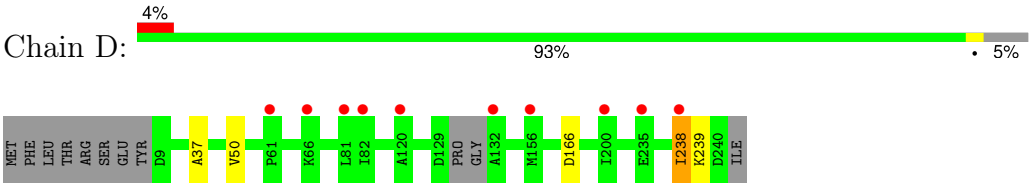
• Molecule 3: Proteasome subunit alpha type-7

Chain Q:



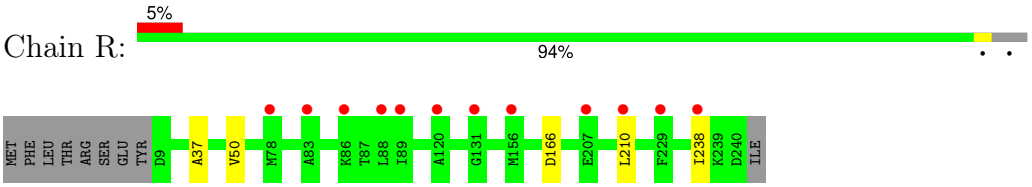
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



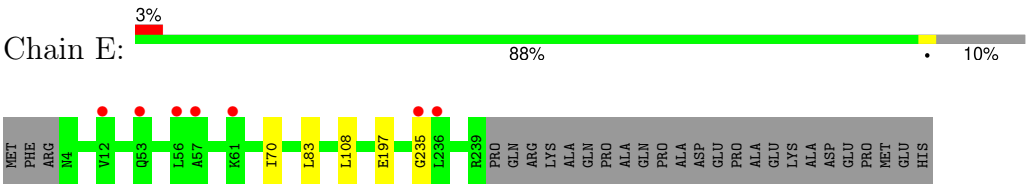
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



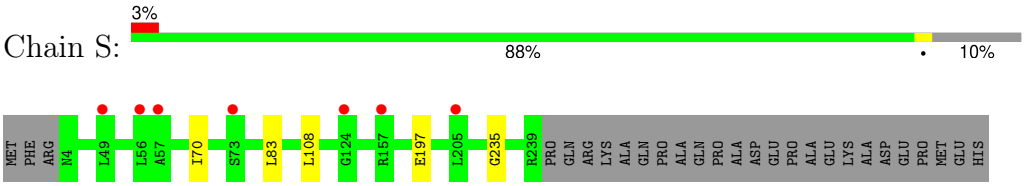
• Molecule 5: Proteasome subunit alpha type-1

Chain E:



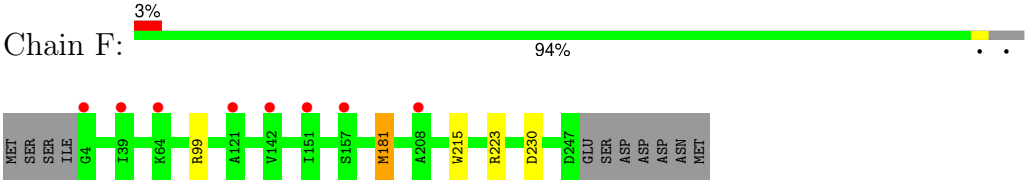
• Molecule 5: Proteasome subunit alpha type-1

Chain S:



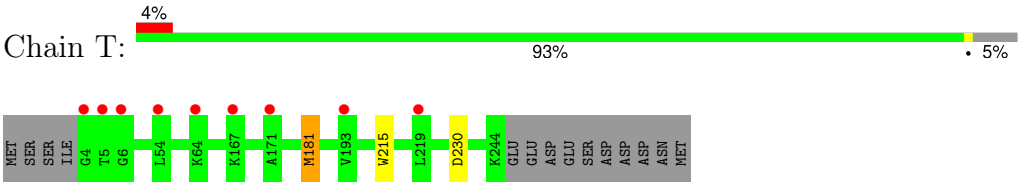
• Molecule 6: Proteasome subunit alpha type-3

Chain F:



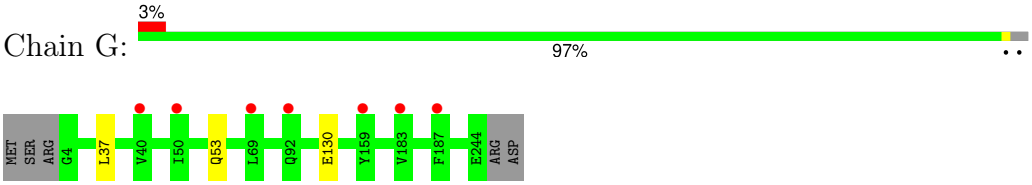
• Molecule 6: Proteasome subunit alpha type-3

Chain T:



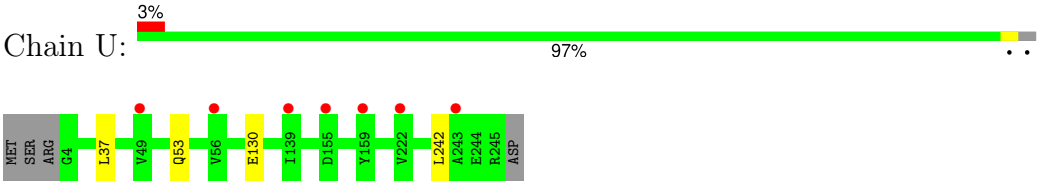
• Molecule 7: Proteasome subunit alpha type-6

Chain G:



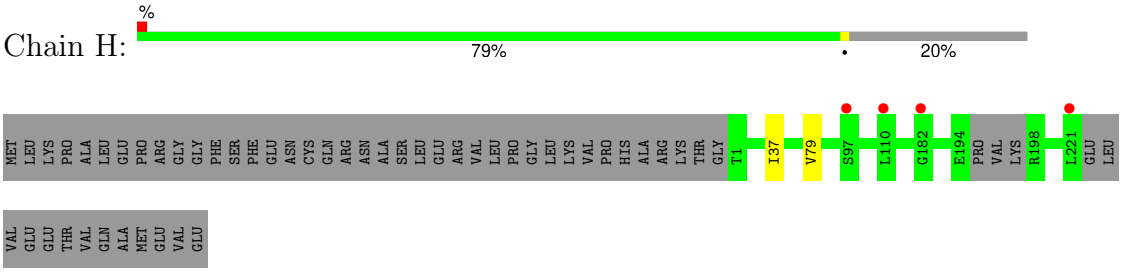
• Molecule 7: Proteasome subunit alpha type-6

Chain U:



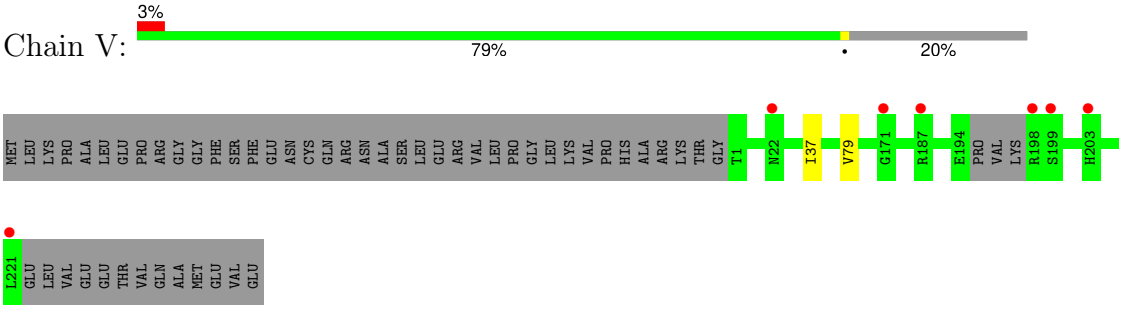
• Molecule 8: Proteasome subunit beta type-10

Chain H:



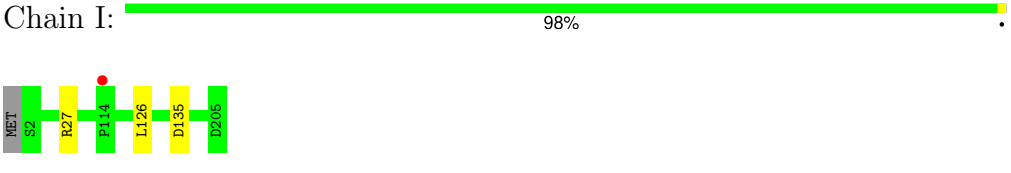
• Molecule 8: Proteasome subunit beta type-10

Chain V:



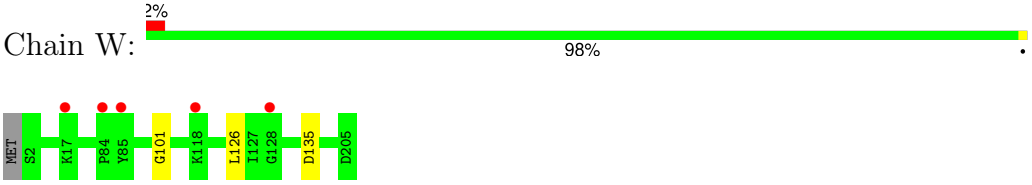
• Molecule 9: Proteasome subunit beta type-3

Chain I:



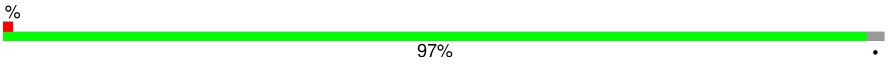
• Molecule 9: Proteasome subunit beta type-3

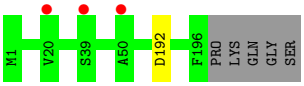
Chain W:



• Molecule 10: Proteasome subunit beta type-2

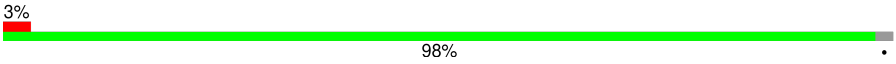
Chain J:

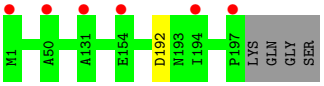




• Molecule 10: Proteasome subunit beta type-2

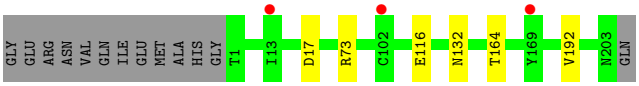
Chain X:





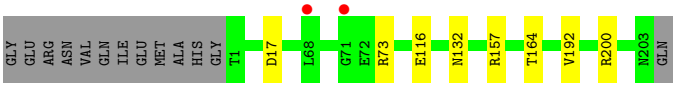
• Molecule 11: Proteasome subunit beta type-8

Chain K:



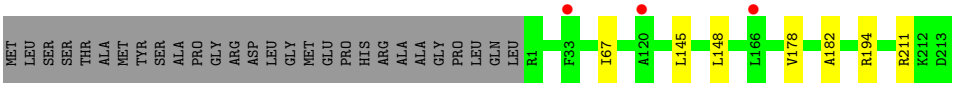
• Molecule 11: Proteasome subunit beta type-8

Chain Y:



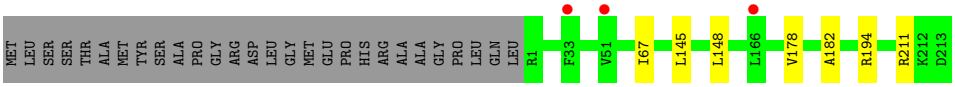
• Molecule 12: Proteasome subunit beta type-1

Chain L:



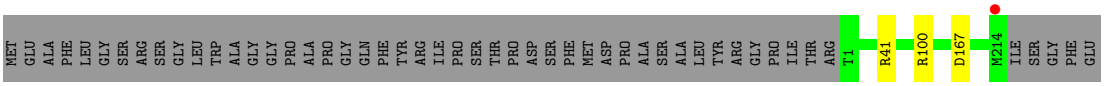
• Molecule 12: Proteasome subunit beta type-1

Chain Z:



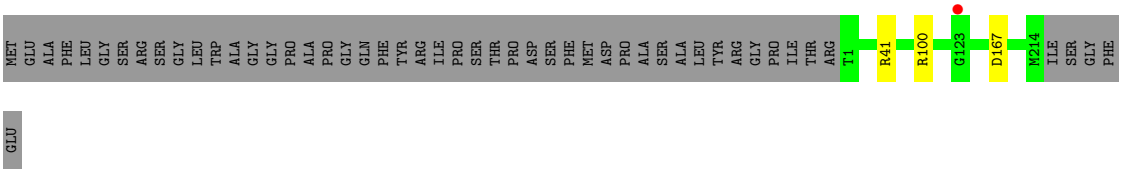
• Molecule 13: Proteasome subunit beta type-4

Chain M:



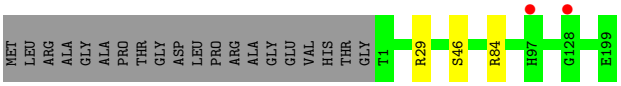
• Molecule 13: Proteasome subunit beta type-4

Chain a:



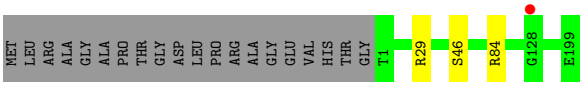
• Molecule 14: Proteasome subunit beta type-9

Chain N:



• Molecule 14: Proteasome subunit beta type-9

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	118.57Å 203.14Å 161.49Å 90.00° 106.82° 90.00°	Depositor
Resolution (Å)	154.58 – 2.77 154.58 – 2.77	Depositor EDS
% Data completeness (in resolution range)	97.0 (154.58-2.77) 97.0 (154.58-2.77)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.248 , 0.291 0.248 , 0.293	Depositor DCC
R_{free} test set	671 reflections (0.36%)	wwPDB-VP
Wilson B-factor (Å^2)	54.0	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 29.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	48431	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SCN, HUJ

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	0.57	0/1826	0.69	1/2474 (0.0%)
1	O	0.57	0/1826	0.68	0/2474
2	B	0.55	0/1961	0.72	1/2640 (0.0%)
2	P	0.54	0/1969	0.72	0/2651
3	C	0.58	0/1822	0.75	1/2458 (0.0%)
3	Q	0.58	0/1873	0.75	2/2526 (0.1%)
4	D	0.54	0/1783	0.64	0/2406
4	R	0.54	0/1796	0.65	0/2426
5	E	0.54	0/1891	0.75	0/2555
5	S	0.54	0/1891	0.74	0/2555
6	F	0.57	0/1946	0.71	2/2620 (0.1%)
6	T	0.57	0/1920	0.70	0/2585
7	G	0.56	0/1909	0.66	0/2581
7	U	0.54	0/1920	0.66	0/2595
8	H	0.51	0/1625	0.72	0/2207
8	V	0.52	0/1625	0.72	0/2207
9	I	0.54	0/1620	0.70	1/2184 (0.0%)
9	W	0.54	0/1620	0.70	0/2184
10	J	0.56	0/1603	0.71	0/2168
10	X	0.57	0/1611	0.72	0/2180
11	K	0.57	0/1609	0.73	1/2170 (0.0%)
11	Y	0.57	0/1609	0.72	2/2170 (0.1%)
12	L	0.55	0/1684	0.76	1/2268 (0.0%)
12	Z	0.55	0/1684	0.76	1/2268 (0.0%)
13	M	0.56	0/1706	0.76	1/2309 (0.0%)
13	a	0.56	0/1706	0.76	1/2309 (0.0%)
14	N	0.54	0/1521	0.70	1/2062 (0.0%)
14	b	0.54	0/1521	0.71	1/2062 (0.0%)
All	All	0.55	0/49077	0.71	17/66294 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	226	ARG	CD-NE-CZ	7.30	133.82	123.60
12	L	211	ARG	NE-CZ-NH1	5.83	123.22	120.30
12	Z	211	ARG	NE-CZ-NH1	5.54	123.07	120.30
6	F	223	ARG	NE-CZ-NH1	5.50	123.05	120.30
14	b	29	ARG	NE-CZ-NH1	5.44	123.02	120.30
13	a	41	ARG	NE-CZ-NH1	5.38	122.99	120.30
13	M	41	ARG	NE-CZ-NH1	5.36	122.98	120.30
6	F	99	ARG	NE-CZ-NH1	5.27	122.94	120.30
9	I	27	ARG	NE-CZ-NH1	5.27	122.94	120.30
3	C	81	ARG	NE-CZ-NH1	5.25	122.93	120.30
14	N	29	ARG	NE-CZ-NH1	5.20	122.90	120.30
11	Y	157	ARG	NE-CZ-NH1	5.14	122.87	120.30
3	Q	81	ARG	NE-CZ-NH1	5.13	122.87	120.30
11	K	73	ARG	NE-CZ-NH1	5.08	122.84	120.30
3	Q	117	ARG	NE-CZ-NH1	5.06	122.83	120.30
11	Y	73	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	176	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1787	0	1782	2	0
1	O	1787	0	1782	2	0
2	B	1932	0	1947	0	0
2	P	1940	0	1951	0	0
3	C	1798	0	1820	2	0
3	Q	1848	0	1865	1	0
4	D	1758	0	1742	1	0
4	R	1769	0	1753	1	0
5	E	1857	0	1845	1	0
5	S	1857	0	1845	1	0
6	F	1911	0	1887	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	1885	0	1871	1	0
7	G	1875	0	1879	1	0
7	U	1886	0	1892	1	0
8	H	1601	0	1634	1	0
8	V	1601	0	1634	1	0
9	I	1591	0	1609	0	0
9	W	1591	0	1609	0	0
10	J	1571	0	1573	0	0
10	X	1578	0	1580	0	0
11	K	1576	0	1522	1	0
11	Y	1576	0	1522	1	0
12	L	1654	0	1656	3	0
12	Z	1654	0	1656	3	0
13	M	1673	0	1650	0	0
13	a	1673	0	1650	0	0
14	N	1493	0	1457	0	0
14	b	1493	0	1457	0	0
15	E	3	0	0	0	0
15	L	3	0	0	0	0
15	Z	3	0	0	0	0
16	G	1	0	0	0	0
16	H	1	0	0	0	0
16	I	2	0	0	0	0
16	K	1	0	0	0	0
16	L	2	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	W	1	0	0	0	0
16	Z	1	0	0	0	0
16	b	1	0	0	0	0
17	K	33	0	0	0	0
17	N	33	0	0	0	0
17	Y	33	0	0	0	0
17	b	33	0	0	0	0
18	B	2	0	0	0	0
18	C	1	0	0	0	0
18	E	1	0	0	0	0
18	F	1	0	0	0	0
18	H	2	0	0	0	0
18	I	4	0	0	0	0
18	J	1	0	0	0	0
18	K	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	L	2	0	0	0	0
18	M	4	0	0	0	0
18	N	3	0	0	0	0
18	O	1	0	0	0	0
18	P	2	0	0	0	0
18	Q	1	0	0	0	0
18	R	4	0	0	0	0
18	S	4	0	0	0	0
18	T	2	0	0	0	0
18	U	1	0	0	0	0
18	V	5	0	0	0	0
18	W	3	0	0	0	0
18	X	3	0	0	0	0
18	Y	5	0	0	0	0
18	Z	4	0	0	0	0
18	a	2	0	0	0	0
18	b	1	0	0	0	0
All	All	48431	0	48070	25	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 0.

All (25) 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)
12:L:145:LEU:HD21	12:L:182:ALA:HB2	1.78	0.65
12:Z:145:LEU:HD21	12:Z:182:ALA:HB2	1.79	0.64
1:A:110:VAL:HG22	1:A:135:ILE:HD13	1.85	0.59
1:O:110:VAL:HG22	1:O:135:ILE:HD13	1.85	0.58
12:Z:148:LEU:HD23	12:Z:178:VAL:HG12	1.97	0.47
5:E:70:ILE:HD13	5:E:108:LEU:HD23	1.96	0.47
12:L:148:LEU:HD23	12:L:178:VAL:HG12	1.97	0.47
5:S:70:ILE:HD13	5:S:108:LEU:HD23	1.96	0.46
3:Q:108:THR:HG21	3:Q:145:TYR:HB3	1.99	0.44
8:V:37:ILE:HG21	8:V:79:VAL:HG11	2.00	0.44
11:K:164:THR:OG1	11:K:192:VAL:HG11	2.18	0.44
1:A:73:LEU:HD23	1:A:86:VAL:HG22	1.98	0.44
11:Y:164:THR:OG1	11:Y:192:VAL:HG11	2.18	0.44
1:O:73:LEU:HD23	1:O:86:VAL:HG22	1.98	0.43
3:C:108:THR:HG21	3:C:145:TYR:HB3	2.01	0.43
6:T:181:MET:N	6:T:181:MET:SD	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:37:ILE:HG21	8:H:79:VAL:HG11	2.01	0.42
6:F:181:MET:SD	6:F:181:MET:N	2.93	0.42
12:Z:145:LEU:HD22	12:Z:178:VAL:HB	2.02	0.42
12:L:145:LEU:HD22	12:L:178:VAL:HB	2.02	0.41
4:R:37:ALA:HB2	4:R:50:VAL:HG23	2.02	0.41
7:U:37:LEU:HD22	7:U:53:GLN:HB2	2.02	0.41
7:G:37:LEU:HD22	7:G:53:GLN:HB2	2.03	0.41
4:D:37:ALA:HB2	4:D:50:VAL:HG23	2.03	0.40
3:C:43:LEU:HD11	3:C:134:VAL:HG22	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	227/234 (97%)	215 (95%)	11 (5%)	1 (0%)	30 58
1	O	227/234 (97%)	215 (95%)	12 (5%)	0	100 100
2	B	241/261 (92%)	233 (97%)	8 (3%)	0	100 100
2	P	242/261 (93%)	234 (97%)	8 (3%)	0	100 100
3	C	221/248 (89%)	212 (96%)	9 (4%)	0	100 100
3	Q	230/248 (93%)	220 (96%)	10 (4%)	0	100 100
4	D	226/241 (94%)	212 (94%)	12 (5%)	2 (1%)	14 38
4	R	230/241 (95%)	213 (93%)	15 (6%)	2 (1%)	14 38
5	E	234/263 (89%)	221 (94%)	12 (5%)	1 (0%)	30 58
5	S	234/263 (89%)	223 (95%)	10 (4%)	1 (0%)	30 58
6	F	242/255 (95%)	237 (98%)	5 (2%)	0	100 100
6	T	239/255 (94%)	235 (98%)	4 (2%)	0	100 100
7	G	239/246 (97%)	234 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	U	240/246 (98%)	236 (98%)	4 (2%)	0	100	100
8	H	214/273 (78%)	205 (96%)	9 (4%)	0	100	100
8	V	214/273 (78%)	203 (95%)	11 (5%)	0	100	100
9	I	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
9	W	202/205 (98%)	193 (96%)	8 (4%)	1 (0%)	25	52
10	J	194/201 (96%)	188 (97%)	6 (3%)	0	100	100
10	X	195/201 (97%)	189 (97%)	6 (3%)	0	100	100
11	K	201/276 (73%)	193 (96%)	7 (4%)	1 (0%)	25	52
11	Y	201/276 (73%)	192 (96%)	8 (4%)	1 (0%)	25	52
12	L	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
12	Z	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
13	M	212/264 (80%)	203 (96%)	9 (4%)	0	100	100
13	a	212/264 (80%)	203 (96%)	9 (4%)	0	100	100
14	N	197/219 (90%)	187 (95%)	10 (5%)	0	100	100
14	b	197/219 (90%)	187 (95%)	10 (5%)	0	100	100
All	All	6135/6854 (90%)	5883 (96%)	242 (4%)	10 (0%)	44	71

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	R	238	ILE
4	D	239	LYS
5	E	235	GLY
11	K	132	ASN
11	Y	132	ASN
4	R	210	LEU
5	S	235	GLY
4	D	238	ILE
1	A	141	GLY
9	W	101	GLY

5.3.2 Protein sidechains (i)

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	188/191 (98%)	186 (99%)	2 (1%)	70	88
1	O	188/191 (98%)	187 (100%)	1 (0%)	86	95
2	B	205/221 (93%)	205 (100%)	0	100	100
2	P	206/221 (93%)	206 (100%)	0	100	100
3	C	193/211 (92%)	190 (98%)	3 (2%)	58	83
3	Q	198/211 (94%)	196 (99%)	2 (1%)	73	89
4	D	193/203 (95%)	191 (99%)	2 (1%)	73	89
4	R	194/203 (96%)	193 (100%)	1 (0%)	86	95
5	E	202/224 (90%)	200 (99%)	2 (1%)	73	89
5	S	202/224 (90%)	200 (99%)	2 (1%)	73	89
6	F	201/212 (95%)	198 (98%)	3 (2%)	60	84
6	T	198/212 (93%)	195 (98%)	3 (2%)	60	84
7	G	205/210 (98%)	204 (100%)	1 (0%)	86	95
7	U	206/210 (98%)	204 (99%)	2 (1%)	73	89
8	H	170/217 (78%)	170 (100%)	0	100	100
8	V	170/217 (78%)	170 (100%)	0	100	100
9	I	173/174 (99%)	171 (99%)	2 (1%)	67	87
9	W	173/174 (99%)	171 (99%)	2 (1%)	67	87
10	J	167/171 (98%)	166 (99%)	1 (1%)	84	94
10	X	168/171 (98%)	167 (99%)	1 (1%)	84	94
11	K	165/222 (74%)	163 (99%)	2 (1%)	67	87
11	Y	165/222 (74%)	162 (98%)	3 (2%)	54	80
12	L	178/199 (89%)	176 (99%)	2 (1%)	70	88
12	Z	178/199 (89%)	176 (99%)	2 (1%)	70	88
13	M	177/215 (82%)	175 (99%)	2 (1%)	70	88
13	a	177/215 (82%)	175 (99%)	2 (1%)	70	88
14	N	153/166 (92%)	151 (99%)	2 (1%)	65	86
14	b	153/166 (92%)	151 (99%)	2 (1%)	65	86
All	All	5146/5672 (91%)	5099 (99%)	47 (1%)	75	91

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	PHE
1	A	182	GLU
3	C	154	HIS
3	C	185	ASP
3	C	214	ASP
4	D	166	ASP
4	D	238	ILE
5	E	83	LEU
5	E	197	GLU
6	F	181	MET
6	F	215	TRP
6	F	230	ASP
7	G	130	GLU
9	I	126	LEU
9	I	135	ASP
10	J	192	ASP
11	K	17	ASP
11	K	116	GLU
12	L	67	ILE
12	L	194	ARG
13	M	100	ARG
13	M	167	ASP
14	N	46	SER
14	N	84	ARG
1	O	182	GLU
3	Q	185	ASP
3	Q	214	ASP
4	R	166	ASP
5	S	83	LEU
5	S	197	GLU
6	T	181	MET
6	T	215	TRP
6	T	230	ASP
7	U	130	GLU
7	U	242	LEU
9	W	126	LEU
9	W	135	ASP
10	X	192	ASP
11	Y	17	ASP
11	Y	116	GLU
11	Y	200	ARG
12	Z	67	ILE
12	Z	194	ARG

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Mol	Chain	Res	Type
13	a	100	ARG
13	a	167	ASP
14	b	46	SER
14	b	84	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	211	ASN
8	H	109	GLN
12	L	79	ASN
13	M	147	GLN
4	R	211	ASN
8	V	109	GLN
12	Z	79	ASN
13	a	147	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 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	$\#\|Z\|>2$
15	SCN	L	301	-	1,2,2	0.19	0	0,1,1	-	-
15	SCN	Z	301	-	1,2,2	0.23	0	0,1,1	-	-
15	SCN	E	301	-	1,2,2	0.50	0	0,1,1	-	-
17	HUJ	b	901	14	27,34,35	0.91	2 (7%)	35,46,49	1.45	6 (17%)
17	HUJ	K	901	11	27,34,35	1.08	2 (7%)	35,46,49	1.45	7 (20%)
17	HUJ	Y	901	11	27,34,35	1.08	2 (7%)	35,46,49	1.44	6 (17%)
17	HUJ	N	901	14	27,34,35	1.33	4 (14%)	35,46,49	1.58	6 (17%)

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	HUJ	N	901	14	-	9/23/32/34	0/2/2/2
17	HUJ	b	901	14	-	7/23/32/34	0/2/2/2
17	HUJ	Y	901	11	-	7/23/32/34	0/2/2/2
17	HUJ	K	901	11	-	6/23/32/34	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	901	HUJ	C12-C11	-4.47	1.33	1.39
17	Y	901	HUJ	N3-N2	3.73	1.41	1.34
17	K	901	HUJ	N3-N2	3.71	1.41	1.34
17	N	901	HUJ	N3-N2	3.59	1.40	1.34
17	b	901	HUJ	N3-N2	3.44	1.40	1.34
17	Y	901	HUJ	N2-N1	3.22	1.40	1.34
17	K	901	HUJ	N2-N1	2.88	1.39	1.34
17	N	901	HUJ	N2-N1	2.72	1.39	1.34
17	b	901	HUJ	N2-N1	2.49	1.39	1.34
17	N	901	HUJ	C11-C16	2.10	1.45	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	b	901	HUJ	N3-N2-N1	-3.57	104.55	107.22
17	Y	901	HUJ	O4-C14-C15	3.39	120.95	115.14
17	K	901	HUJ	N3-N2-N1	-3.38	104.70	107.22
17	b	901	HUJ	O4-C14-C15	3.32	120.83	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	K	901	HUJ	O4-C14-C15	3.31	120.82	115.14
17	N	901	HUJ	O4-C14-C15	3.31	120.81	115.14
17	N	901	HUJ	C16-C11-C10	-3.14	117.61	124.25
17	N	901	HUJ	N3-N2-N1	-3.03	104.96	107.22
17	b	901	HUJ	O4-C14-C13	-2.91	119.39	124.30
17	K	901	HUJ	O4-C14-C13	-2.89	119.42	124.30
17	Y	901	HUJ	O4-C14-C13	-2.89	119.43	124.30
17	b	901	HUJ	C19-O4-C14	2.88	121.74	117.51
17	b	901	HUJ	C8-N1-C7	2.83	136.48	129.82
17	Y	901	HUJ	N3-N2-N1	-2.73	105.18	107.22
17	N	901	HUJ	C8-N1-C7	2.66	136.06	129.82
17	Y	901	HUJ	C6-C5-N	2.59	120.17	115.19
17	Y	901	HUJ	O-C5-C6	-2.43	115.72	121.08
17	K	901	HUJ	C18-O3-C15	2.35	121.11	114.74
17	Y	901	HUJ	C19-O4-C14	2.21	120.76	117.51
17	K	901	HUJ	C17-O2-C16	2.20	120.71	114.74
17	b	901	HUJ	C18-O3-C15	2.11	120.48	114.74
17	K	901	HUJ	C6-C5-N	2.11	119.24	115.19
17	N	901	HUJ	O1-C10-C11	-2.06	117.26	121.03
17	N	901	HUJ	O4-C14-C13	-2.04	120.87	124.30
17	K	901	HUJ	C8-N1-C7	2.02	134.56	129.82

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	901	HUJ	C9-C8-N1-C7
17	K	901	HUJ	C9-C8-N1-N2
17	N	901	HUJ	N1-C8-C9-N4
17	Y	901	HUJ	C9-C8-N1-C7
17	Y	901	HUJ	C9-C8-N1-N2
17	Y	901	HUJ	N1-C8-C9-N4
17	Y	901	HUJ	C15-C14-O4-C19
17	b	901	HUJ	C15-C14-O4-C19
17	N	901	HUJ	C14-C15-O3-C18
17	N	901	HUJ	C13-C14-O4-C19
17	b	901	HUJ	C13-C14-O4-C19
17	Y	901	HUJ	C13-C14-O4-C19
17	N	901	HUJ	C15-C14-O4-C19
17	K	901	HUJ	C13-C14-O4-C19
17	N	901	HUJ	N4-C10-C11-C16
17	N	901	HUJ	O1-C10-C11-C16

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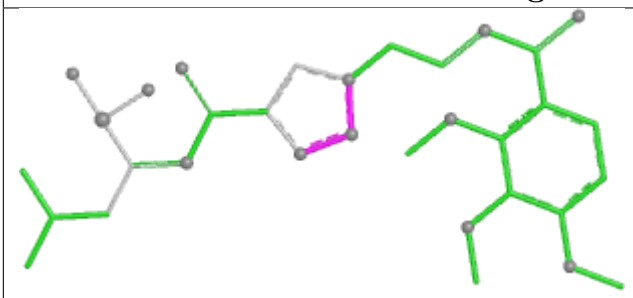
Mol	Chain	Res	Type	Atoms
17	N	901	HUJ	C16-C15-O3-C18
17	K	901	HUJ	C15-C14-O4-C19
17	b	901	HUJ	C9-C8-N1-C7
17	b	901	HUJ	N1-C8-C9-N4
17	b	901	HUJ	O1-C10-C11-C16
17	b	901	HUJ	N4-C10-C11-C16
17	Y	901	HUJ	O1-C10-C11-C16
17	Y	901	HUJ	N4-C10-C11-C16
17	K	901	HUJ	O1-C10-C11-C16
17	K	901	HUJ	N4-C10-C11-C16
17	N	901	HUJ	C9-C8-N1-C7
17	N	901	HUJ	C9-C8-N1-N2
17	b	901	HUJ	C9-C8-N1-N2

There are no ring outliers.

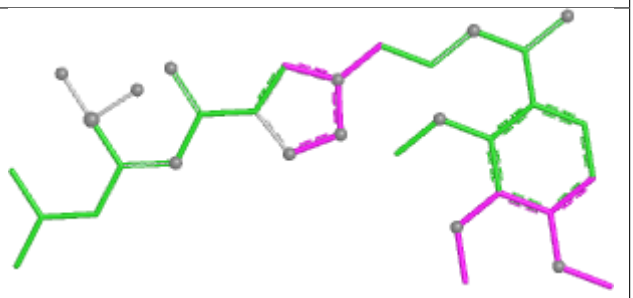
No monomer is involved in short contacts.

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

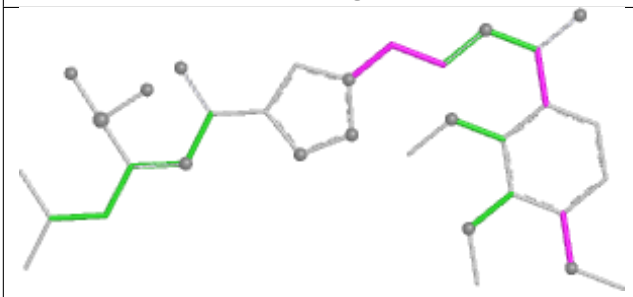
Ligand HUJ b 901



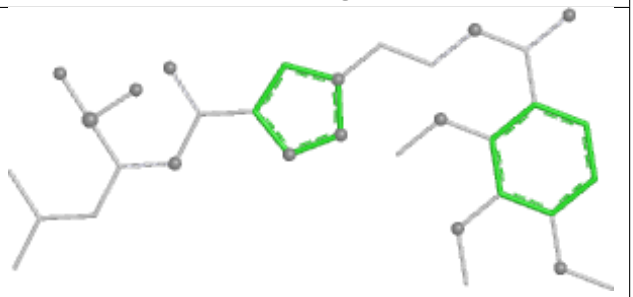
Bond lengths



Bond angles

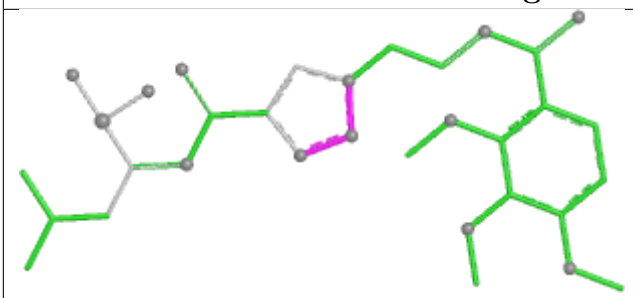


Torsions

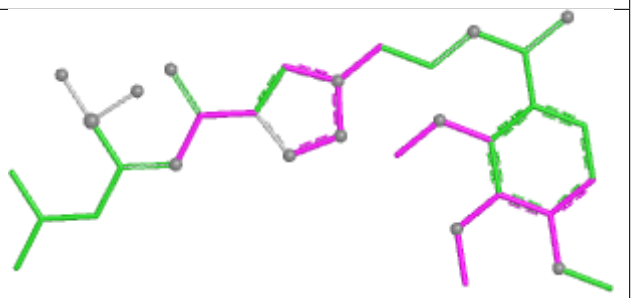


Rings

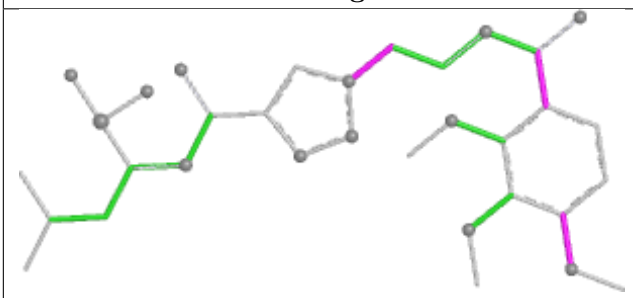
Ligand HUJ K 901



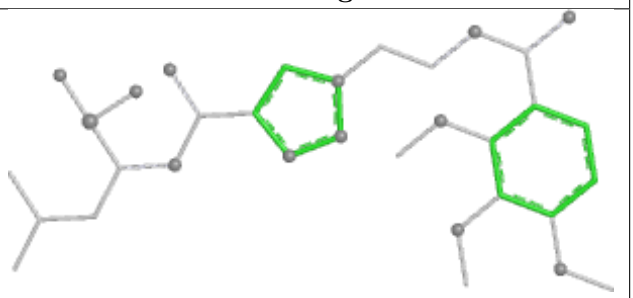
Bond lengths



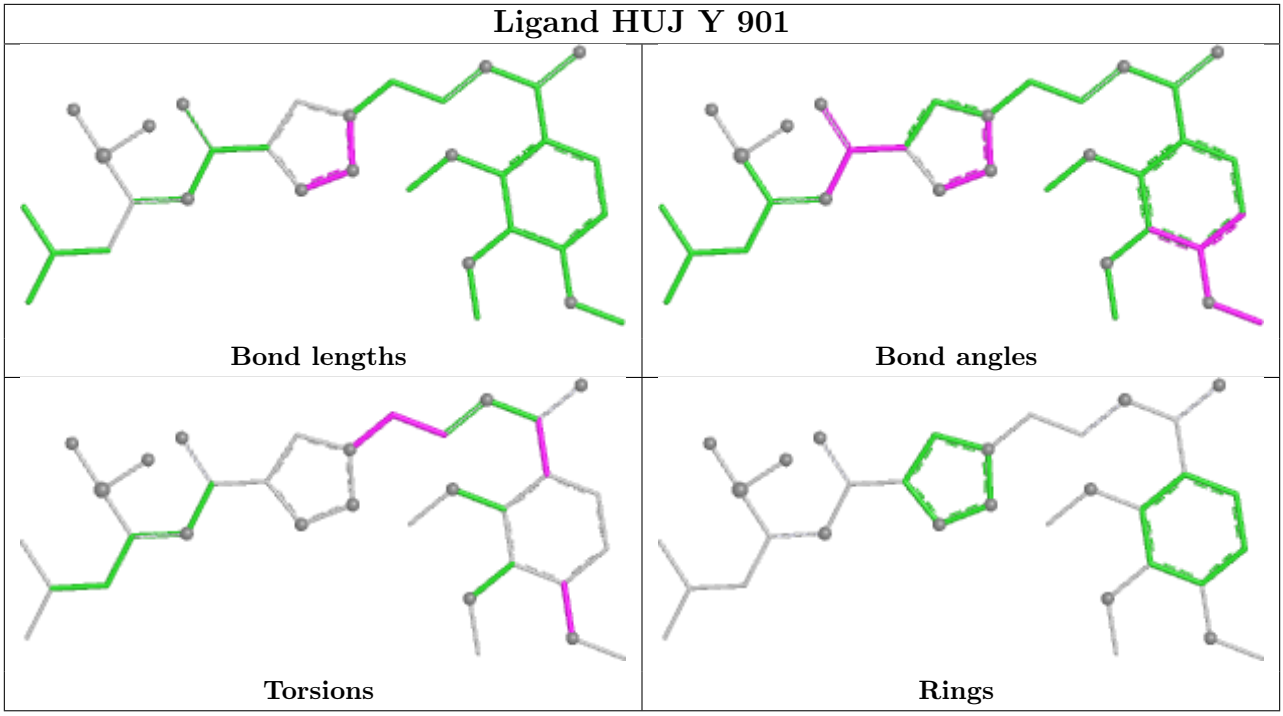
Bond angles

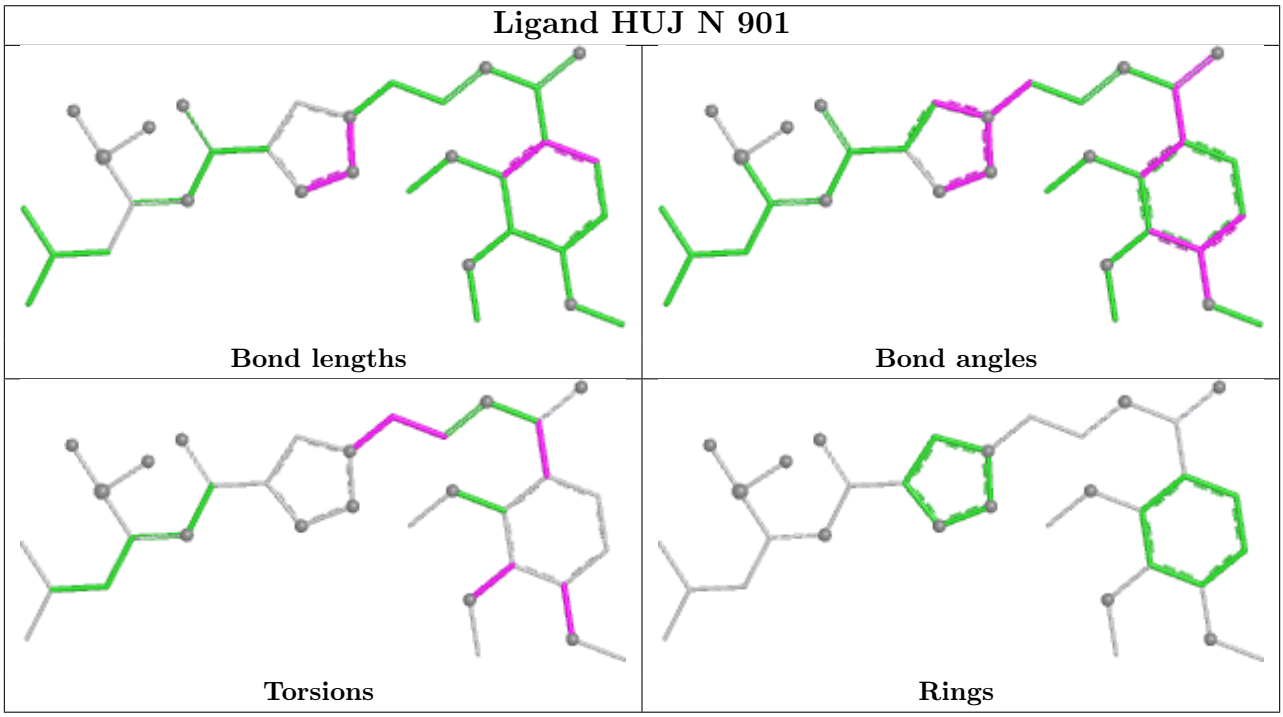


Torsions



Rings





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, 95^{th} 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	229/234 (97%)	0.56	6 (2%)	57	51	47, 72, 112, 125	6 (2%)
1	O	229/234 (97%)	0.54	4 (1%)	69	64	34, 70, 107, 141	5 (2%)
2	B	245/261 (93%)	0.60	14 (5%)	30	26	45, 74, 117, 176	12 (4%)
2	P	246/261 (94%)	0.51	2 (0%)	82	79	41, 75, 111, 166	5 (2%)
3	C	227/248 (91%)	0.65	7 (3%)	51	46	48, 79, 125, 175	5 (2%)
3	Q	234/248 (94%)	0.58	7 (2%)	52	47	37, 78, 122, 161	6 (2%)
4	D	230/241 (95%)	0.56	10 (4%)	40	35	44, 79, 112, 153	7 (3%)
4	R	232/241 (96%)	0.63	12 (5%)	34	29	42, 81, 116, 153	3 (1%)
5	E	236/263 (89%)	0.59	7 (2%)	52	47	46, 77, 119, 152	0
5	S	236/263 (89%)	0.44	7 (2%)	52	47	43, 69, 117, 170	2 (0%)
6	F	244/255 (95%)	0.58	8 (3%)	49	44	47, 78, 120, 141	6 (2%)
6	T	241/255 (94%)	0.49	9 (3%)	45	40	44, 71, 105, 131	2 (0%)
7	G	241/246 (97%)	0.65	7 (2%)	54	48	47, 82, 119, 156	4 (1%)
7	U	242/246 (98%)	0.51	7 (2%)	54	48	39, 73, 108, 140	5 (2%)
8	H	218/273 (79%)	0.40	4 (1%)	67	62	42, 65, 109, 130	2 (0%)
8	V	218/273 (79%)	0.41	7 (3%)	50	45	40, 64, 104, 148	3 (1%)
9	I	204/205 (99%)	0.22	1 (0%)	87	84	34, 59, 84, 126	2 (0%)
9	W	204/205 (99%)	0.36	5 (2%)	58	52	39, 60, 83, 125	0
10	J	196/201 (97%)	0.36	3 (1%)	71	67	38, 63, 91, 125	2 (1%)
10	X	197/201 (98%)	0.32	6 (3%)	52	47	40, 63, 89, 121	4 (2%)
11	K	203/276 (73%)	0.24	3 (1%)	71	67	41, 62, 87, 107	0
11	Y	203/276 (73%)	0.35	2 (0%)	79	75	40, 60, 92, 117	0
12	L	213/241 (88%)	0.29	3 (1%)	73	68	35, 58, 91, 118	2 (0%)
12	Z	213/241 (88%)	0.23	3 (1%)	73	68	32, 57, 86, 117	2 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	214/264 (81%)	0.22	1 (0%) 87 84	40, 63, 85, 122	1 (0%)
13	a	214/264 (81%)	0.27	1 (0%) 87 84	38, 61, 87, 106	0
14	N	199/219 (90%)	0.29	2 (1%) 79 75	42, 61, 89, 103	1 (0%)
14	b	199/219 (90%)	0.27	1 (0%) 87 84	33, 60, 84, 106	2 (1%)
All	All	6207/6854 (90%)	0.44	149 (2%) 59 53	32, 68, 110, 176	89 (1%)

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	194	ILE	4.5
12	L	33	PHE	4.4
7	G	159	TYR	4.0
7	G	40	VAL	3.9
5	E	236	LEU	3.8
3	C	138	PHE	3.7
11	K	102	CYS	3.5
4	D	156	MET	3.4
4	R	238	ILE	3.3
8	H	221	LEU	3.2
4	R	131	GLY	3.2
9	W	128	GLY	3.2
1	O	231	ALA	3.1
5	S	57	ALA	3.1
2	B	237	ILE	3.1
6	T	193	VAL	3.1
3	Q	219	ILE	3.0
10	X	154	GLU	3.0
8	V	221	LEU	3.0
6	F	208	ALA	2.8
14	N	97	HIS	2.8
10	J	50	ALA	2.8
9	I	114	PRO	2.8
2	B	11	ILE	2.8
7	U	159	TYR	2.8
7	U	139	ILE	2.7
10	J	20	VAL	2.7
4	R	120	ALA	2.7
3	Q	195	LEU	2.7
4	R	86	LYS	2.7
5	E	61	LYS	2.7
1	O	176	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
7	G	183	VAL	2.7
6	T	4	GLY	2.7
11	K	169	TYR	2.6
2	B	247	ALA	2.6
10	X	197	PRO	2.6
9	W	84	PRO	2.5
1	A	135	ILE	2.5
11	Y	68	LEU	2.5
6	F	142	VAL	2.5
7	U	155	ASP	2.5
2	P	61	PHE	2.5
1	A	159	ALA	2.5
3	Q	22	ALA	2.5
4	D	238	ILE	2.5
12	Z	166	LEU	2.5
12	Z	33	PHE	2.5
5	E	235	GLY	2.5
2	P	44	LEU	2.4
5	S	124	GLY	2.4
14	b	128	GLY	2.4
5	S	56	LEU	2.4
7	G	69	LEU	2.4
1	A	52	LYS	2.4
2	B	64	LYS	2.4
7	U	49	VAL	2.4
6	F	121	ALA	2.4
10	X	131	ALA	2.4
13	a	123	GLY	2.4
14	N	128	GLY	2.4
5	S	49	LEU	2.4
2	B	46	ALA	2.4
6	F	4	GLY	2.4
3	C	42	VAL	2.4
4	D	81	LEU	2.3
3	C	191	VAL	2.3
2	B	16	GLY	2.3
4	R	156	MET	2.3
6	F	64	LYS	2.3
7	U	222	VAL	2.3
10	J	39	SER	2.3
3	Q	203	GLY	2.3
6	T	6	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
8	V	171	GLY	2.3
2	B	61	PHE	2.3
5	E	53	GLN	2.3
4	R	83	ALA	2.3
2	B	206	LEU	2.3
12	L	166	LEU	2.3
8	V	187	ARG	2.3
8	V	198	ARG	2.3
7	G	92	GLN	2.3
7	G	187	PHE	2.3
2	B	147	LEU	2.3
4	R	210	LEU	2.3
8	H	110	LEU	2.3
13	M	214	MET	2.2
6	F	151	ILE	2.2
9	W	118	LYS	2.2
5	S	157	ARG	2.2
8	V	203	HIS	2.2
2	B	213	ILE	2.2
3	Q	52	LYS	2.2
5	S	205	LEU	2.2
6	T	54	LEU	2.2
5	S	73	SER	2.2
8	V	199	SER	2.2
4	R	78	MET	2.2
10	X	1	MET	2.2
3	C	16	LEU	2.2
4	R	88	LEU	2.2
1	A	54	ILE	2.2
7	U	56	VAL	2.2
5	E	56	LEU	2.2
4	R	207	GLU	2.1
2	B	76	VAL	2.1
9	W	17	LYS	2.1
4	D	120	ALA	2.1
6	T	171	ALA	2.1
3	Q	86	ARG	2.1
4	D	61	PRO	2.1
2	B	33	THR	2.1
6	F	157	SER	2.1
4	D	82	ILE	2.1
5	E	12	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
6	T	219	LEU	2.1
5	E	57	ALA	2.1
1	A	16	GLY	2.1
8	H	182	GLY	2.1
4	D	235	GLU	2.1
1	O	232	ILE	2.1
3	C	181	ILE	2.1
6	F	39	ILE	2.1
7	G	50	ILE	2.1
12	Z	51	VAL	2.1
11	Y	71	GLY	2.1
4	D	66	LYS	2.1
6	T	167	LYS	2.1
9	W	85	TYR	2.1
10	X	50	ALA	2.1
6	T	64	LYS	2.0
6	T	5	THR	2.0
4	D	200	ILE	2.0
10	X	194	ILE	2.0
11	K	13	ILE	2.0
4	R	229	PHE	2.0
8	H	97	SER	2.0
3	C	172	LEU	2.0
1	A	231	ALA	2.0
1	O	40	ALA	2.0
3	C	180	ALA	2.0
4	D	132	ALA	2.0
7	U	243	ALA	2.0
4	R	89	ILE	2.0
2	B	44	LEU	2.0
3	Q	138	PHE	2.0
8	V	22	ASN	2.0
12	L	120	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

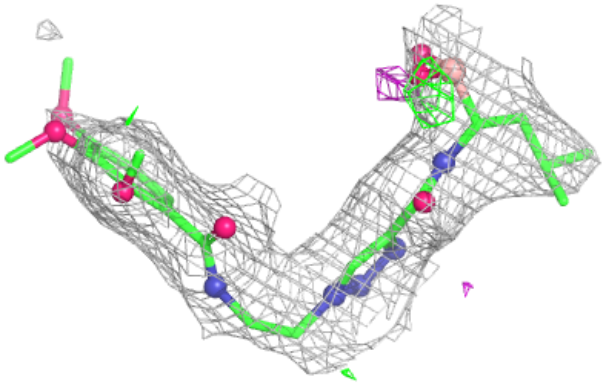
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

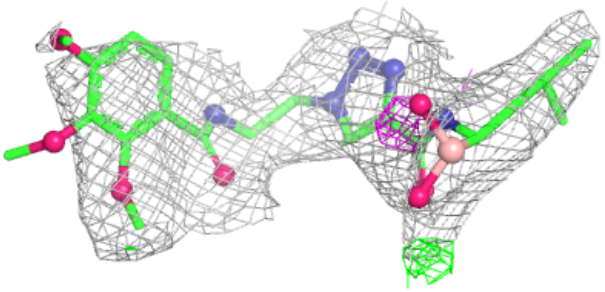
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	NA	Z	302	1/1	0.78	0.13	62,62,62,62	0
16	NA	I	301	1/1	0.79	0.14	66,66,66,66	0
17	HUJ	K	901	33/34	0.80	0.14	53,77,118,131	2
16	NA	N	902	1/1	0.82	0.11	49,49,49,49	0
17	HUJ	Y	901	33/34	0.82	0.17	56,93,126,129	2
17	HUJ	b	901	33/34	0.83	0.18	40,66,132,147	0
16	NA	L	303	1/1	0.84	0.13	68,68,68,68	0
17	HUJ	N	901	33/34	0.86	0.12	42,63,82,83	11
15	SCN	Z	301	3/3	0.87	0.19	65,65,72,81	0
15	SCN	L	301	3/3	0.88	0.12	46,46,64,71	0
16	NA	I	302	1/1	0.89	0.08	58,58,58,58	0
16	NA	L	302	1/1	0.91	0.10	68,68,68,68	0
15	SCN	E	301	3/3	0.91	0.11	67,67,68,74	0
16	NA	G	301	1/1	0.92	0.07	58,58,58,58	0
16	NA	U	301	1/1	0.94	0.08	60,60,60,60	0
16	NA	H	301	1/1	0.95	0.05	62,62,62,62	0
16	NA	b	902	1/1	0.95	0.06	61,61,61,61	0
16	NA	W	301	1/1	0.95	0.07	66,66,66,66	0
16	NA	K	902	1/1	0.98	0.04	48,48,48,48	0

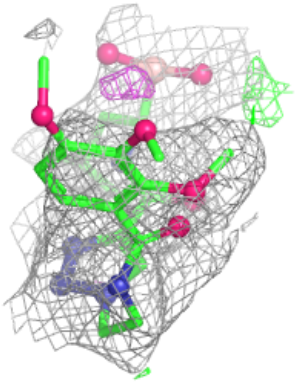
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HUJ K 901:

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

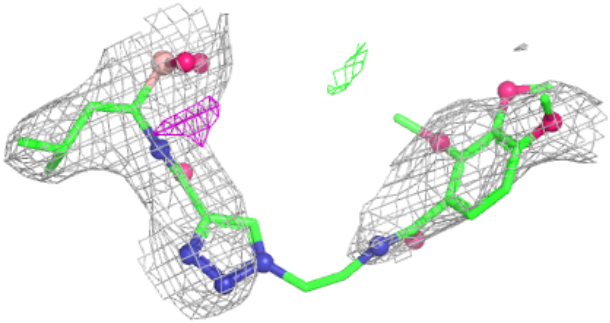


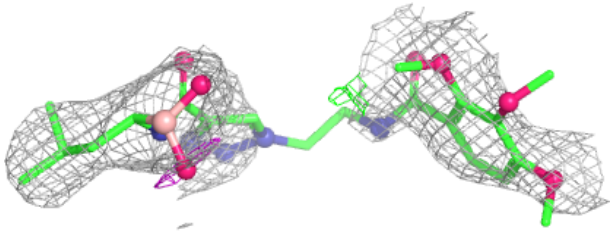


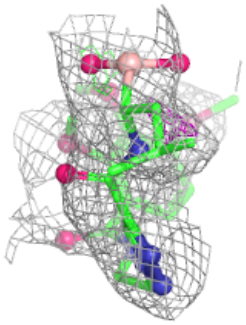


Electron density around HUJ Y 901:

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

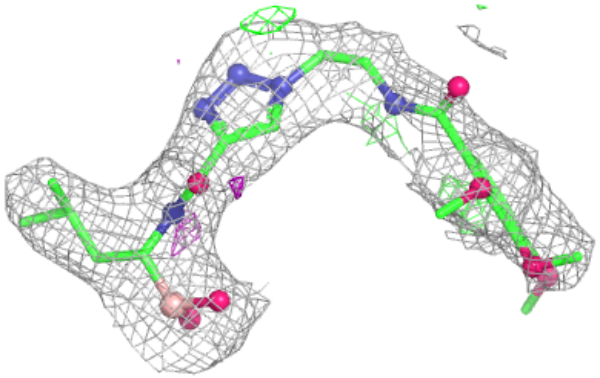


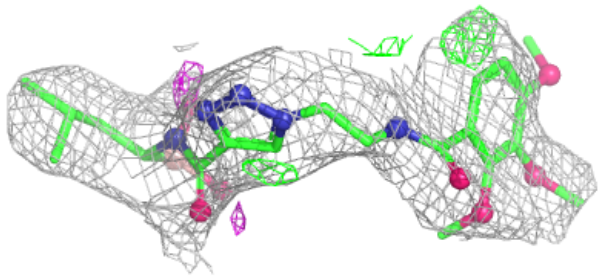


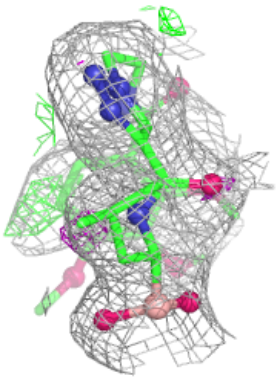


Electron density around HUJ b 901:

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

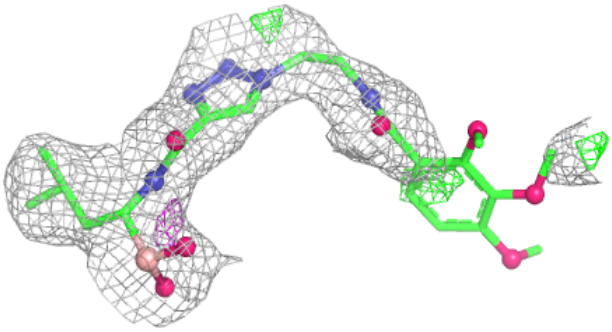


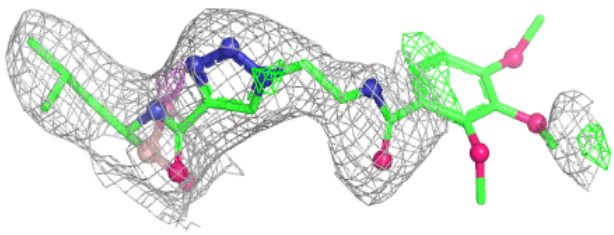


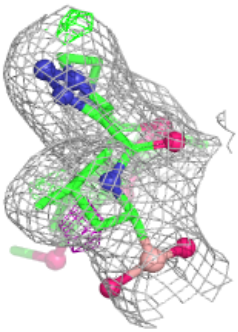


Electron density around HUJ N 901:

$2mF_o$-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 (i)

There are no such residues in this entry.