Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2021 – 02:12 pm BST

PDB ID	:	7AWE
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 following versions of software and data (see references ⓘ) were used in the production of this report:

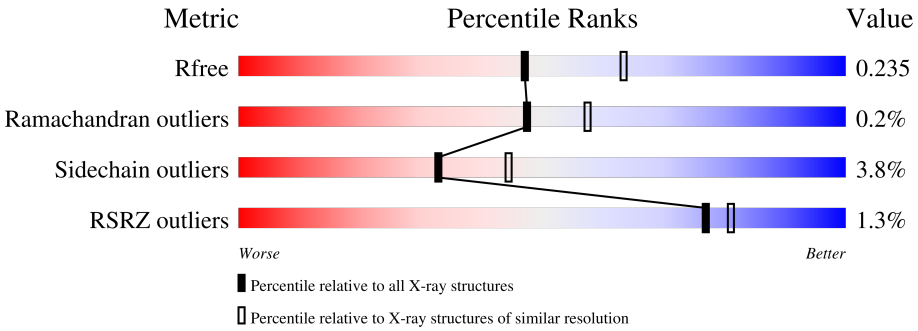
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 2.29 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}	130704	6980 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (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 <=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	2%, 97%
1	O	242	2%, 98%
2	B	229	97%
2	P	229	97%
3	C	256	2%, 91%, 5%
3	Q	256	2%, 95%

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Mol	Chain	Length	Quality of chain
4	D	237	92%
4	R	237	4% 95%
5	E	232	2% 94% 6%
5	S	232	3% 95% 5%
6	F	236	% 97%
6	T	236	2% 97%
7	G	242	3% 96%
7	U	242	96%
8	H	199	98%
8	V	199	98%
9	I	223	4% 98%
9	W	223	4% 97%
10	J	204	% 98%
10	X	204	97%
11	K	197	98%
11	Y	197	% 97%
12	L	203	96%
12	Z	203	96%
13	M	213	96%
13	a	213	96%
14	N	214	96%
14	b	214	96%

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 (three-letter code: 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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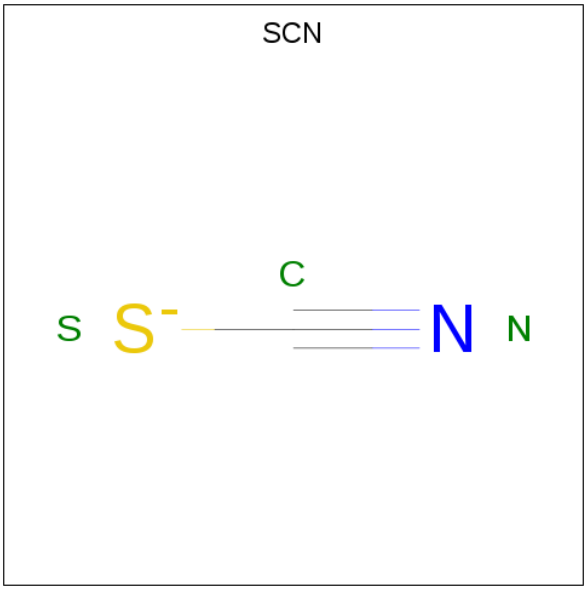
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	I	1	Total Na 1 1	0	0
15	J	2	Total Na 2 2	0	0
15	L	1	Total Na 1 1	0	0
15	M	1	Total Na 1 1	0	0
15	O	1	Total Na 1 1	0	0
15	V	1	Total Na 1 1	0	0
15	W	1	Total Na 1 1	0	0
15	X	1	Total Na 1 1	0	0
15	Z	1	Total Na 1 1	0	0
15	a	1	Total Na 1 1	0	0

- Molecule 16 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

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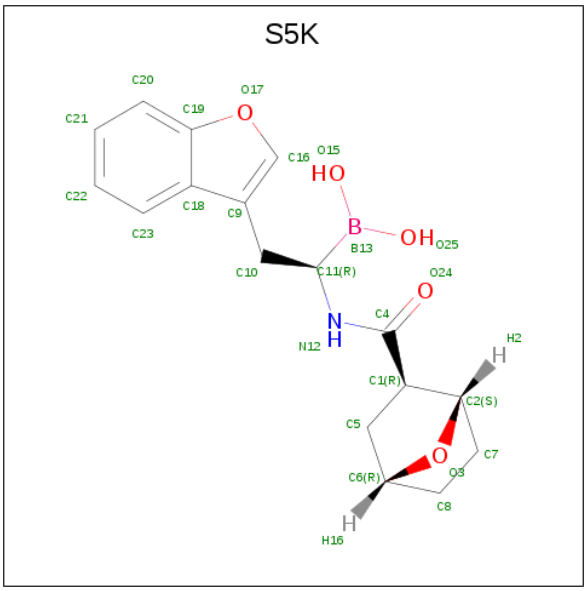
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	K	1	Total C N S 3 1 1 1	0	0
16	K	1	Total C N S 3 1 1 1	0	0
16	M	1	Total C N S 3 1 1 1	0	0
16	M	1	Total C N S 3 1 1 1	0	0
16	M	1	Total C N S 3 1 1 1	0	0
16	T	1	Total C N S 3 1 1 1	0	0
16	U	1	Total C N S 3 1 1 1	0	0
16	Z	1	Total C N S 3 1 1 1	0	0
16	a	1	Total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

- 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 (three-letter code: S5K) (formula: $C_{17}H_{20}BNO_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 18 is water.

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

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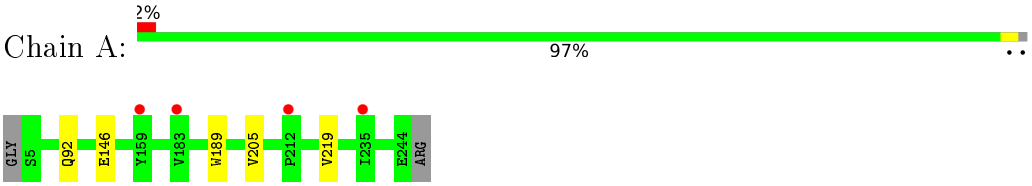
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	Q	40	Total O 40 40	0	0
18	R	29	Total O 29 29	0	0
18	S	22	Total O 22 22	0	0
18	T	58	Total O 58 58	0	0
18	U	43	Total O 43 43	0	0
18	V	57	Total O 57 57	0	0
18	W	52	Total O 52 52	0	0
18	X	68	Total O 68 68	0	0
18	Y	42	Total O 42 42	0	0
18	Z	62	Total O 62 62	0	0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

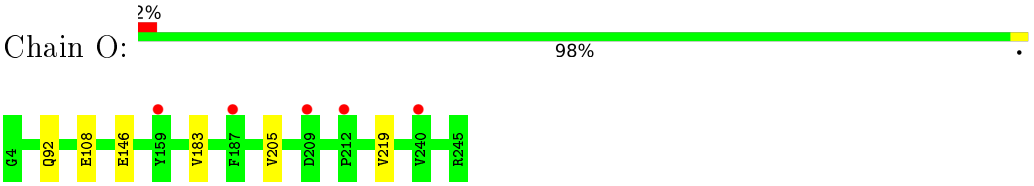
3 Residue-property plots (i)

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.

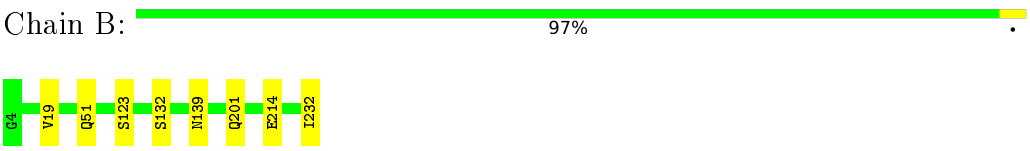
- Molecule 1: Proteasome subunit alpha type-6



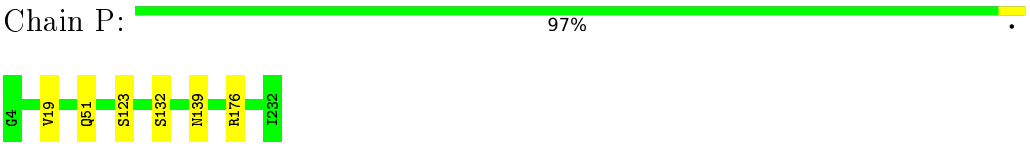
- Molecule 1: Proteasome subunit alpha type-6



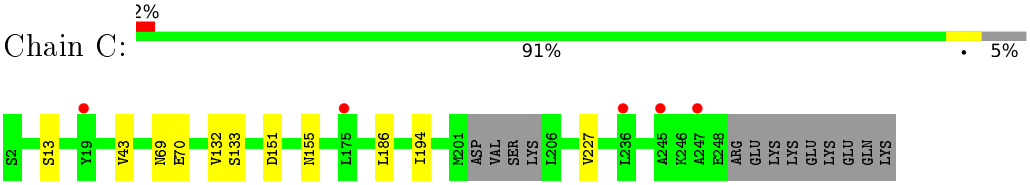
- Molecule 2: Proteasome subunit alpha type-2



- Molecule 2: Proteasome subunit alpha type-2

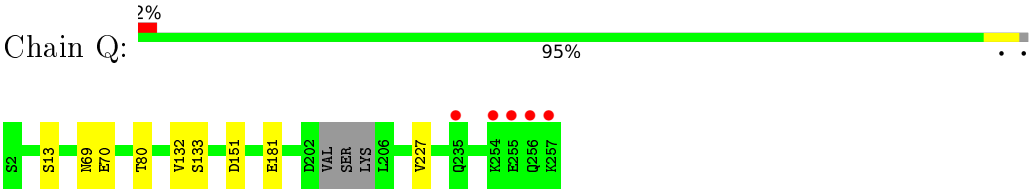


- Molecule 3: Proteasome subunit alpha type-4



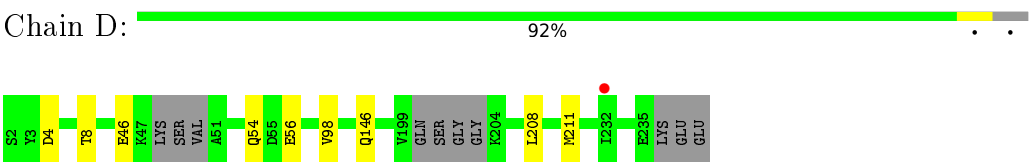
- Molecule 3: Proteasome subunit alpha type-4

Chain Q:



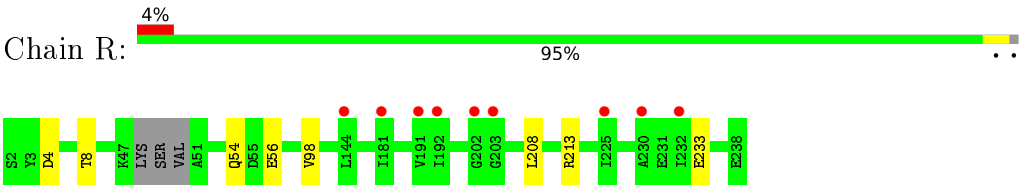
• Molecule 4: Proteasome subunit alpha type-7

Chain D:



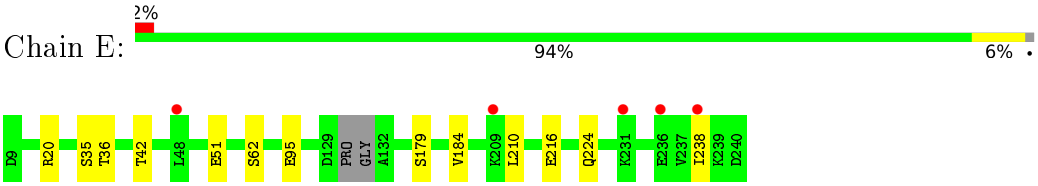
• Molecule 4: Proteasome subunit alpha type-7

Chain R:



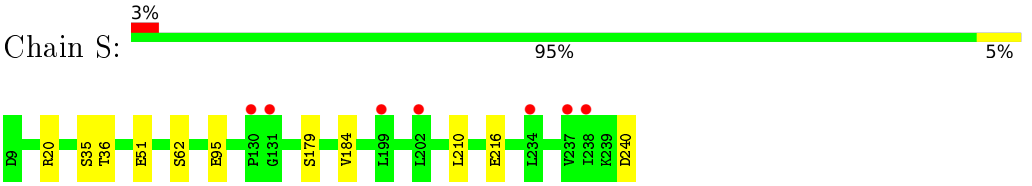
• Molecule 5: Proteasome subunit alpha type-5

Chain E:



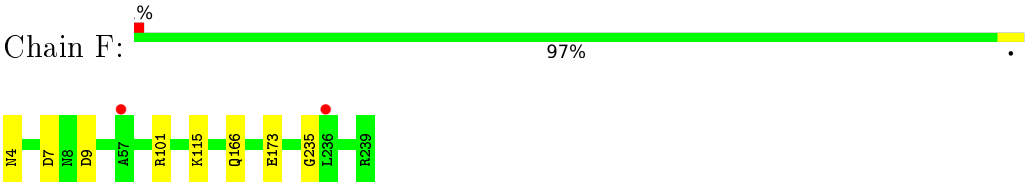
• Molecule 5: Proteasome subunit alpha type-5

Chain S:



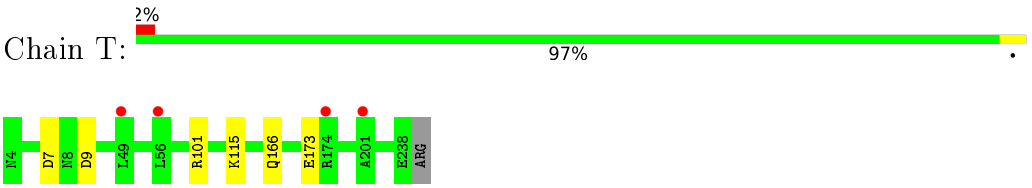
• Molecule 6: Proteasome subunit alpha type-1

Chain F:



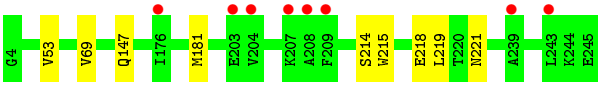
• Molecule 6: Proteasome subunit alpha type-1

Chain T:



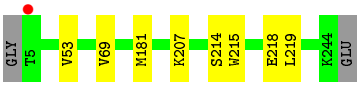
• Molecule 7: Proteasome subunit alpha type-3

Chain G:



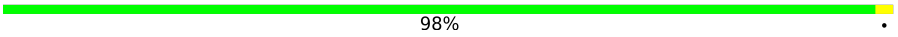
• Molecule 7: Proteasome subunit alpha type-3

Chain U:



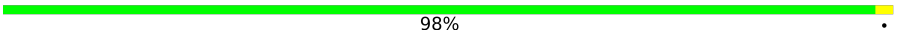
• Molecule 8: Proteasome subunit beta type-9

Chain H:



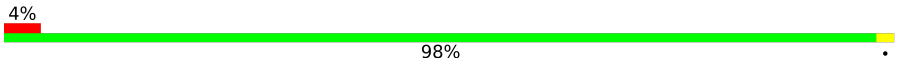
• Molecule 8: Proteasome subunit beta type-9

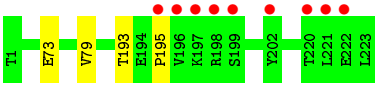
Chain V:



• Molecule 9: Proteasome subunit beta type-10

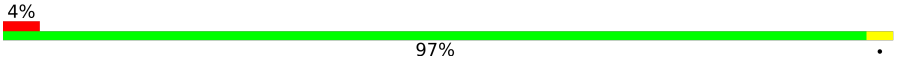
Chain I:

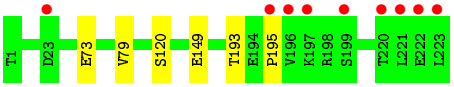




• Molecule 9: Proteasome subunit beta type-10

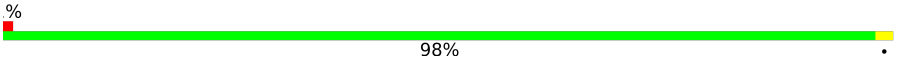
Chain W:

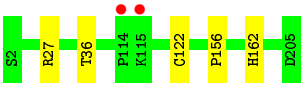




• Molecule 10: Proteasome subunit beta type-3

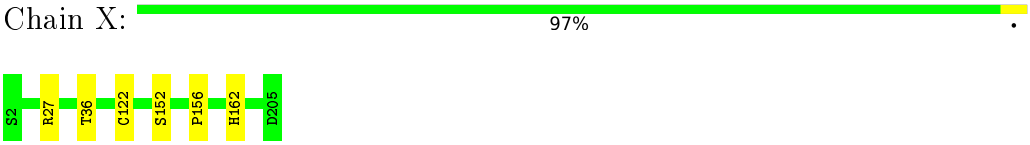
Chain J:





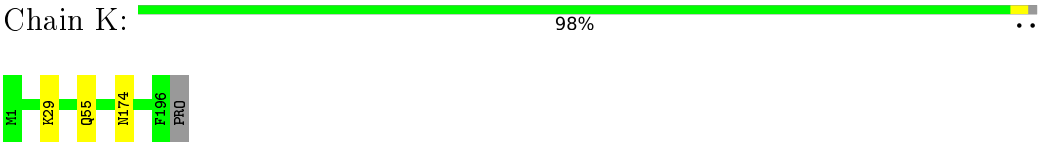
• Molecule 10: Proteasome subunit beta type-3

Chain X:



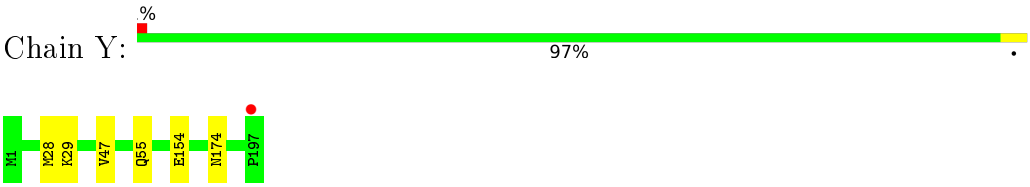
• Molecule 11: Proteasome subunit beta type-2

Chain K:



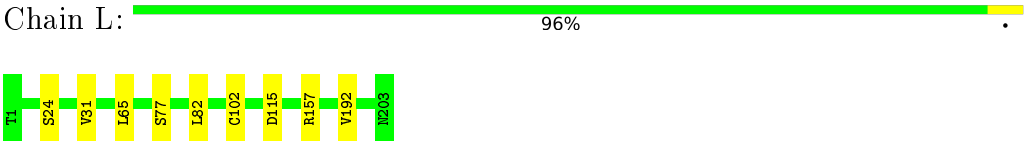
• Molecule 11: Proteasome subunit beta type-2

Chain Y:



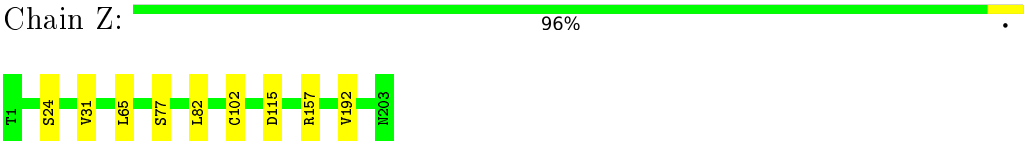
• Molecule 12: Proteasome subunit beta type-8

Chain L:



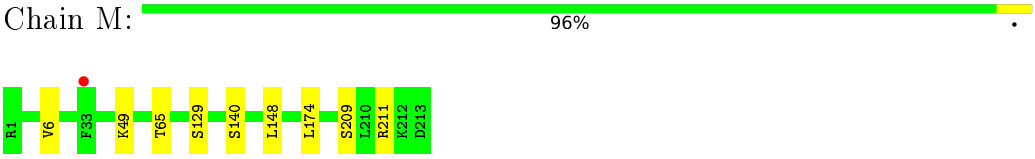
• Molecule 12: Proteasome subunit beta type-8

Chain Z:



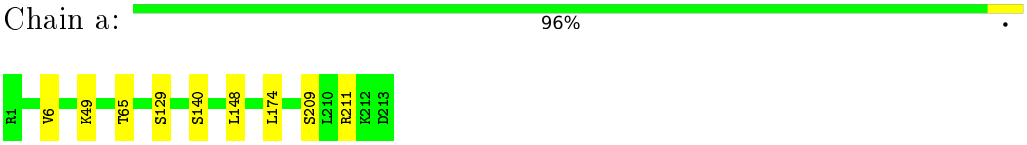
• Molecule 13: Proteasome subunit beta type-1

Chain M:



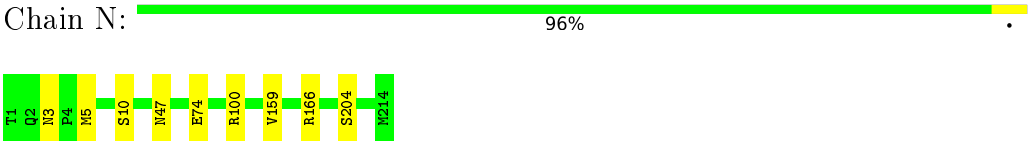
• Molecule 13: Proteasome subunit beta type-1

Chain a:



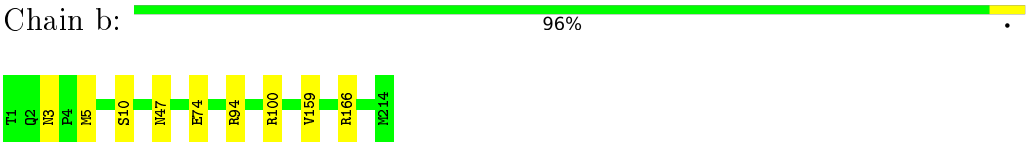
• Molecule 14: Proteasome subunit beta type-4

Chain N:



• Molecule 14: Proteasome subunit beta type-4

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	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
$< I/\sigma(I) >$ [1]	1.70 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.7 (18-SEP-2020)	Depositor
R, R_{free}	0.178 , 0.214 0.203 , 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)	0.29 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[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: S5K, NA, SCN

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	0.38	0/1905	0.60	0/2576
1	O	0.39	0/1920	0.59	0/2595
2	B	0.39	0/1826	0.61	0/2474
2	P	0.40	0/1826	0.59	0/2474
3	C	0.39	0/1941	0.58	0/2614
3	Q	0.39	0/2032	0.56	0/2731
4	D	0.37	0/1822	0.55	0/2458
4	R	0.36	0/1873	0.54	0/2526
5	E	0.40	0/1783	0.57	0/2406
5	S	0.40	0/1796	0.57	0/2426
6	F	0.39	0/1891	0.60	0/2555
6	T	0.41	0/1880	0.60	0/2541
7	G	0.38	0/1929	0.57	0/2597
7	U	0.39	0/1916	0.58	0/2580
8	H	0.42	0/1521	0.60	0/2062
8	V	0.42	0/1521	0.61	0/2062
9	I	0.43	0/1667	0.63	0/2266
9	W	0.43	0/1667	0.63	0/2266
10	J	0.47	0/1620	0.64	0/2184
10	X	0.47	0/1620	0.63	0/2184
11	K	0.44	0/1603	0.63	0/2168
11	Y	0.44	0/1611	0.62	0/2180
12	L	0.45	0/1609	0.65	0/2170
12	Z	0.45	0/1609	0.65	0/2170
13	M	0.48	0/1684	0.67	0/2268
13	a	0.48	0/1684	0.67	0/2268
14	N	0.41	0/1706	0.64	0/2309
14	b	0.42	0/1706	0.64	0/2309
All	All	0.42	0/49168	0.61	0/66419

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	238/242 (98%)	237 (100%)	0	1 (0%)	34 40
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%)	34 40
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%)	34 40
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%)	34 40
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%)	29 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	W	221/223 (99%)	214 (97%)	6 (3%)	1 (0%)	29 34
10	J	202/204 (99%)	195 (96%)	6 (3%)	1 (0%)	29 34
10	X	202/204 (99%)	196 (97%)	5 (2%)	1 (0%)	29 34
11	K	194/197 (98%)	188 (97%)	5 (3%)	1 (0%)	29 34
11	Y	195/197 (99%)	189 (97%)	5 (3%)	1 (0%)	29 34
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%)	47 57

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 (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	205/206 (100%)	201 (98%)	4 (2%)	55 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	206/206 (100%)	200 (97%)	6 (3%)	42	56
2	B	188/188 (100%)	180 (96%)	8 (4%)	29	38
2	P	188/188 (100%)	182 (97%)	6 (3%)	39	52
3	C	203/216 (94%)	192 (95%)	11 (5%)	22	28
3	Q	213/216 (99%)	204 (96%)	9 (4%)	30	39
4	D	193/201 (96%)	184 (95%)	9 (5%)	26	34
4	R	198/201 (98%)	191 (96%)	7 (4%)	36	48
5	E	193/194 (100%)	180 (93%)	13 (7%)	16	19
5	S	194/194 (100%)	183 (94%)	11 (6%)	20	26
6	F	202/202 (100%)	195 (96%)	7 (4%)	36	48
6	T	201/202 (100%)	195 (97%)	6 (3%)	41	54
7	G	199/199 (100%)	190 (96%)	9 (4%)	27	36
7	U	198/199 (100%)	191 (96%)	7 (4%)	36	48
8	H	153/153 (100%)	150 (98%)	3 (2%)	55	70
8	V	153/153 (100%)	149 (97%)	4 (3%)	46	60
9	I	175/175 (100%)	172 (98%)	3 (2%)	60	74
9	W	175/175 (100%)	170 (97%)	5 (3%)	42	56
10	J	173/173 (100%)	169 (98%)	4 (2%)	50	65
10	X	173/173 (100%)	168 (97%)	5 (3%)	42	56
11	K	167/168 (99%)	165 (99%)	2 (1%)	71	82
11	Y	168/168 (100%)	163 (97%)	5 (3%)	41	54
12	L	165/165 (100%)	156 (94%)	9 (6%)	21	27
12	Z	165/165 (100%)	156 (94%)	9 (6%)	21	27
13	M	178/178 (100%)	169 (95%)	9 (5%)	24	31
13	a	178/178 (100%)	169 (95%)	9 (5%)	24	31
14	N	177/177 (100%)	168 (95%)	9 (5%)	24	31
14	b	177/177 (100%)	168 (95%)	9 (5%)	24	31
All	All	5158/5190 (99%)	4960 (96%)	198 (4%)	33	44

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	GLN

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Mol	Chain	Res	Type
1	A	146	GLU
1	A	205	VAL
1	A	219	VAL
2	B	19	VAL
2	B	51	GLN
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	132	VAL
3	C	133	SER
3	C	151	ASP
3	C	155	ASN
3	C	186	LEU
3	C	194	ILE
3	C	227	VAL
4	D	4	ASP
4	D	8	THR
4	D	46	GLU
4	D	54	GLN
4	D	56	GLU
4	D	98	VAL
4	D	146	GLN
4	D	208	LEU
4	D	211	MET
5	E	20	ARG
5	E	35	SER
5	E	36	THR
5	E	42	THR
5	E	51	GLU
5	E	62	SER
5	E	95	GLU
5	E	179	SER
5	E	184	VAL
5	E	210	LEU
5	E	216	GLU

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Mol	Chain	Res	Type
5	E	224	GLN
5	E	238	ILE
6	F	4	ASN
6	F	7	ASP
6	F	9	ASP
6	F	101	ARG
6	F	115	LYS
6	F	166	GLN
6	F	173	GLU
7	G	53	VAL
7	G	69	VAL
7	G	147	GLN
7	G	181	MET
7	G	214	SER
7	G	215	TRP
7	G	218	GLU
7	G	219	LEU
7	G	221	ASN
8	H	84	ARG
8	H	176	VAL
8	H	191	ASN
9	I	73	GLU
9	I	79	VAL
9	I	193	THR
10	J	27	ARG
10	J	36	THR
10	J	122	CYS
10	J	162	HIS
11	K	29	LYS
11	K	55	GLN
12	L	24	SER
12	L	31	VAL
12	L	65	LEU
12	L	77	SER
12	L	82	LEU
12	L	102	CYS
12	L	115	ASP
12	L	157	ARG
12	L	192	VAL
13	M	6	VAL
13	M	49	LYS
13	M	65	THR

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Mol	Chain	Res	Type
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	3	ASN
14	N	5	MET
14	N	10	SER
14	N	47	ASN
14	N	74	GLU
14	N	100	ARG
14	N	159	VAL
14	N	166	ARG
14	N	204	SER
1	O	92	GLN
1	O	108	GLU
1	O	146	GLU
1	O	183	VAL
1	O	205	VAL
1	O	219	VAL
2	P	19	VAL
2	P	51	GLN
2	P	123	SER
2	P	132	SER
2	P	139	ASN
2	P	176	ARG
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	227	VAL
4	R	4	ASP
4	R	8	THR
4	R	54	GLN
4	R	56	GLU
4	R	98	VAL
4	R	208	LEU

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Mol	Chain	Res	Type
4	R	233	GLU
5	S	20	ARG
5	S	35	SER
5	S	36	THR
5	S	51	GLU
5	S	62	SER
5	S	95	GLU
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	101	ARG
6	T	115	LYS
6	T	166	GLN
6	T	173	GLU
7	U	53	VAL
7	U	69	VAL
7	U	181	MET
7	U	214	SER
7	U	215	TRP
7	U	218	GLU
7	U	219	LEU
8	V	71	GLU
8	V	84	ARG
8	V	176	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
10	X	27	ARG
10	X	36	THR
10	X	122	CYS
10	X	152	SER
10	X	162	HIS
11	Y	28	MET
11	Y	29	LYS
11	Y	47	VAL

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Mol	Chain	Res	Type
11	Y	55	GLN
11	Y	154	GLU
12	Z	24	SER
12	Z	31	VAL
12	Z	65	LEU
12	Z	77	SER
12	Z	82	LEU
12	Z	102	CYS
12	Z	115	ASP
12	Z	157	ARG
12	Z	192	VAL
13	a	6	VAL
13	a	49	LYS
13	a	65	THR
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	94	ARG
14	b	100	ARG
14	b	159	VAL
14	b	166	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	51	GLN
2	B	139	ASN
3	C	109	GLN
5	E	41	GLN
5	E	155	HIS
5	E	164	GLN
5	E	214	ASN
6	F	4	ASN
6	F	175	HIS

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Mol	Chain	Res	Type
8	H	66	HIS
9	I	152	GLN
9	I	203	HIS
12	L	146	ASN
13	M	79	ASN
13	M	108	ASN
13	M	131	GLN
1	O	172	GLN
2	P	139	ASN
3	Q	198	ASN
3	Q	240	HIS
4	R	146	GLN
5	S	41	GLN
5	S	155	HIS
5	S	164	GLN
5	S	214	ASN
5	S	221	GLN
5	S	224	GLN
6	T	4	ASN
6	T	175	HIS
6	T	185	ASN
8	V	66	HIS
8	V	97	HIS
12	Z	146	ASN
13	a	79	ASN
13	a	108	ASN
13	a	131	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides 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	M	302	-	1,2,2	0.12	0	0,1,1	0.00	-
16	SCN	U	301	-	1,2,2	0.08	0	0,1,1	0.00	-
17	S5K	H	901	8	19,27,27	0.86	1 (5%)	23,39,39	1.48	4 (17%)
16	SCN	K	201	-	1,2,2	0.31	0	0,1,1	0.00	-
16	SCN	a	302	-	1,2,2	0.16	0	0,1,1	0.00	-
16	SCN	M	304	-	1,2,2	0.51	0	0,1,1	0.00	-
16	SCN	Z	903	-	1,2,2	0.25	0	0,1,1	0.00	-
16	SCN	T	301	-	1,2,2	0.42	0	0,1,1	0.00	-
16	SCN	F	301	-	1,2,2	0.67	0	0,1,1	0.00	-
17	S5K	Z	901	12	19,27,27	0.80	0	23,39,39	1.44	4 (17%)
16	SCN	M	303	-	1,2,2	0.43	0	0,1,1	0.00	-
16	SCN	a	303	-	1,2,2	0.57	0	0,1,1	0.00	-
16	SCN	K	202	-	1,2,2	0.63	0	0,1,1	0.00	-
17	S5K	L	901	12	19,27,27	0.81	1 (5%)	23,39,39	1.46	2 (8%)
17	S5K	V	901	8	19,27,27	0.81	1 (5%)	23,39,39	1.41	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	S5K	L	901	12	-	6/10/33/33	0/5/4/4
17	S5K	Z	901	12	-	4/10/33/33	0/5/4/4
17	S5K	H	901	8	-	4/10/33/33	0/5/4/4
17	S5K	V	901	8	-	5/10/33/33	0/5/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	901	S5K	C18-C19	-2.25	1.38	1.43
17	L	901	S5K	C18-C19	-2.16	1.38	1.43
17	V	901	S5K	C18-C19	-2.08	1.39	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	L	901	S5K	C2-O3-C6	-5.13	96.89	108.92
17	V	901	S5K	C2-O3-C6	-4.90	97.43	108.92
17	H	901	S5K	C2-O3-C6	-4.65	98.01	108.92
17	Z	901	S5K	C2-O3-C6	-4.63	98.06	108.92
17	L	901	S5K	C23-C18-C19	-2.87	118.56	120.38
17	V	901	S5K	C23-C18-C19	-2.74	118.65	120.38
17	H	901	S5K	C23-C18-C19	-2.72	118.66	120.38
17	Z	901	S5K	C23-C18-C19	-2.71	118.67	120.38
17	H	901	S5K	O3-C6-C5	-2.29	102.12	105.07
17	Z	901	S5K	O3-C2-C1	-2.08	99.28	103.45
17	Z	901	S5K	O3-C6-C5	-2.07	102.40	105.07
17	H	901	S5K	O3-C2-C7	-2.05	100.84	104.36
17	V	901	S5K	O3-C6-C5	-2.05	102.43	105.07

There are no chirality outliers.

All (19) torsion outliers are listed below:

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

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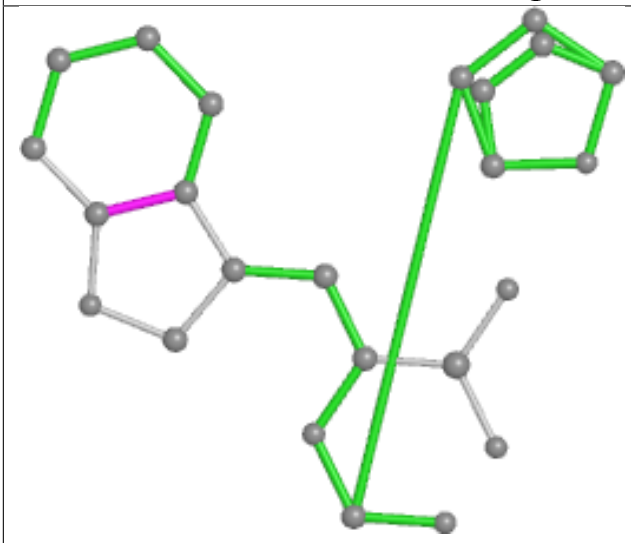
Mol	Chain	Res	Type	Atoms
17	L	901	S5K	C5-C1-C4-N12
17	V	901	S5K	C5-C1-C4-N12

There are no ring outliers.

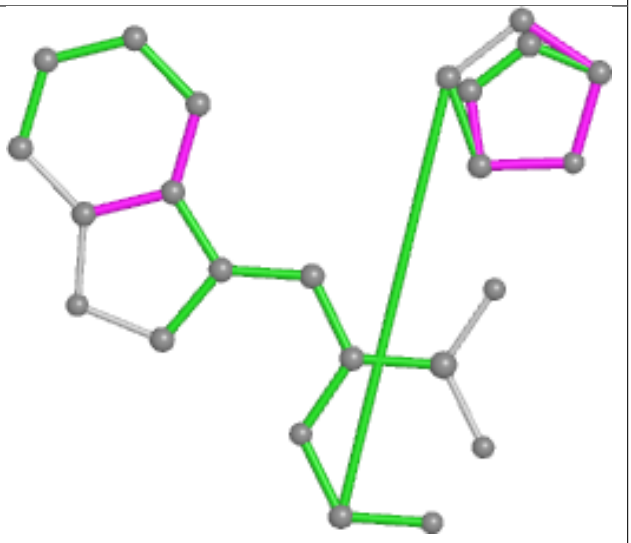
No monomer is involved in short contacts.

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.

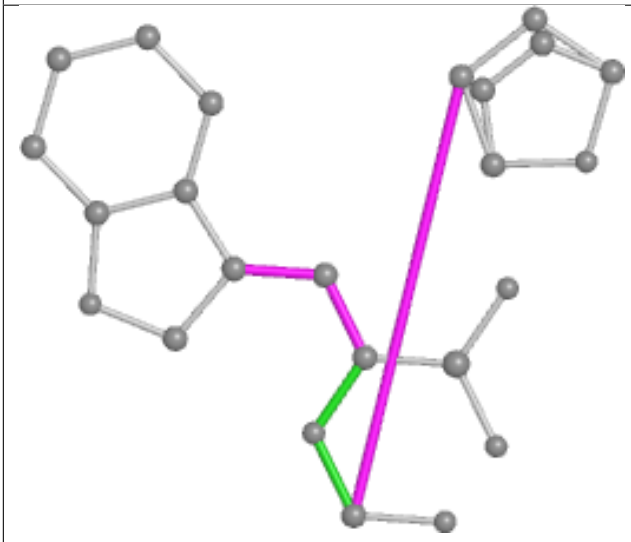
Ligand S5K H 901



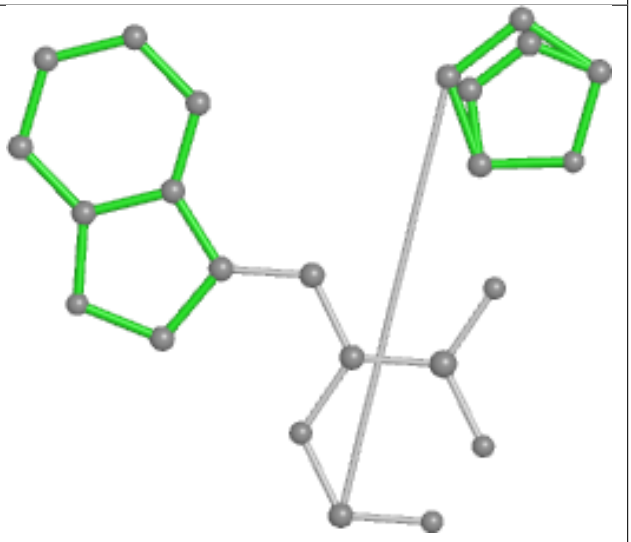
Bond lengths



Bond angles

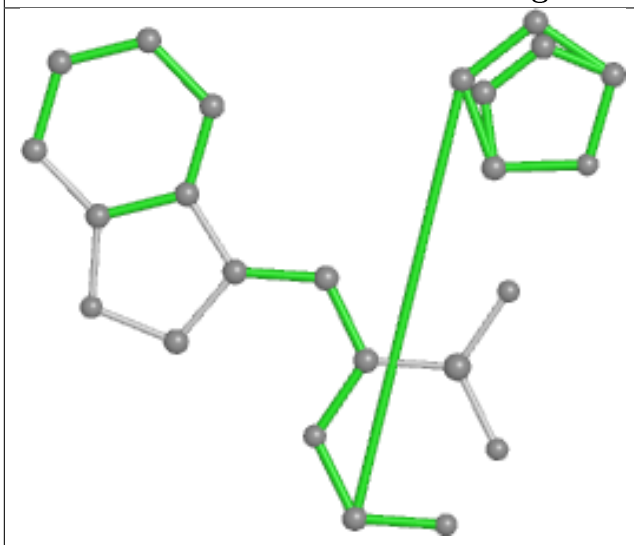


Torsions

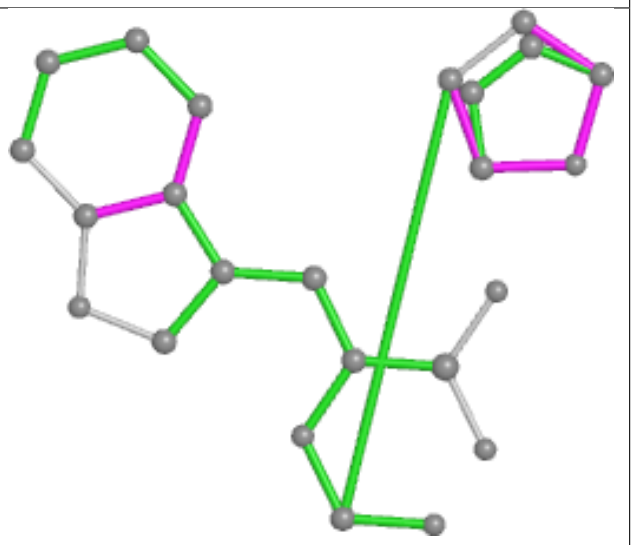


Rings

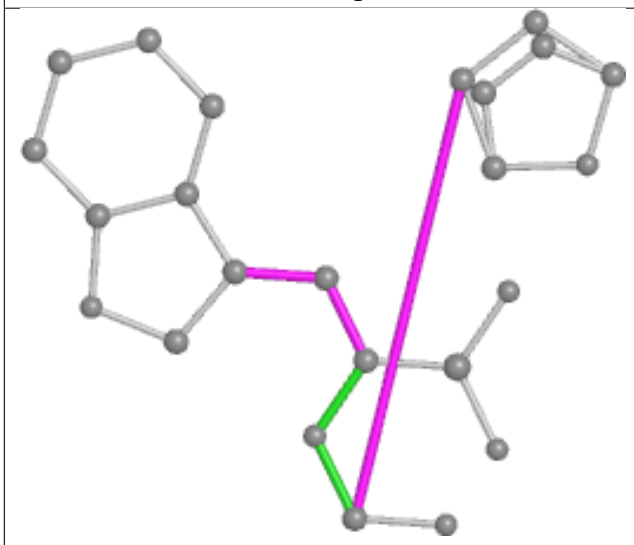
Ligand S5K Z 901



Bond lengths



Bond angles



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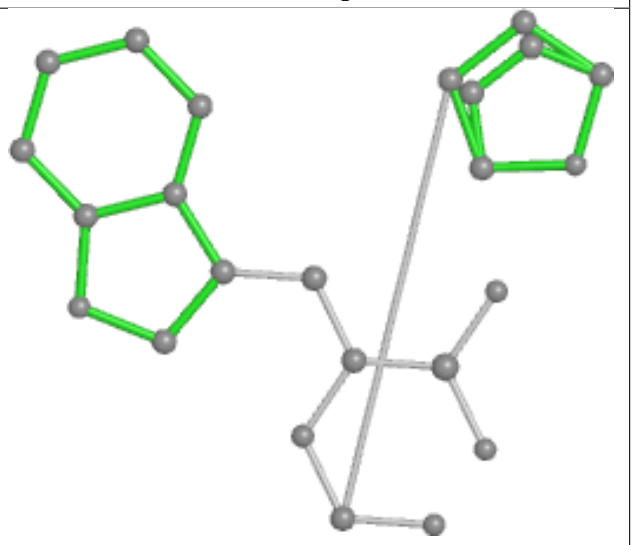
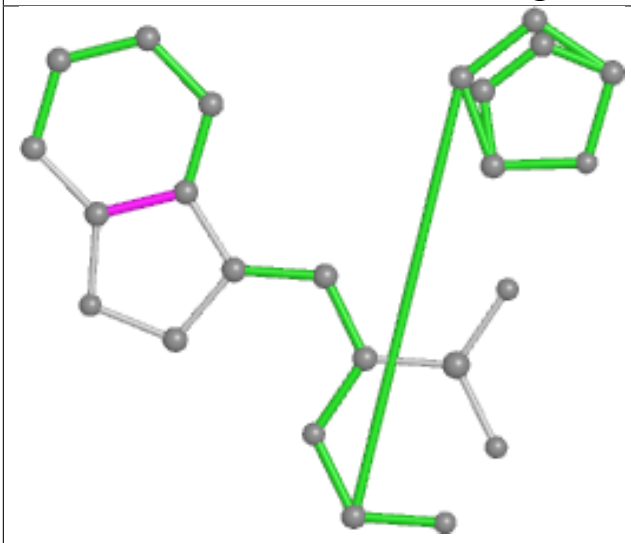
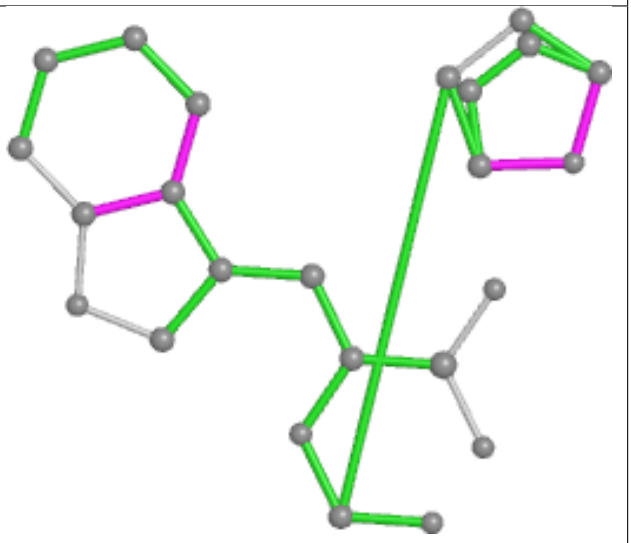


Rings

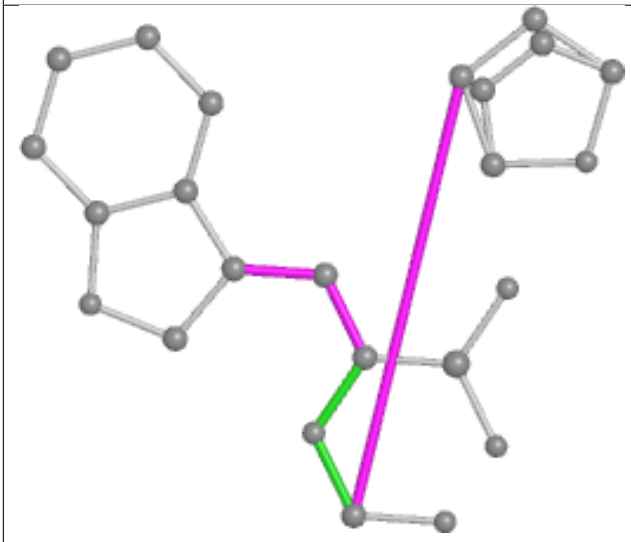
Ligand S5K L 901



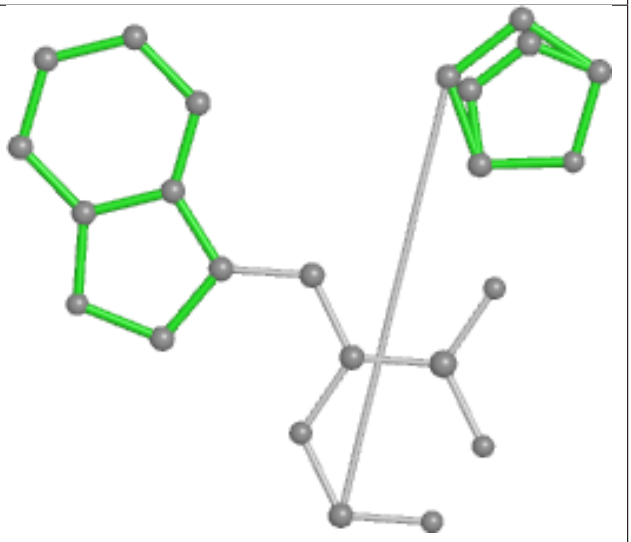
Bond lengths



Bond angles

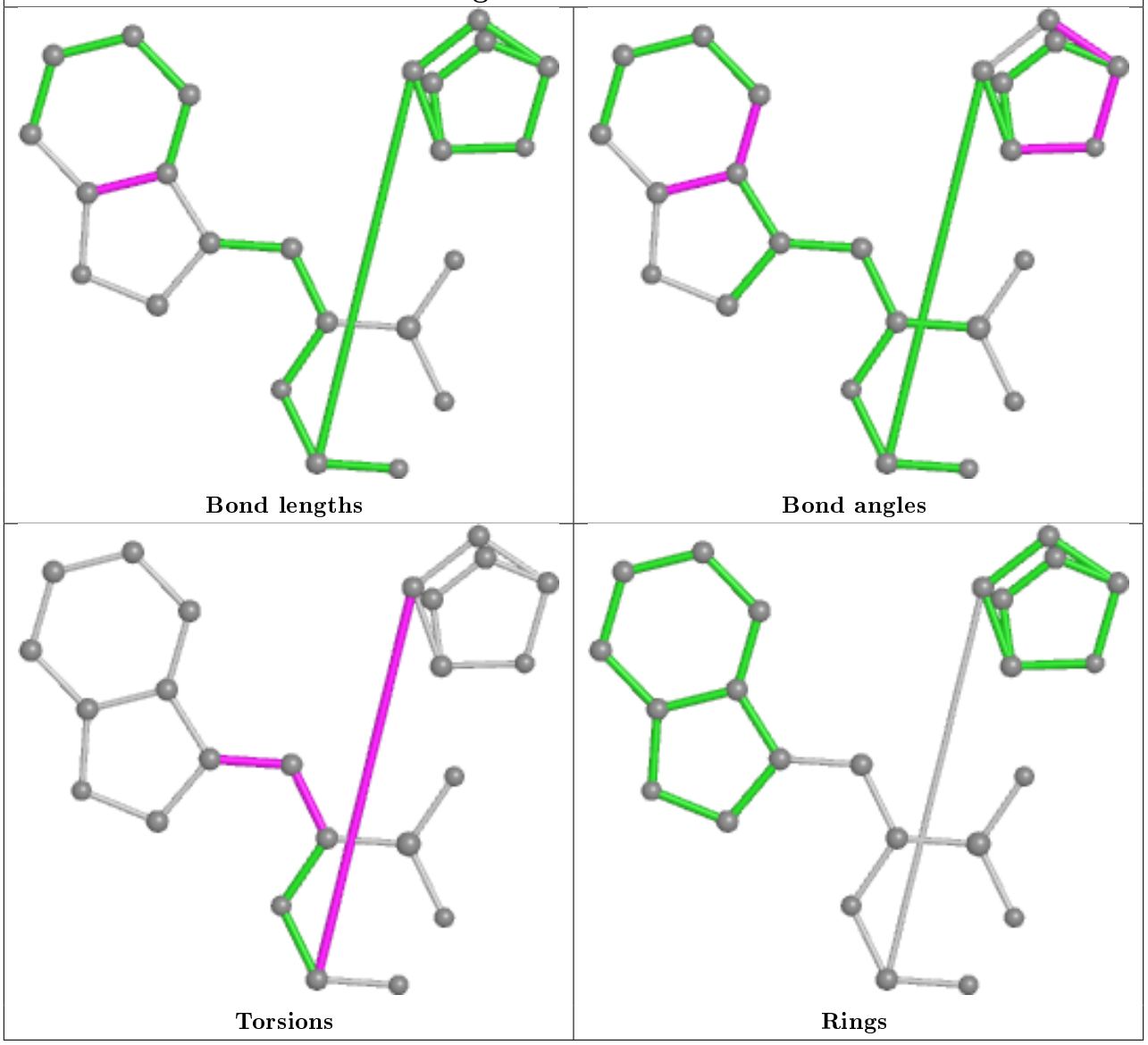


Torsions



Rings

Ligand S5K V 901



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	240/242 (99%)	0.17	4 (1%) 70 75	46, 68, 108, 129	9 (3%)
1	O	242/242 (100%)	0.09	5 (2%) 63 69	40, 62, 92, 121	9 (3%)
2	B	229/229 (100%)	0.04	0 100 100	43, 61, 90, 99	9 (3%)
2	P	229/229 (100%)	-0.10	0 100 100	43, 59, 85, 97	9 (3%)
3	C	243/256 (94%)	0.10	5 (2%) 63 69	40, 64, 95, 152	13 (5%)
3	Q	253/256 (98%)	0.19	5 (1%) 65 70	40, 65, 134, 192	2 (0%)
4	D	227/237 (95%)	0.16	1 (0%) 92 94	45, 71, 116, 154	13 (5%)
4	R	234/237 (98%)	0.19	9 (3%) 40 45	48, 71, 108, 133	16 (6%)
5	E	230/232 (99%)	0.22	5 (2%) 62 68	38, 69, 98, 129	10 (4%)
5	S	232/232 (100%)	0.19	7 (3%) 50 56	38, 71, 96, 122	17 (7%)
6	F	236/236 (100%)	0.18	2 (0%) 86 89	43, 64, 97, 131	11 (4%)
6	T	235/236 (99%)	0.09	4 (1%) 70 75	43, 61, 95, 119	4 (1%)
7	G	242/242 (100%)	0.32	8 (3%) 46 52	47, 69, 104, 138	12 (4%)
7	U	240/242 (99%)	0.14	1 (0%) 92 94	41, 61, 90, 104	8 (3%)
8	H	199/199 (100%)	-0.04	0 100 100	38, 50, 67, 73	1 (0%)
8	V	199/199 (100%)	-0.10	0 100 100	35, 47, 66, 76	3 (1%)
9	I	223/223 (100%)	0.09	9 (4%) 38 43	36, 52, 101, 125	6 (2%)
9	W	223/223 (100%)	0.09	9 (4%) 38 43	37, 50, 101, 120	4 (1%)
10	J	204/204 (100%)	-0.13	2 (0%) 82 86	32, 45, 66, 86	2 (0%)
10	X	204/204 (100%)	-0.17	0 100 100	34, 45, 65, 78	3 (1%)
11	K	196/197 (99%)	-0.03	0 100 100	36, 50, 64, 82	2 (1%)
11	Y	197/197 (100%)	-0.11	1 (0%) 91 93	36, 50, 70, 91	3 (1%)
12	L	203/203 (100%)	-0.16	0 100 100	32, 47, 67, 81	1 (0%)
12	Z	203/203 (100%)	-0.20	0 100 100	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	1 (0%) 91 93	30, 45, 66, 89	3 (1%)
13	a	213/213 (100%)	-0.15	0 100 100	30, 44, 66, 89	5 (2%)
14	N	214/214 (100%)	-0.15	0 100 100	31, 48, 68, 85	2 (0%)
14	b	214/214 (100%)	-0.15	0 100 100	30, 46, 68, 85	1 (0%)
All	All	6217/6254 (99%)	0.03	78 (1%) 77 81	30, 56, 95, 192	179 (2%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	254	LYS	5.8
9	W	220	THR	5.6
9	I	221	LEU	5.6
5	S	130	PRO	5.3
9	I	196	VAL	5.1
3	Q	257	LYS	4.9
9	W	221	LEU	4.6
7	G	207	LYS	4.5
9	I	195	PRO	4.4
3	Q	255	GLU	4.2
9	W	195	PRO	3.9
7	G	176	ILE	3.4
9	W	223	LEU	3.4
3	Q	256	GLN	3.4
9	W	199	SER	3.4
9	W	196	VAL	3.3
9	I	198	ARG	3.2
9	I	222	GLU	3.2
4	R	232	ILE	3.1
5	S	131	GLY	3.1
1	A	159	TYR	3.0
5	S	238	ILE	3.0
5	S	237	VAL	3.0
3	C	236	LEU	3.0
11	Y	197	PRO	3.0
6	T	201	ALA	2.9
1	O	209	ASP	2.9
1	A	235	ILE	2.9
7	G	239	ALA	2.8
5	S	202	LEU	2.8
5	E	236	GLU	2.8
1	O	187	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
3	Q	235	GLN	2.7
9	I	199	SER	2.7
10	J	114	PRO	2.7
6	F	57	ALA	2.7
6	T	56	LEU	2.7
6	F	236	LEU	2.6
1	O	212	PRO	2.6
9	I	197	LYS	2.6
9	I	220	THR	2.6
3	C	175	LEU	2.6
3	C	247	ALA	2.6
4	R	225	ILE	2.6
9	W	197	LYS	2.6
7	G	243	LEU	2.5
4	R	191	VAL	2.5
7	G	204	VAL	2.5
5	S	234	LEU	2.5
13	M	33	PHE	2.5
1	A	183	VAL	2.4
1	O	240	VAL	2.4
9	W	222	GLU	2.4
10	J	115	LYS	2.3
4	R	144	LEU	2.3
5	E	231	LYS	2.3
5	E	238	ILE	2.3
1	O	159	TYR	2.3
7	G	203	GLU	2.3
5	E	48	LEU	2.3
6	T	174	ARG	2.3
9	W	23	ASP	2.3
7	G	208	ALA	2.3
6	T	49	LEU	2.2
4	R	203	GLY	2.2
5	S	199	LEU	2.2
4	R	202	GLY	2.2
4	R	181	ILE	2.2
7	U	5	THR	2.1
4	D	232	ILE	2.1
5	E	209	LYS	2.1
3	C	19	TYR	2.1
9	I	202	TYR	2.1
4	R	192	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	245	ALA	2.0
1	A	212	PRO	2.0
7	G	209	PHE	2.0
4	R	230	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
17	S5K	V	901	24/24	0.78	0.37	62,70,72,72	0
17	S5K	H	901	24/24	0.81	0.32	61,71,74,74	0
16	SCN	M	303	3/3	0.86	0.18	60,60,61,62	0
16	SCN	Z	903	3/3	0.90	0.10	71,71,72,72	0
16	SCN	F	301	3/3	0.91	0.10	65,65,66,67	0
16	SCN	a	303	3/3	0.91	0.18	64,64,65,66	0
15	NA	X	301	1/1	0.92	0.09	43,43,43,43	0
15	NA	a	301	1/1	0.92	0.11	61,61,61,61	0
15	NA	J	301	1/1	0.92	0.07	44,44,44,44	0
15	NA	J	302	1/1	0.92	0.12	55,55,55,55	0
15	NA	M	301	1/1	0.93	0.14	51,51,51,51	0
16	SCN	K	202	3/3	0.93	0.15	69,69,69,70	0
16	SCN	a	302	3/3	0.93	0.18	69,69,69,69	0
16	SCN	T	301	3/3	0.95	0.09	78,78,79,79	0
15	NA	W	301	1/1	0.95	0.07	40,40,40,40	0
15	NA	H	902	1/1	0.95	0.16	51,51,51,51	0
15	NA	A	301	1/1	0.96	0.05	48,48,48,48	0
15	NA	Z	902	1/1	0.96	0.09	38,38,38,38	0
16	SCN	M	304	3/3	0.96	0.09	68,68,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	SCN	K	201	3/3	0.96	0.10	70,70,70,70	0
16	SCN	U	301	3/3	0.96	0.11	69,69,69,69	0
15	NA	V	902	1/1	0.97	0.12	52,52,52,52	0
15	NA	O	301	1/1	0.97	0.09	42,42,42,42	0
16	SCN	M	302	3/3	0.97	0.12	68,68,68,68	0
17	S5K	Z	901	24/24	0.97	0.13	30,35,38,38	0
17	S5K	L	901	24/24	0.98	0.13	31,34,36,37	0
15	NA	L	902	1/1	0.98	0.08	34,34,34,34	0
15	NA	I	301	1/1	0.98	0.08	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.