Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 08:23 pm GMT

PDB ID	:	5CZ6
Title	:	Yeast 20S proteasome beta5-T1A mutant in complex with Syringolin A, propeptide expressed in trans
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2015-07-31
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

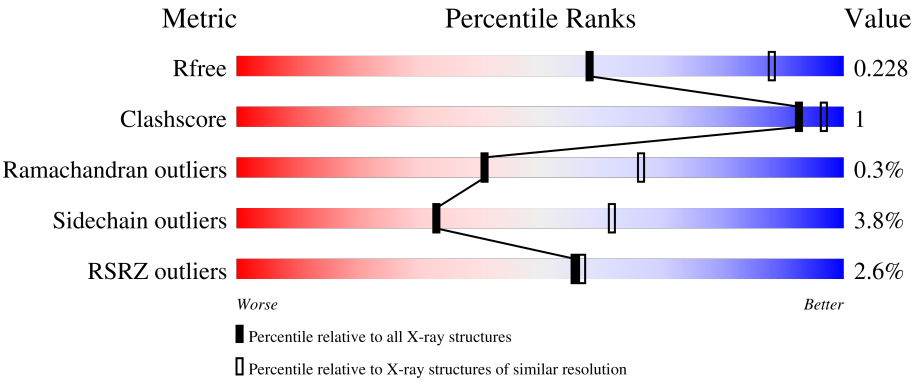
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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.



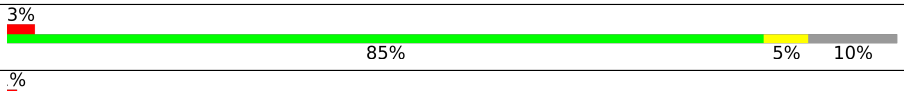
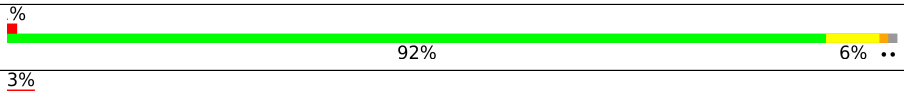
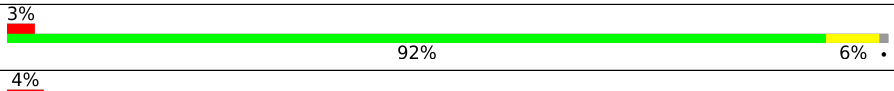
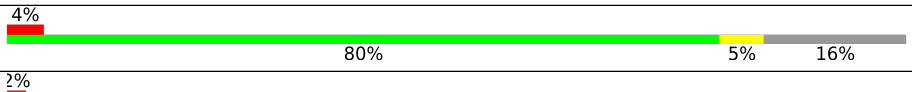
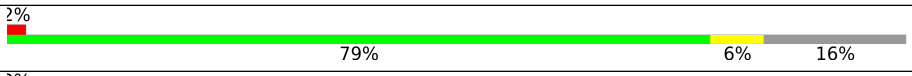
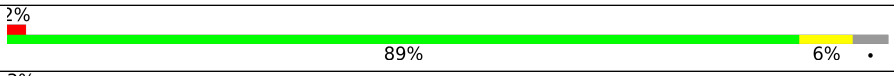
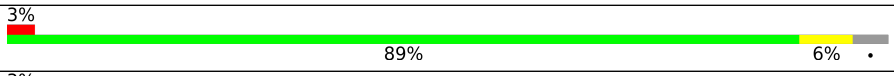
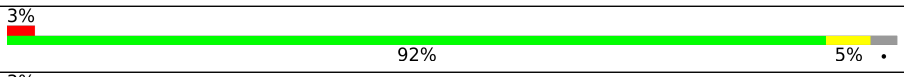
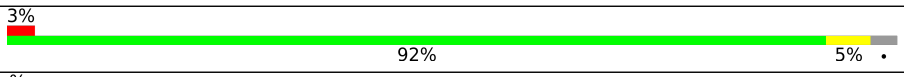
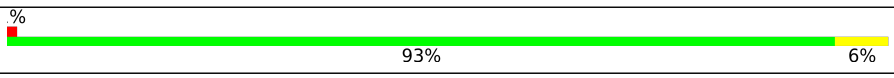
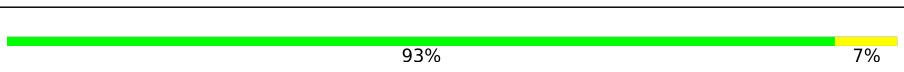
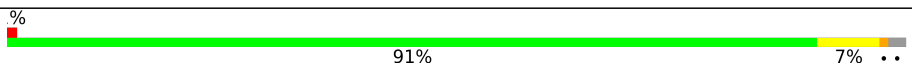
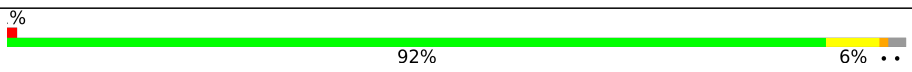
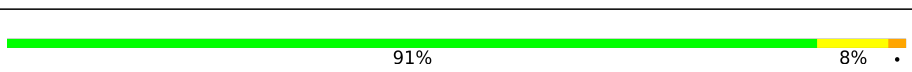
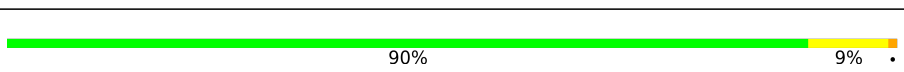
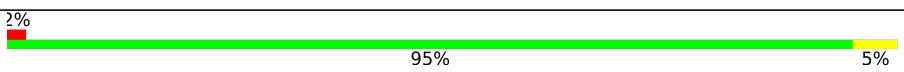
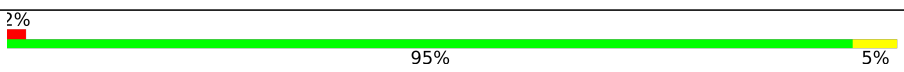
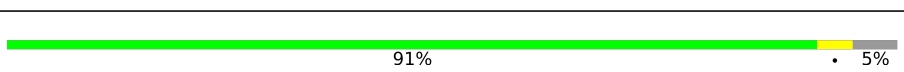
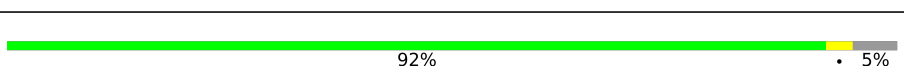
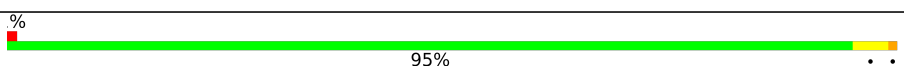
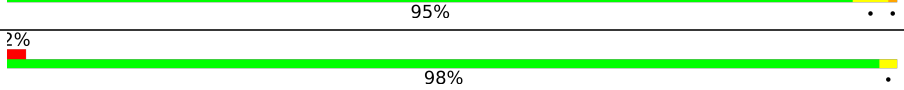
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	250	4% 98% ·
1	O	250	4% 97% ·
2	B	258	4% 86% 8% · 5%
2	P	258	5% 86% 7% · 5%
3	C	254	6% 86% 7% · 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 49891 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1642	1044	280	311	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1642	1044	280	311	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	ALA	THR	engineered mutation	UNP P30656
Y	1	ALA	THR	engineered mutation	UNP P30656

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

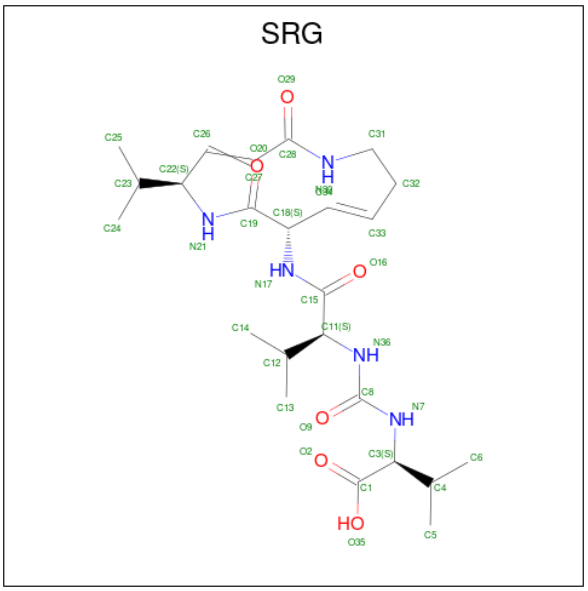
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	H	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0
15	K	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	W	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is (2S)-2-[[(2S)-1-[[(5S,8S,9E)-2,7-dioxo-5-propan-2-yl-1,6-diazacyclododeca-3,9-dien-8-yl]amino]-3-methyl-1-oxo-butan-2-yl]carbamoylamino]-3-methyl-butanoic acid (three-letter code: SRG) (formula: $C_{24}H_{39}N_5O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			35	24	5	6		
17	V	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	17	Total	O	0	0
			17	17		
18	B	10	Total	O	0	0
			10	10		
18	C	9	Total	O	0	0
			9	9		
18	D	16	Total	O	0	0
			16	16		
18	E	12	Total	O	0	0
			12	12		
18	F	10	Total	O	0	0
			10	10		
18	G	16	Total	O	0	0
			16	16		
18	H	24	Total	O	0	0
			24	24		
18	I	16	Total	O	0	0
			16	16		
18	J	14	Total	O	0	0
			14	14		
18	K	15	Total	O	0	0
			15	15		
18	L	28	Total	O	0	0
			28	28		
18	M	22	Total	O	0	0
			22	22		
18	N	11	Total	O	0	0
			11	11		
18	O	6	Total	O	0	0
			6	6		
18	P	12	Total	O	0	0
			12	12		
18	Q	15	Total	O	0	0
			15	15		
18	R	19	Total	O	0	0
			19	19		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	S	11	Total O 11 11	0	0
18	T	17	Total O 17 17	0	0
18	U	17	Total O 17 17	0	0
18	V	15	Total O 15 15	0	0
18	W	5	Total O 5 5	0	0
18	X	13	Total O 13 13	0	0
18	Y	20	Total O 20 20	0	0
18	Z	25	Total O 25 25	0	0
18	a	28	Total O 28 28	0	0
18	b	25	Total O 25 25	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-2

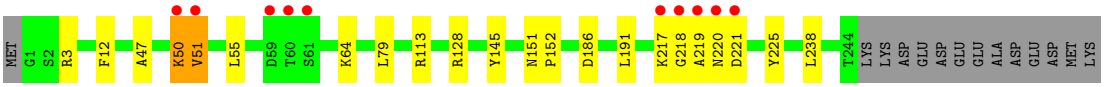
Chain A:

• Molecule 1: Proteasome subunit alpha type-2

Chain O:

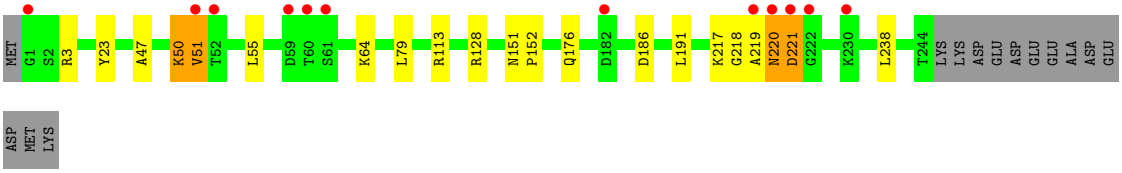
• Molecule 2: Proteasome subunit alpha type-3

Chain B:



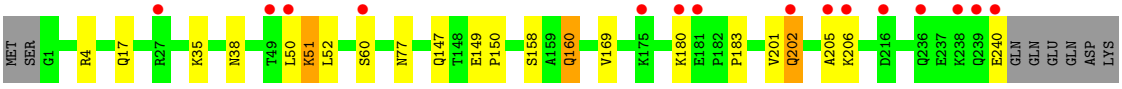
• Molecule 2: Proteasome subunit alpha type-3

Chain P:



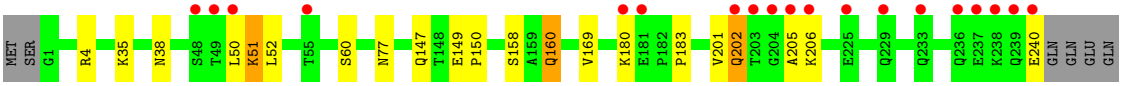
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



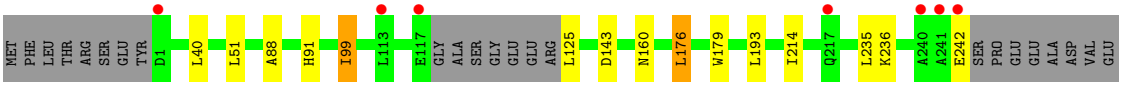
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



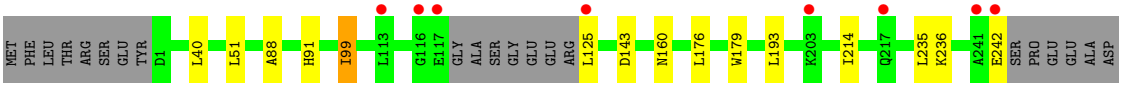
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



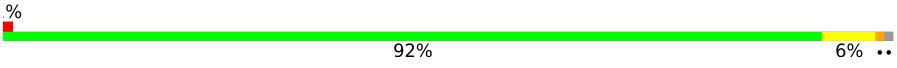
• Molecule 4: Proteasome subunit alpha type-5

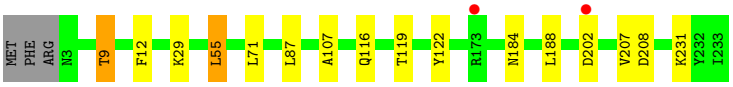
Chain R:



• Molecule 5: Proteasome subunit alpha type-6

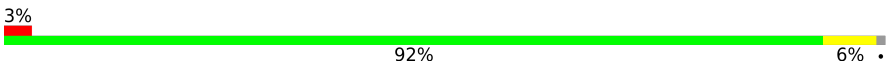
Chain E:





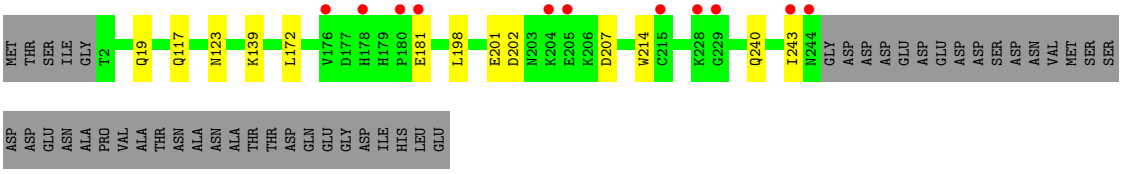
• Molecule 5: Proteasome subunit alpha type-6

Chain S:

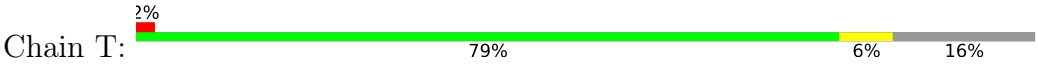


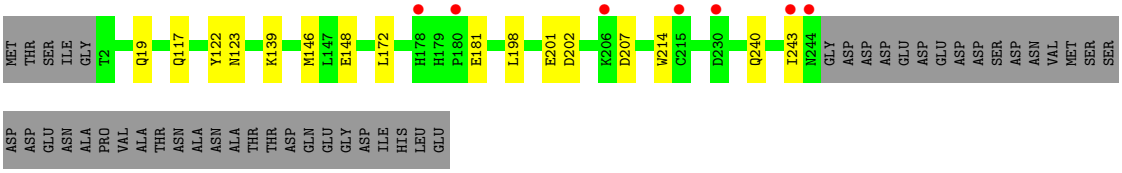
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:

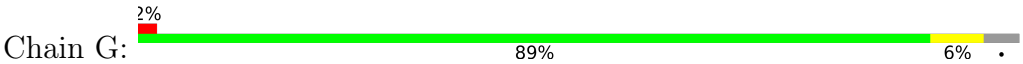


• Molecule 6: Probable proteasome subunit alpha type-7

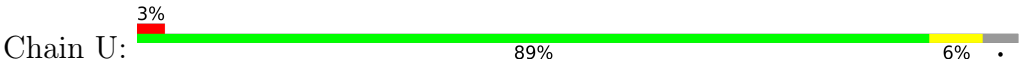




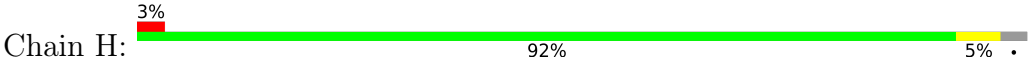
• Molecule 7: Proteasome subunit alpha type-1

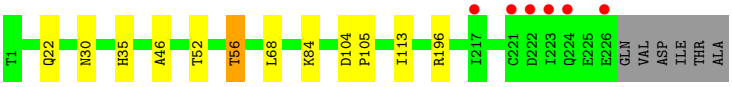


• Molecule 7: Proteasome subunit alpha type-1

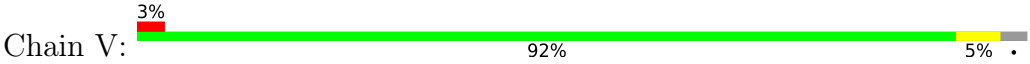


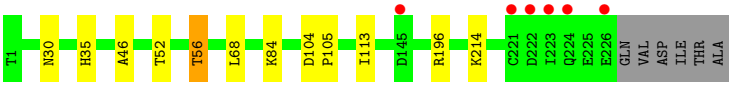
• Molecule 8: Proteasome subunit beta type-2



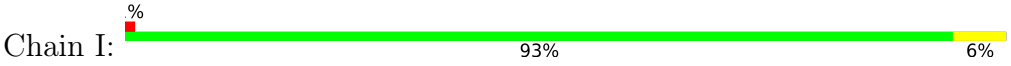


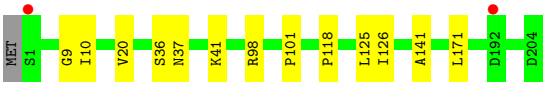
• Molecule 8: Proteasome subunit beta type-2



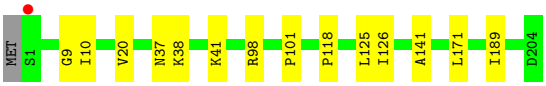


• Molecule 9: Proteasome subunit beta type-3

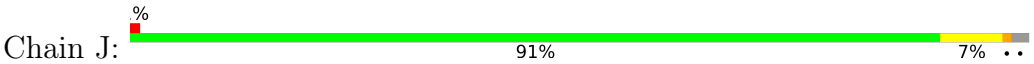


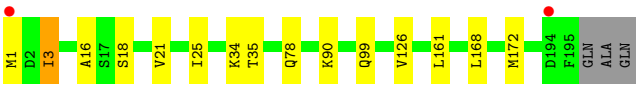


• Molecule 9: Proteasome subunit beta type-3

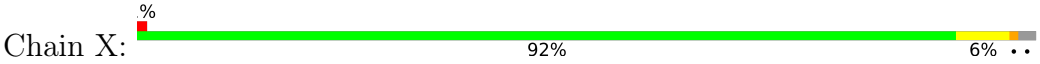


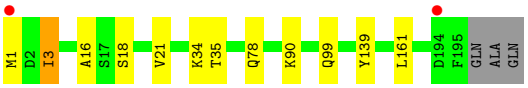
• Molecule 10: Proteasome subunit beta type-4



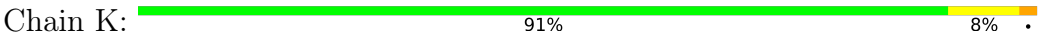


• Molecule 10: Proteasome subunit beta type-4

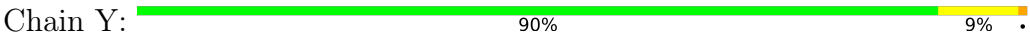


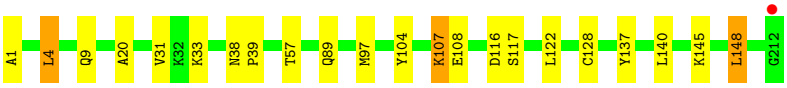


• Molecule 11: Proteasome subunit beta type-5

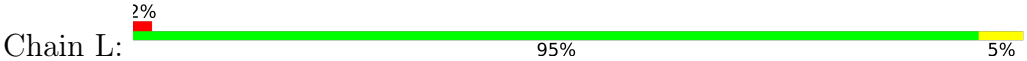


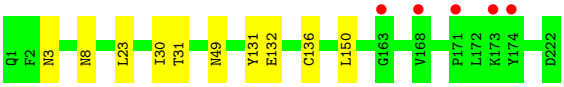
• Molecule 11: Proteasome subunit beta type-5





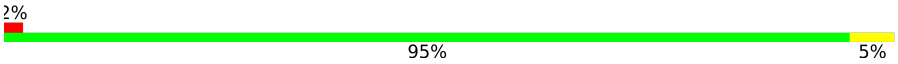
• Molecule 12: Proteasome subunit beta type-6

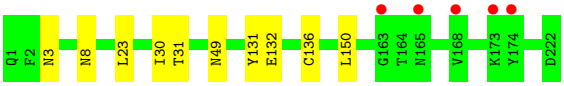




• Molecule 12: Proteasome subunit beta type-6

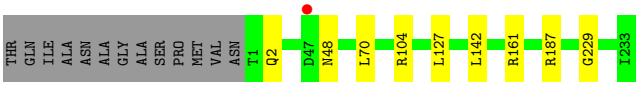
Chain Z:





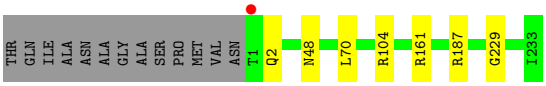
• Molecule 13: Proteasome subunit beta type-7

Chain M:



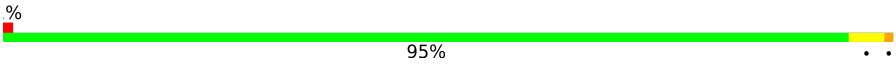
• Molecule 13: Proteasome subunit beta type-7

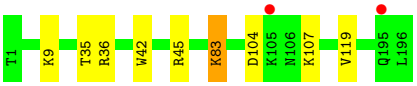
Chain a:



• Molecule 14: Proteasome subunit beta type-1

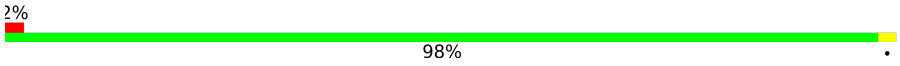
Chain N:

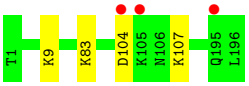




• Molecule 14: Proteasome subunit beta type-1

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	135.04Å 301.44Å 145.75Å 90.00° 113.27° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (15.00-2.70) 97.5 (15.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.194 , 0.226 0.198 , 0.228	Depositor DCC
R_{free} test set	14147 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	56.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	49891	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SRG, MG, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.28	0/1952	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.28	0/1934	0.50	0/2618
2	P	0.28	0/1934	0.50	0/2618
3	C	0.28	0/1910	0.51	0/2586
3	Q	0.28	0/1910	0.51	0/2586
4	D	0.27	0/1837	0.48	0/2475
4	R	0.27	0/1837	0.48	0/2475
5	E	0.27	0/1800	0.47	0/2433
5	S	0.27	0/1800	0.47	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.28	0/1945	0.47	0/2634
7	U	0.27	0/1945	0.47	0/2634
8	H	0.26	0/1750	0.47	0/2373
8	V	0.27	0/1750	0.47	0/2373
9	I	0.28	0/1611	0.48	0/2174
9	W	0.28	0/1611	0.49	0/2174
10	J	0.27	0/1589	0.48	0/2142
10	X	0.27	0/1589	0.48	0/2142
11	K	0.30	0/1679	0.49	1/2271 (0.0%)
11	Y	0.33	0/1679	0.50	1/2271 (0.0%)
12	L	0.29	0/1795	0.48	0/2420
12	Z	0.29	0/1795	0.48	0/2420
13	M	0.28	0/1855	0.51	0/2514
13	a	0.28	0/1855	0.51	0/2514
14	N	0.26	0/1541	0.48	0/2087
14	b	0.26	0/1541	0.47	0/2087
All	All	0.28	0/50260	0.48	2/67956 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Y	4	LEU	CA-CB-CG	5.82	128.68	115.30
11	K	4	LEU	CA-CB-CG	5.09	127.02	115.30

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	1915	0	1929	1	0
1	O	1915	0	1929	4	0
2	B	1904	0	1904	11	0
2	P	1904	0	1904	10	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	5	0
5	E	1773	0	1775	5	0
5	S	1773	0	1775	4	0
6	F	1892	0	1883	2	0
6	T	1892	0	1883	5	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	5	0
8	H	1719	0	1718	6	0
8	V	1719	0	1718	7	0
9	I	1581	0	1574	11	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	7	0
11	K	1642	0	1593	10	0
11	Y	1642	0	1593	10	0
12	L	1757	0	1711	3	0
12	Z	1757	0	1711	2	0
13	M	1824	0	1832	1	0
13	a	1824	0	1832	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1512	0	1481	5	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	W	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	H	35	0	37	6	0
17	V	35	0	37	1	0
18	A	17	0	0	0	0
18	B	10	0	0	0	0
18	C	9	0	0	0	0
18	D	16	0	0	0	0
18	E	12	0	0	0	0
18	F	10	0	0	0	0
18	G	16	0	0	0	0
18	H	24	0	0	0	0
18	I	16	0	0	0	0
18	J	14	0	0	0	0
18	K	15	0	0	0	0
18	L	28	0	0	0	0
18	M	22	0	0	0	0
18	N	11	0	0	0	0
18	O	6	0	0	0	0
18	P	12	0	0	0	0
18	Q	15	0	0	0	0
18	R	19	0	0	0	0
18	S	11	0	0	0	0
18	T	17	0	0	2	0
18	U	17	0	0	0	0
18	V	15	0	0	0	0
18	W	5	0	0	0	0
18	X	13	0	0	0	0
18	Y	20	0	0	1	0
18	Z	25	0	0	0	0
18	a	28	0	0	0	0
18	b	25	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	49891	0	49198	134	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 1.

All (134) 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)
17:H:301:SRG:H6	9:I:125:LEU:CD2	2.05	0.87
17:H:301:SRG:H6	9:I:125:LEU:HD21	1.67	0.77
8:V:52:THR:O	8:V:56:THR:OG1	2.03	0.76
8:H:52:THR:O	8:H:56:THR:OG1	2.04	0.76
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.22	0.74
2:B:3:ARG:HB3	5:E:122:TYR:OH	1.99	0.62
8:V:46:ALA:HA	17:V:301:SRG:H24A	1.82	0.62
17:H:301:SRG:H6	9:I:125:LEU:HD23	1.82	0.62
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.39	0.58
11:Y:1:ALA:CB	11:Y:33:LYS:HZ3	2.17	0.58
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.39	0.57
17:H:301:SRG:C6	9:I:125:LEU:HD21	2.34	0.57
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.41	0.56
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.90	0.54
14:N:35:THR:HG21	14:N:45:ARG:HE	1.72	0.54
5:S:12:PHE:H	6:T:19:GLN:HE22	1.54	0.54
8:H:46:ALA:HA	17:H:301:SRG:H24A	1.89	0.53
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.90	0.53
12:L:131:TYR:O	12:L:132:GLU:HG2	2.09	0.53
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.43	0.52
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.09	0.52
3:C:51:LYS:O	3:C:52:LEU:HB2	2.08	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.57	0.52
10:J:25:ILE:O	10:X:139:TYR:OH	2.28	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.57	0.52
2:B:12:PHE:H	3:C:17:GLN:HE22	1.58	0.51
5:E:12:PHE:H	6:F:19:GLN:HE22	1.59	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.12	0.50
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.42	0.50
12:L:131:TYR:C	12:L:132:GLU:HG2	2.32	0.50
2:P:217:LYS:C	2:P:219:ALA:H	2.15	0.50
8:V:84:LYS:HA	8:V:113:ILE:HD11	1.94	0.50
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.59	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:23:PHE:O	7:U:26:THR:HB	2.12	0.49
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.95	0.49
8:H:84:LYS:HA	8:H:113:ILE:HD11	1.93	0.49
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.95	0.49
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.78	0.49
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.48	0.48
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.95	0.48
12:Z:131:TYR:C	12:Z:132:GLU:HG2	2.32	0.48
2:B:217:LYS:C	2:B:219:ALA:H	2.15	0.48
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.96	0.48
11:Y:89:GLN:HG2	18:Y:417:HOH:O	2.14	0.48
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.97	0.47
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.96	0.47
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.79	0.47
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.97	0.47
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.97	0.47
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.78	0.47
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.45	0.46
6:T:148:GLU:HG2	18:T:301:HOH:O	2.15	0.46
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.95	0.46
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.98	0.46
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.50	0.46
3:C:35:LYS:HG2	3:C:158:SER:O	2.16	0.45
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.99	0.45
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.99	0.45
11:Y:97:MET:HB2	11:Y:117:SER:HB3	1.99	0.45
17:H:301:SRG:C6	9:I:125:LEU:CD2	2.88	0.45
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.85	0.45
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.52	0.45
7:U:73:VAL:HG12	7:U:133:THR:HB	1.98	0.45
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.17	0.44
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.00	0.44
7:G:73:VAL:HG12	7:G:133:THR:HB	1.98	0.44
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.47	0.44
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.00	0.44
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.53	0.43
6:F:198:LEU:HD12	6:F:243:ILE:HG22	1.99	0.43
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.00	0.43
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.48	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.81	0.43
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:209:ASN:O	9:W:38:LYS:NZ	2.52	0.43
8:V:35:HIS:CB	8:V:56:THR:HG21	2.49	0.43
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.00	0.43
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.01	0.43
6:T:198:LEU:HD12	6:T:243:ILE:HG22	1.99	0.43
4:D:91:HIS:HB3	4:D:99:ILE:HG22	2.01	0.43
4:R:91:HIS:HB3	4:R:99:ILE:HG22	2.01	0.43
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.01	0.43
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.00	0.43
9:I:101:PRO:HB3	9:I:126:ILE:HD12	2.01	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.43
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.84	0.43
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.01	0.43
2:P:176:GLN:HG3	3:Q:52:LEU:HD13	2.01	0.43
14:N:35:THR:CG2	14:N:45:ARG:HE	2.32	0.42
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.49	0.42
10:X:1:MET:HB3	10:X:34:LYS:HE3	2.01	0.42
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.01	0.42
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.01	0.42
9:W:101:PRO:HB3	9:W:126:ILE:HD12	2.01	0.42
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	2.01	0.42
11:K:53:GLN:O	11:K:57:THR:OG1	2.36	0.42
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.49	0.42
8:H:35:HIS:HB2	8:H:56:THR:HG21	2.02	0.42
11:K:107:LYS:HG3	11:K:108:GLU:HG3	2.02	0.42
10:J:1:MET:HB3	10:J:34:LYS:HE3	2.01	0.42
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.50	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.50	0.42
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.01	0.42
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.01	0.42
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	2.01	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.41
2:P:3:ARG:HB3	5:S:122:TYR:OH	2.20	0.41
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.50	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
10:J:1:MET:CB	10:J:34:LYS:HE3	2.51	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.58	0.41
10:X:1:MET:CB	10:X:34:LYS:HE3	2.51	0.41
2:B:50:LYS:O	2:B:51:VAL:C	2.59	0.41
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.56	0.41
5:S:9:THR:HG21	5:S:119:THR:HA	2.02	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.03	0.41
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.03	0.40
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.50	0.40
2:P:220:ASN:O	2:P:221:ASP:HB2	2.21	0.40
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.40
2:B:145:TYR:OH	2:B:217:LYS:N	2.54	0.40
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.03	0.40
9:I:98:ARG:O	9:I:126:ILE:HD11	2.20	0.40
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.57	0.40
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.57	0.40
5:E:9:THR:HG21	5:E:119:THR:HA	2.02	0.40
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.04	0.40
9:W:98:ARG:O	9:W:126:ILE:HD11	2.21	0.40
2:B:219:ALA:HB2	2:B:225:TYR:HB2	2.02	0.40
11:K:211:ILE:HG21	8:V:214:LYS:HE3	2.03	0.40
10:J:168:LEU:O	10:J:172:MET:HB2	2.21	0.40
6:T:146:MET:HE2	18:T:301:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34 60
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34 60
2	B	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	9 23
2	P	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	9 23
3	C	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12 30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12	30
4	D	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
4	R	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
5	E	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	239 (100%)	0	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	223 (96%)	7 (3%)	1 (0%)	34	60
13	a	231/246 (94%)	223 (96%)	7 (3%)	1 (0%)	34	60
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6284/6614 (95%)	6143 (98%)	123 (2%)	18 (0%)	41	66

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
2	P	51	VAL
2	P	221	ASP
3	Q	202	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2	THR
2	B	218	GLY
2	B	220	ASN
1	O	2	THR
2	P	218	GLY
2	P	220	ASN
3	C	205	ALA
3	Q	205	ALA
3	C	183	PRO
3	Q	183	PRO
13	M	229	GLY
13	a	229	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	209/209 (100%)	205 (98%)	4 (2%)	57	82
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	82
2	B	203/216 (94%)	196 (97%)	7 (3%)	37	66
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	66
3	C	212/226 (94%)	200 (94%)	12 (6%)	20	44
3	Q	212/226 (94%)	200 (94%)	12 (6%)	20	44
4	D	194/215 (90%)	183 (94%)	11 (6%)	20	44
4	R	194/215 (90%)	183 (94%)	11 (6%)	20	44
5	E	190/193 (98%)	179 (94%)	11 (6%)	20	43
5	S	190/193 (98%)	179 (94%)	11 (6%)	20	43
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	51
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	51
7	G	206/210 (98%)	197 (96%)	9 (4%)	28	56
7	U	206/210 (98%)	197 (96%)	9 (4%)	28	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	H	185/190 (97%)	180 (97%)	5 (3%)	44 74
8	V	185/190 (97%)	181 (98%)	4 (2%)	52 79
9	I	172/173 (99%)	170 (99%)	2 (1%)	71 88
9	W	172/173 (99%)	169 (98%)	3 (2%)	60 84
10	J	173/175 (99%)	168 (97%)	5 (3%)	42 71
10	X	173/175 (99%)	168 (97%)	5 (3%)	42 71
11	K	168/168 (100%)	160 (95%)	8 (5%)	25 53
11	Y	168/168 (100%)	160 (95%)	8 (5%)	25 53
12	L	185/185 (100%)	179 (97%)	6 (3%)	39 68
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39 68
13	M	199/208 (96%)	193 (97%)	6 (3%)	41 70
13	a	199/208 (96%)	193 (97%)	6 (3%)	41 70
14	N	162/162 (100%)	158 (98%)	4 (2%)	47 76
14	b	162/162 (100%)	158 (98%)	4 (2%)	47 76
All	All	5318/5538 (96%)	5118 (96%)	200 (4%)	33 62

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	79	LEU
2	B	113	ARG
2	B	186	ASP
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	50	LEU
3	C	51	LYS
3	C	60	SER
3	C	77	ASN
3	C	147	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	40	LEU
4	D	51	LEU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	207	VAL
5	E	208	ASP
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	207	ASP
6	F	214	TRP
6	F	240	GLN
7	G	26	THR
7	G	75	ASN
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	22	GLN
8	H	30	ASN
8	H	56	THR
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	3	ILE
10	J	35	THR
10	J	78	GLN
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	9	GLN
11	K	57	THR
11	K	104	TYR
11	K	107	LYS
11	K	116	ASP
11	K	140	LEU
11	K	148	LEU
12	L	3	ASN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	136	CYS
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	62	SER
1	O	122	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	79	LEU
2	P	113	ARG
2	P	186	ASP
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	50	LEU
3	Q	51	LYS
3	Q	60	SER
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	40	LEU
4	R	51	LEU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	207	VAL
5	S	208	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	207	ASP
6	T	214	TRP
6	T	240	GLN
7	U	26	THR
7	U	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	56	THR
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	125	LEU
9	W	171	LEU
10	X	3	ILE
10	X	35	THR
10	X	78	GLN
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	57	THR
11	Y	104	TYR
11	Y	107	LYS
11	Y	116	ASP
11	Y	140	LEU
11	Y	148	LEU
12	Z	3	ASN
12	Z	23	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	Z	31	THR
12	Z	49	ASN
12	Z	136	CYS
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	66	HIS
8	H	165	ASN
9	I	37	ASN
9	I	203	GLN
10	J	55	GLN
10	J	63	ASN
10	J	146	HIS
11	K	85	ASN
11	K	176	ASN
11	K	190	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	17	GLN
3	Q	38	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
8	V	35	HIS
9	W	37	ASN
10	X	55	GLN
10	X	146	HIS
11	Y	85	ASN
11	Y	176	ASN
11	Y	190	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	a	102	GLN
13	a	194	ASN
13	a	213	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

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
17	SRG	V	301	8	33,35,35	2.03	4 (12%)	43,47,47	2.41	5 (11%)
17	SRG	H	301	8	33,35,35	2.26	6 (18%)	43,47,47	2.77	10 (23%)

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	SRG	V	301	8	-	16/53/53/53	0/0/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SRG	H	301	8	-	21/53/53/53	0/0/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	SRG	C27-C26	9.59	1.54	1.32
17	V	301	SRG	C27-C26	8.96	1.53	1.32
17	H	301	SRG	C27-C28	-4.92	1.38	1.48
17	V	301	SRG	C28-N30	4.03	1.43	1.34
17	V	301	SRG	C19-N21	3.07	1.40	1.34
17	V	301	SRG	C27-C28	-2.78	1.42	1.48
17	H	301	SRG	C32-C33	-2.70	1.34	1.50
17	H	301	SRG	C23-C22	-2.17	1.50	1.54
17	H	301	SRG	C11-C15	-2.14	1.47	1.52
17	H	301	SRG	C8-N36	-2.12	1.31	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	H	301	SRG	C31-C32-C33	-10.37	100.90	111.95
17	H	301	SRG	C22-C26-C27	-9.58	109.52	126.78
17	V	301	SRG	C31-C32-C33	-9.20	102.14	111.95
17	V	301	SRG	C22-C26-C27	-9.02	110.52	126.78
17	H	301	SRG	C27-C28-N30	5.36	125.06	114.97
17	V	301	SRG	C26-C27-C28	-4.91	110.41	122.69
17	V	301	SRG	C27-C28-N30	4.50	123.45	114.97
17	H	301	SRG	O29-C28-N30	-4.23	115.24	122.23
17	H	301	SRG	C26-C27-C28	-4.07	112.51	122.69
17	V	301	SRG	O29-C28-N30	-3.82	115.92	122.23
17	H	301	SRG	C23-C22-C26	-2.98	109.14	113.10
17	H	301	SRG	C25-C23-C22	-2.67	107.12	111.21
17	H	301	SRG	C12-C11-N36	-2.55	105.12	111.43
17	H	301	SRG	C32-C33-C34	-2.49	114.25	125.39
17	H	301	SRG	C31-N30-C28	2.11	125.64	122.54

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	SRG	N17-C18-C34-C33
17	H	301	SRG	C19-C18-C34-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	H	301	SRG	C26-C22-C23-C24
17	H	301	SRG	N21-C22-C26-C27
17	H	301	SRG	C23-C22-C26-C27
17	H	301	SRG	C22-C26-C27-C28
17	H	301	SRG	C27-C28-N30-C31
17	H	301	SRG	O29-C28-N30-C31
17	H	301	SRG	N30-C31-C32-C33
17	V	301	SRG	N17-C18-C34-C33
17	V	301	SRG	C19-C18-C34-C33
17	V	301	SRG	N21-C22-C26-C27
17	V	301	SRG	C23-C22-C26-C27
17	V	301	SRG	C22-C26-C27-C28
17	V	301	SRG	C27-C28-N30-C31
17	V	301	SRG	O29-C28-N30-C31
17	V	301	SRG	N30-C31-C32-C33
17	H	301	SRG	C1-C3-C4-C5
17	H	301	SRG	C1-C3-C4-C6
17	H	301	SRG	N7-C3-C4-C6
17	H	301	SRG	N7-C3-C4-C5
17	V	301	SRG	N7-C3-C4-C6
17	V	301	SRG	C1-C3-C4-C6
17	H	301	SRG	C26-C27-C28-N30
17	H	301	SRG	C26-C27-C28-O29
17	H	301	SRG	C12-C11-N36-C8
17	V	301	SRG	C1-C3-C4-C5
17	V	301	SRG	N7-C3-C4-C5
17	V	301	SRG	C12-C11-N36-C8
17	H	301	SRG	C34-C18-C19-O20
17	H	301	SRG	C34-C18-C19-N21
17	H	301	SRG	N17-C18-C19-O20
17	V	301	SRG	C26-C27-C28-O29
17	H	301	SRG	N21-C22-C23-C24
17	V	301	SRG	C34-C18-C19-O20
17	H	301	SRG	N17-C18-C19-N21
17	V	301	SRG	N17-C18-C19-O20

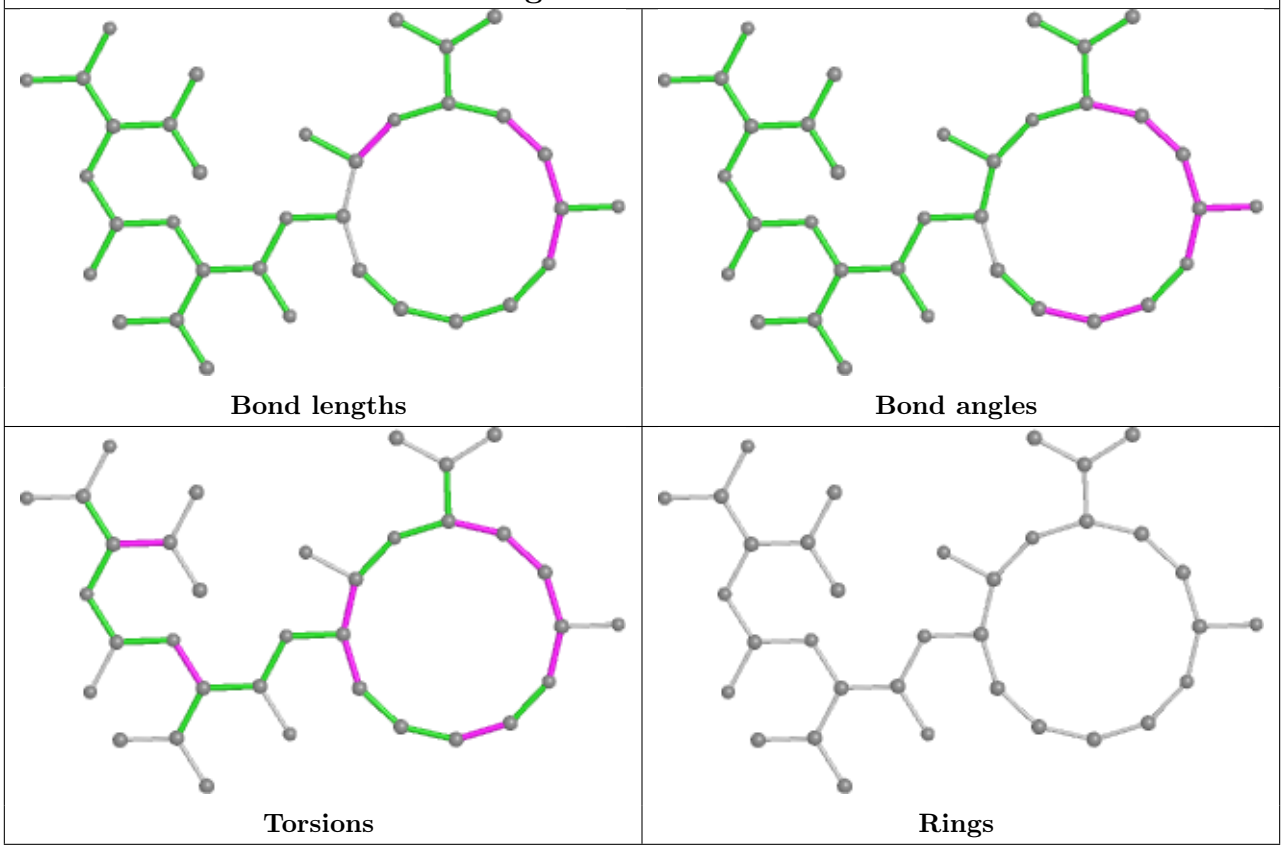
There are no ring outliers.

2 monomers are involved in 7 short contacts:

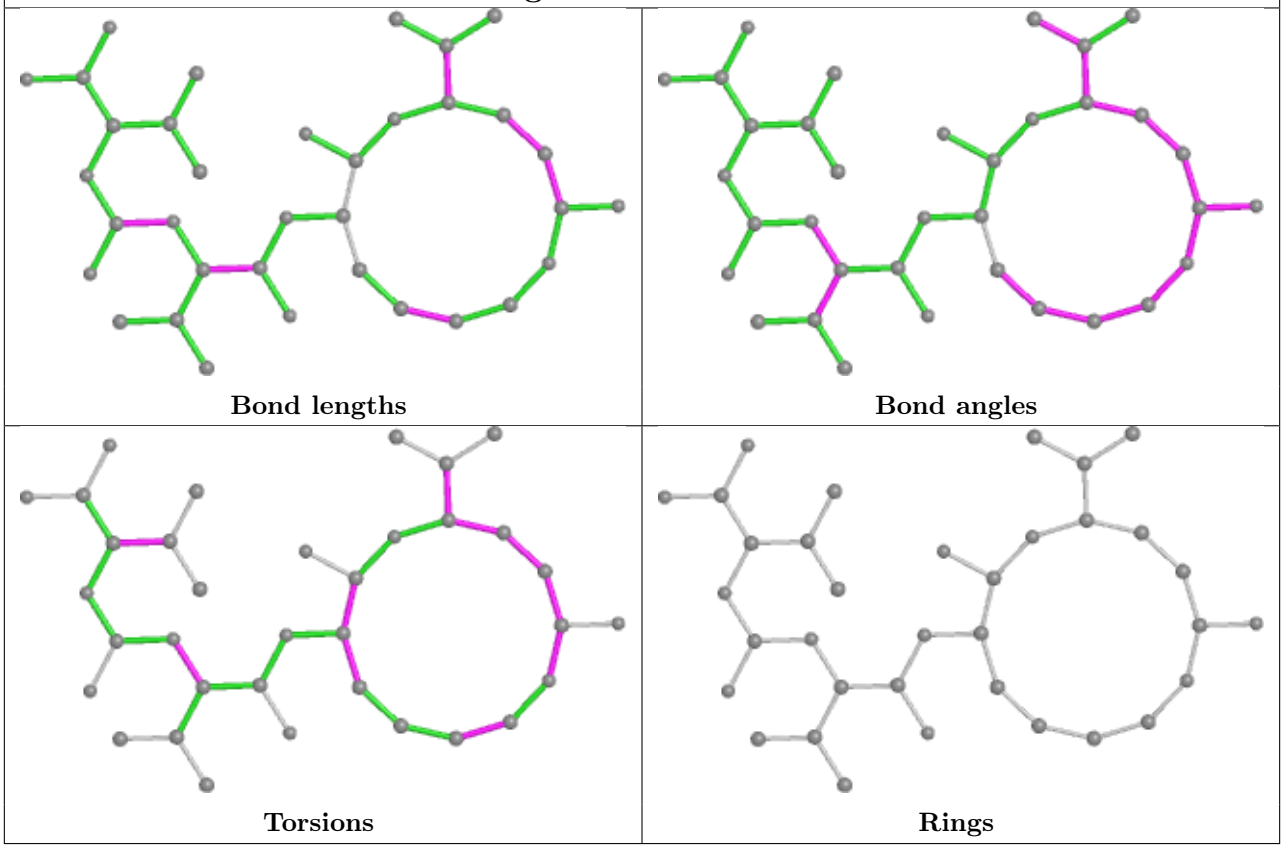
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	V	301	SRG	1	0
17	H	301	SRG	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 SRG V 301



Ligand SRG H 301



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	250/250 (100%)	-0.34	9 (3%)	42	42	43, 55, 89, 131	0
1	O	250/250 (100%)	-0.25	9 (3%)	42	42	47, 63, 107, 139	0
2	B	244/258 (94%)	-0.23	10 (4%)	37	36	44, 62, 101, 152	0
2	P	244/258 (94%)	-0.19	12 (4%)	29	28	48, 65, 107, 147	0
3	C	240/254 (94%)	-0.16	15 (6%)	20	19	42, 65, 122, 145	0
3	Q	240/254 (94%)	0.03	19 (7%)	12	10	46, 73, 152, 177	0
4	D	235/260 (90%)	-0.29	7 (2%)	50	51	47, 66, 97, 135	0
4	R	235/260 (90%)	-0.24	8 (3%)	45	45	47, 67, 104, 134	0
5	E	231/234 (98%)	-0.26	2 (0%)	84	85	49, 67, 99, 142	0
5	S	231/234 (98%)	-0.16	6 (2%)	56	57	49, 71, 104, 149	0
6	F	243/288 (84%)	-0.29	11 (4%)	33	31	43, 60, 110, 140	0
6	T	243/288 (84%)	-0.26	7 (2%)	51	52	43, 66, 115, 144	0
7	G	241/252 (95%)	-0.42	6 (2%)	57	59	38, 56, 88, 138	0
7	U	241/252 (95%)	-0.26	7 (2%)	51	52	44, 60, 94, 143	0
8	H	226/232 (97%)	-0.33	6 (2%)	54	55	33, 51, 83, 147	0
8	V	226/232 (97%)	-0.32	6 (2%)	54	55	41, 54, 83, 152	0
9	I	204/205 (99%)	-0.59	2 (0%)	82	83	39, 51, 80, 106	0
9	W	204/205 (99%)	-0.53	1 (0%)	91	92	42, 54, 84, 109	0
10	J	195/198 (98%)	-0.44	2 (1%)	82	83	40, 55, 79, 130	0
10	X	195/198 (98%)	-0.41	2 (1%)	82	83	42, 57, 82, 141	0
11	K	212/212 (100%)	-0.29	1 (0%)	91	92	42, 59, 83, 101	0
11	Y	212/212 (100%)	-0.37	1 (0%)	91	92	45, 57, 83, 101	0
12	L	222/222 (100%)	-0.46	5 (2%)	60	62	40, 54, 88, 125	0
12	Z	222/222 (100%)	-0.43	5 (2%)	60	62	38, 52, 88, 124	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.57	1 (0%) 92 93	37, 52, 72, 92	0
13	a	233/246 (94%)	-0.57	1 (0%) 92 93	37, 50, 70, 88	0
14	N	196/196 (100%)	-0.59	2 (1%) 82 83	37, 47, 73, 101	0
14	b	196/196 (100%)	-0.56	3 (1%) 73 76	37, 49, 75, 110	0
All	All	6344/6614 (95%)	-0.34	166 (2%) 56 57	33, 58, 99, 177	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	W	1	SER	7.8
1	A	2	THR	7.4
10	X	1	MET	6.5
3	Q	50	LEU	6.1
12	L	174	TYR	6.0
8	V	224	GLN	5.9
12	Z	174	TYR	5.8
2	B	221	ASP	5.8
3	Q	49	THR	5.7
4	R	117	GLU	5.3
7	U	242	GLN	5.2
1	O	1	MET	5.1
3	C	206	LYS	5.1
3	C	205	ALA	5.0
2	P	51	VAL	5.0
2	P	221	ASP	4.8
1	O	2	THR	4.7
1	A	1	MET	4.7
2	B	51	VAL	4.7
1	O	4	ARG	4.6
3	Q	206	LYS	4.6
3	Q	236	GLN	4.6
4	R	116	GLY	4.5
3	C	50	LEU	4.5
2	P	1	GLY	4.5
8	V	222	ASP	4.4
2	P	59	ASP	4.4
5	S	202	ASP	4.4
9	I	1	SER	4.3
10	J	1	MET	4.2
4	R	113	LEU	4.2
1	A	249	ALA	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	R	241	ALA	4.0
2	P	220	ASN	3.9
6	T	178	HIS	3.9
5	E	202	ASP	3.9
8	H	222	ASP	3.8
6	T	243	ILE	3.7
6	F	181	GLU	3.7
14	b	105	LYS	3.7
14	b	195	GLN	3.7
3	C	238	LYS	3.6
6	F	244	ASN	3.6
14	N	195	GLN	3.6
2	P	61	SER	3.6
2	B	219	ALA	3.5
12	Z	165	ASN	3.5
3	Q	240	GLU	3.4
3	Q	204	GLY	3.4
2	P	52	THR	3.4
3	C	239	GLN	3.4
4	R	217	GLN	3.4
3	C	49	THR	3.3
4	D	113	LEU	3.3
7	G	241	GLU	3.3
1	O	52	SER	3.2
8	V	226	GLU	3.2
2	B	220	ASN	3.2
2	B	218	GLY	3.2
3	Q	205	ALA	3.2
12	Z	163	GLY	3.2
3	Q	203	THR	3.1
8	H	226	GLU	3.1
2	P	182	ASP	3.1
3	Q	239	GLN	3.1
2	P	219	ALA	3.1
10	X	194	ASP	3.1
1	O	249	ALA	3.1
7	G	3	TYR	3.0
8	V	223	ILE	3.0
2	B	59	ASP	3.0
1	O	250	LEU	3.0
3	C	240	GLU	3.0
8	V	221	CYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	61	SER	3.0
6	T	244	ASN	2.9
7	U	51	PRO	2.9
3	Q	237	GLU	2.9
3	Q	55	THR	2.9
2	B	217	LYS	2.9
2	P	60	THR	2.9
6	T	180	PRO	2.9
4	D	117	GLU	2.8
4	D	242	GLU	2.8
6	F	243	ILE	2.8
3	Q	225	GLU	2.8
1	O	201	GLU	2.8
7	G	240	ALA	2.8
1	A	3	ASP	2.8
6	T	230	ASP	2.8
6	T	215	CYS	2.8
7	U	206	GLY	2.7
6	F	204	LYS	2.7
4	R	125	LEU	2.7
3	C	236	GLN	2.7
3	Q	202	GLN	2.7
5	S	227	GLU	2.7
3	C	180	LYS	2.7
10	J	194	ASP	2.7
6	F	215	CYS	2.7
8	H	224	GLN	2.6
12	L	173	LYS	2.6
12	Z	173	LYS	2.6
4	R	242	GLU	2.6
8	H	223	ILE	2.6
12	L	163	GLY	2.5
6	F	180	PRO	2.5
1	A	201	GLU	2.5
8	H	221	CYS	2.5
4	D	241	ALA	2.5
3	Q	238	LYS	2.5
14	N	105	LYS	2.5
12	L	168	VAL	2.5
1	A	4	ARG	2.5
13	M	47	ASP	2.5
11	K	212	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	S	173	ARG	2.5
6	F	229	GLY	2.5
3	C	60	SER	2.5
2	B	60	THR	2.4
3	Q	180	LYS	2.4
1	A	228	PRO	2.4
7	G	68	ARG	2.4
7	U	3	TYR	2.4
6	F	178	HIS	2.4
11	Y	212	GLY	2.4
3	Q	181	GLU	2.4
5	E	173	ARG	2.4
1	O	3	ASP	2.3
8	H	217	ILE	2.3
7	U	2	GLY	2.3
12	L	171	PRO	2.3
5	S	180	LYS	2.3
8	V	145	ASP	2.3
1	A	229	THR	2.3
4	D	240	ALA	2.3
5	S	233	ILE	2.3
2	B	50	LYS	2.3
9	I	192	ASP	2.2
3	C	175	LYS	2.2
12	Z	168	VAL	2.2
6	F	176	VAL	2.2
4	D	217	GLN	2.2
7	G	242	GLN	2.2
7	U	188	GLU	2.2
4	R	203	LYS	2.2
14	b	104	ASP	2.1
3	C	181	GLU	2.1
7	U	179	LYS	2.1
3	C	216	ASP	2.1
1	O	203	GLU	2.1
6	F	205	GLU	2.1
3	C	202	GLN	2.1
3	Q	48	SER	2.1
3	Q	229	GLN	2.1
13	a	1	THR	2.1
2	P	222	GLY	2.1
1	A	231	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Q	233	GLN	2.0
3	C	27	ARG	2.0
2	P	230	LYS	2.0
4	D	1	ASP	2.0
7	G	51	PRO	2.0
6	F	228	LYS	2.0
6	T	206	LYS	2.0
5	S	210	LEU	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.

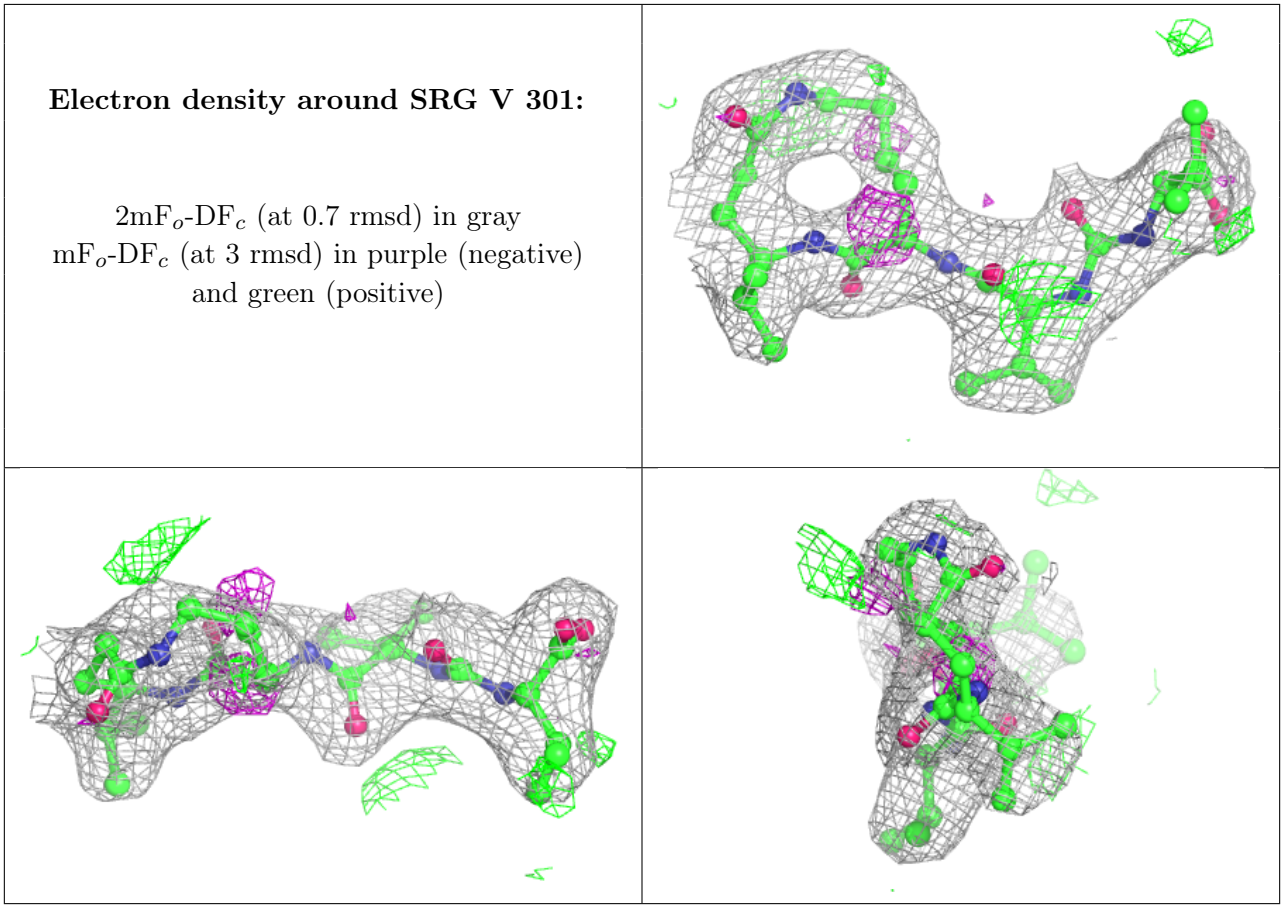
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	SRG	V	301	35/35	0.90	0.21	47,52,62,70	0
15	MG	Z	301	1/1	0.91	0.30	69,69,69,69	0
15	MG	I	301	1/1	0.91	0.45	70,70,70,70	0
15	MG	H	302	1/1	0.92	0.16	64,64,64,64	0
17	SRG	H	301	35/35	0.93	0.17	47,51,66,71	0
15	MG	W	301	1/1	0.95	0.62	76,76,76,76	0
15	MG	G	301	1/1	0.95	0.12	56,56,56,56	0
15	MG	L	301	1/1	0.97	0.11	59,59,59,59	0
15	MG	N	201	1/1	0.97	0.06	47,47,47,47	0
15	MG	K	301	1/1	0.97	0.07	53,53,53,53	0
16	CL	U	301	1/1	0.99	0.28	30,30,30,30	0
15	MG	I	302	1/1	0.99	0.04	55,55,55,55	0
16	CL	G	302	1/1	0.99	0.20	30,30,30,30	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.

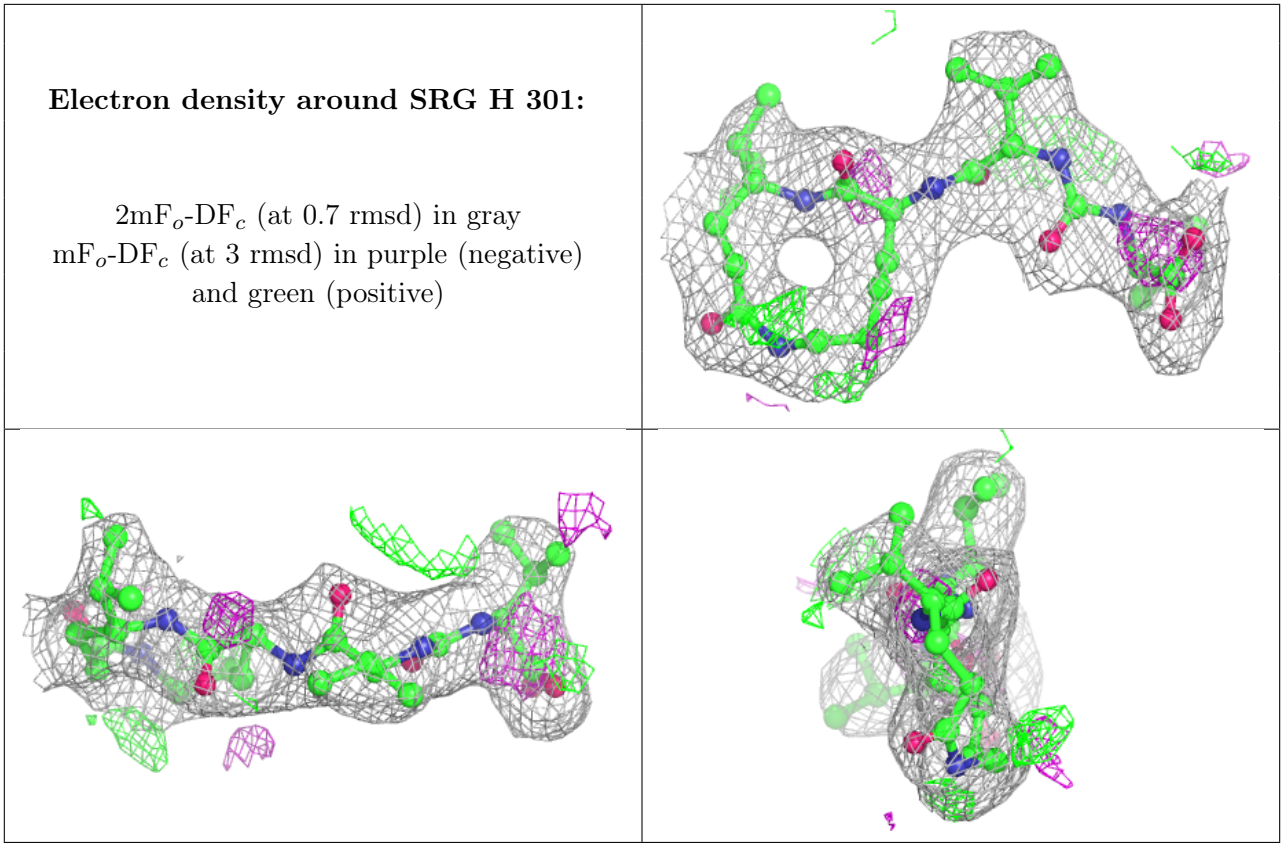
Electron density around SRG V 301:

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



Electron density around SRG H 301:

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



6.5 Other polymers

There are no such residues in this entry.