Full wwPDB X-ray Structure Validation Report (i)

Jan 13, 2024 – 12:57 pm GMT

PDB ID	:	6HVY
Title	:	Yeast 20S proteasome in complex with 5 (7- and 6-membered ring)
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2018-10-11
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 (i) symbol.

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

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

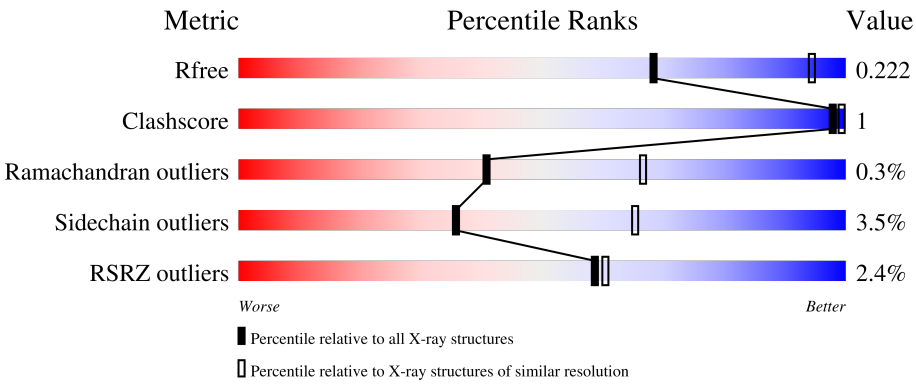
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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	3% 98% •
1	O	250	2% 98% •
2	B	258	2% 89% 6% 5%
2	P	258	4% 89% 5% 5%
3	C	254	6% 88% 6% • 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	254	8% 89% 5% 6%
4	D	260	2% 86% 10%
4	R	260	2% 85% 5% 10%
5	E	234	3% 94% 5%
5	S	234	3% 92% 6%
6	F	288	2% 80% 16%
6	T	288	3% 80% 16%
7	G	252	2% 91% 5%
7	U	252	2% 91% 5%
8	H	232	3% 94%
8	V	232	2% 93%
9	I	205	94% 5%
9	W	205	% 94% 5%
10	J	198	2% 94%
10	X	198	2% 94%
11	K	212	94%
11	Y	212	94%
12	L	222	96%
12	Z	222	% 96%
13	M	246	% 92% 5%
13	a	246	92% 5%
14	N	196	% 94% 6%
14	b	196	% 97%

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 50142 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
			Total	C	N	O	S			
1	A	250	1915	1219	315	377	4	0	0	0
1	O	250	1915	1219	315	377	4	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	226	1726	1086	299	334	7	0	1	0
8	V	226	1726	1086	299	334	7	0	1	0

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	212	1644	1045	280	312	7	0	0	0
11	Y	212	1644	1045	280	312	7	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
15	G	1	1	1	0	0
15	I	2	2	2	0	0

Continued on next page...

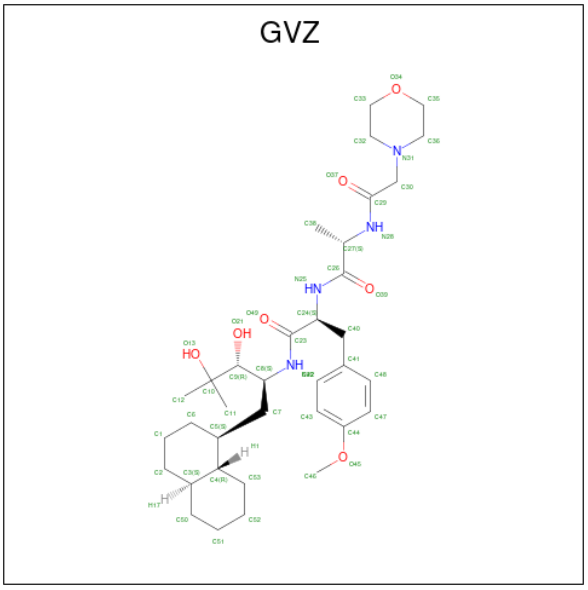
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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 (2 {S})- {N}-[(2 {S},3 {R})-1-[(1 {S},4 {a} {S},8 {a} {R})-1,2,3,4,4 {a} ,5,6,7,8,8 {a}-decahydronaphthalen-1-yl]-4-methyl-3,4-bis(oxidanyl)pentan-2-yl]-3-(4-met hoxyphenyl)-2-[[(2 {S})-2-(2-morpholin-4-ylethanoylamino)propanoyl]amino]propanamide (three-letter code: GVZ) (formula: $C_{35}H_{56}N_4O_7$).



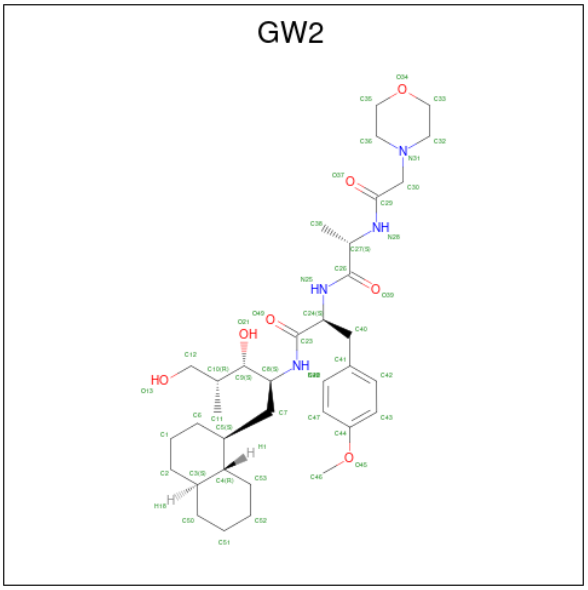
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	1	Total C N O 46 35 4 7	0	1

Continued on next page...

Continued from previous page...

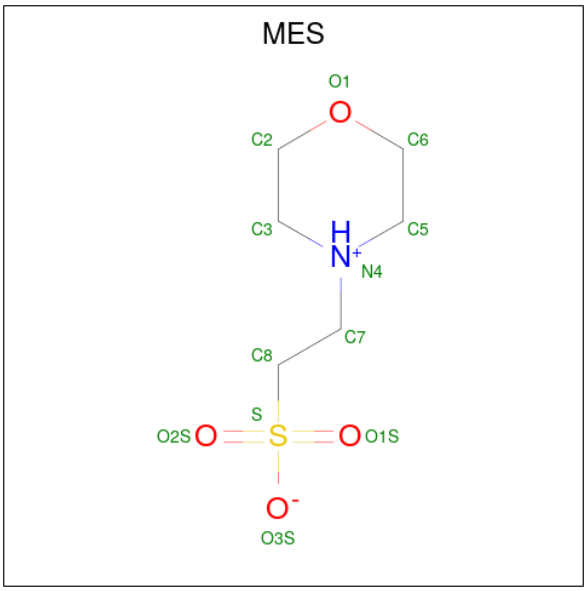
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
17	V	1	46	35	4	7	0	1

- Molecule 18 is (2 {S})- {N}-[(2 {S},3 {S},4 {R})-1-[(1 {S},4 {a} {S},8 {a} {R})-1,2,3,4,4 {a},5,6,7,8,8 {a}-decahydronaphthalen-1-yl]-4-methyl-3,5-bis(oxidanyl)pentan-2-yl]-3-(4-methoxyphenyl)-2-[[(2 {S})-2-(2-morpholin-4-ylethanoylamino)propanoyl]amino]propanamide (three-letter code: GW2) (formula: $C_{35}H_{56}N_4O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
18	H	1	46	35	4	7	0	1
18	V	1	46	35	4	7	0	1

- Molecule 19 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
19	H	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
19	V	1	12	6	1	4	1	0	0

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
20	A	26	26	26	0	0
			Total	O		
20	B	16	16	16	0	0
			Total	O		
20	C	20	20	20	0	0
			Total	O		
20	D	4	4	4	0	0
			Total	O		
20	E	9	9	9	0	0
			Total	O		
20	F	16	16	16	0	0
			Total	O		
20	G	23	23	23	0	0
			Total	O		
20	H	28	28	28	0	0
			Total	O		
20	I	30	30	30	0	0
			Total	O		
20	J	19	19	19	0	0

Continued on next page...

Continued from previous page...

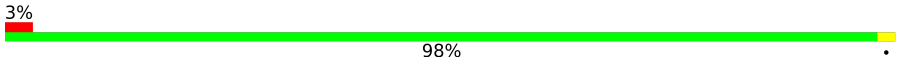
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	K	21	Total O 21 21	0	0
20	L	22	Total O 22 22	0	0
20	M	22	Total O 22 22	0	0
20	N	19	Total O 19 19	0	0
20	O	13	Total O 13 13	0	0
20	P	25	Total O 25 25	0	0
20	Q	10	Total O 10 10	0	0
20	R	20	Total O 20 20	0	0
20	S	13	Total O 13 13	0	0
20	T	12	Total O 12 12	0	0
20	U	22	Total O 22 22	0	0
20	V	18	Total O 18 18	0	0
20	W	17	Total O 17 17	0	0
20	X	24	Total O 24 24	0	0
20	Y	33	Total O 33 33	0	0
20	Z	21	Total O 21 21	0	0
20	a	25	Total O 25 25	0	0
20	b	16	Total O 16 16	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.

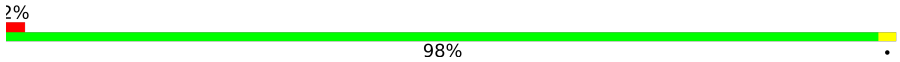
• Molecule 1: Proteasome subunit alpha type-2

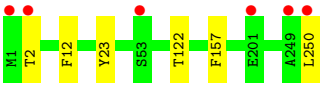
Chain A:



• Molecule 1: Proteasome subunit alpha type-2

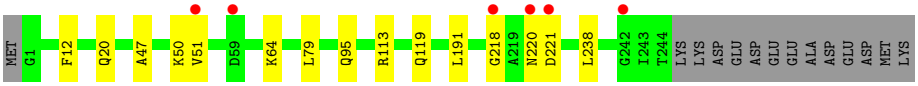
Chain O:





• Molecule 2: Proteasome subunit alpha type-3

Chain B:

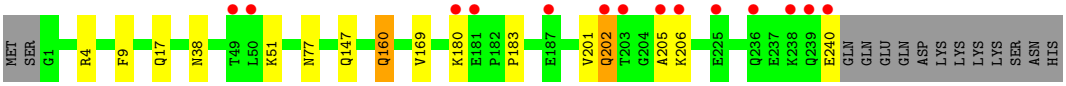


• Molecule 2: Proteasome subunit alpha type-3

Chain P:

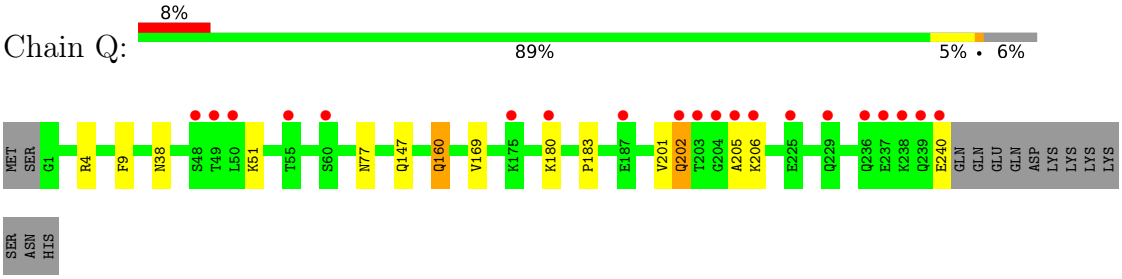
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



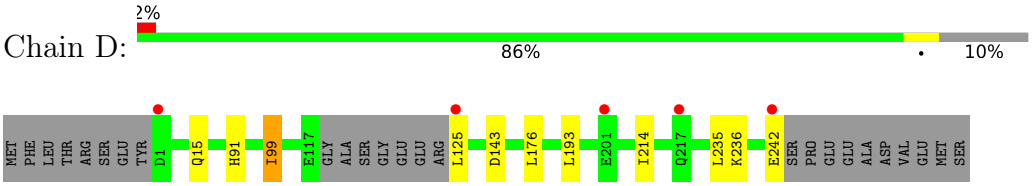
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



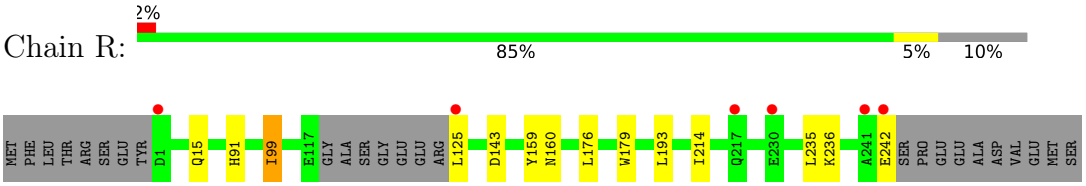
- Molecule 4: Proteasome subunit alpha type-5

Chain D:



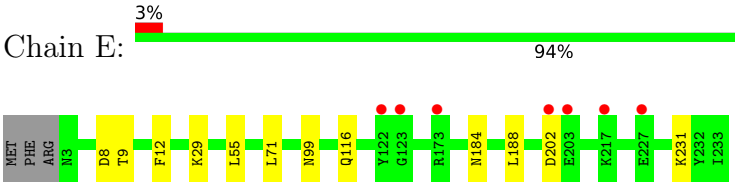
- Molecule 4: Proteasome subunit alpha type-5

Chain R:



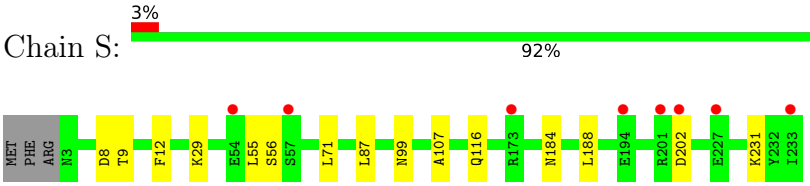
- Molecule 5: Proteasome subunit alpha type-6

Chain E:



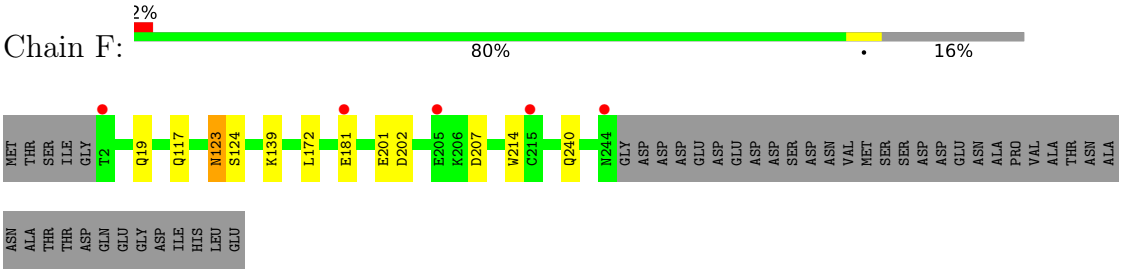
- Molecule 5: Proteasome subunit alpha type-6

Chain S:



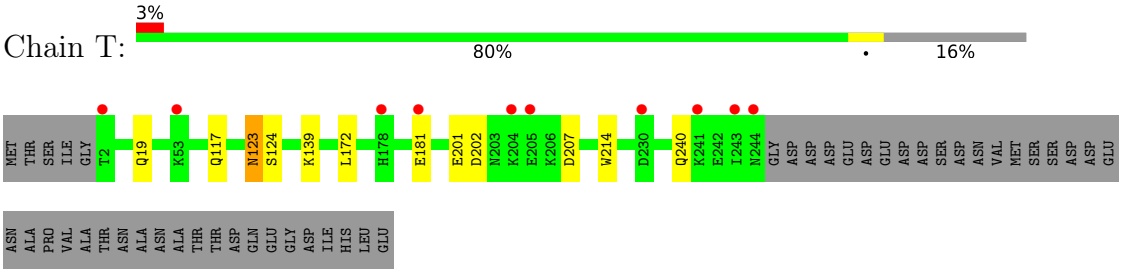
- Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



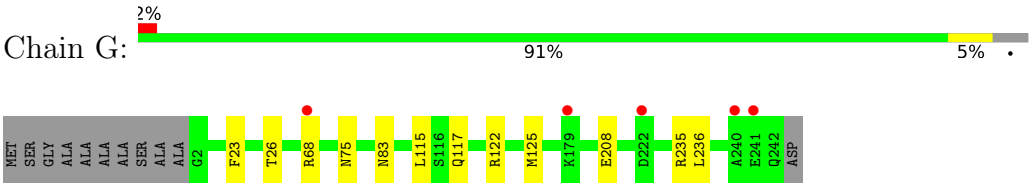
- Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



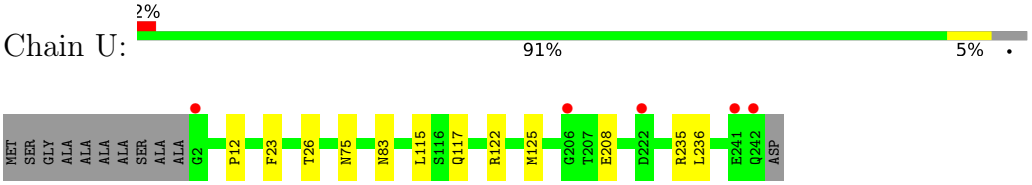
- Molecule 7: Proteasome subunit alpha type-1

Chain G:



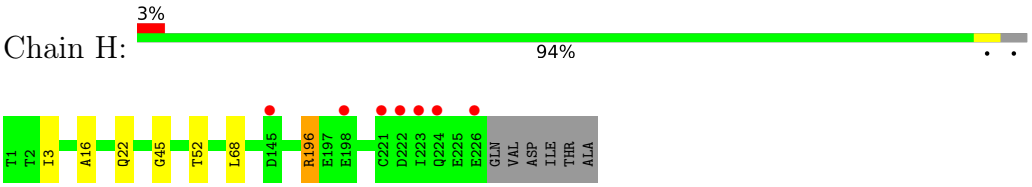
- Molecule 7: Proteasome subunit alpha type-1

Chain U:



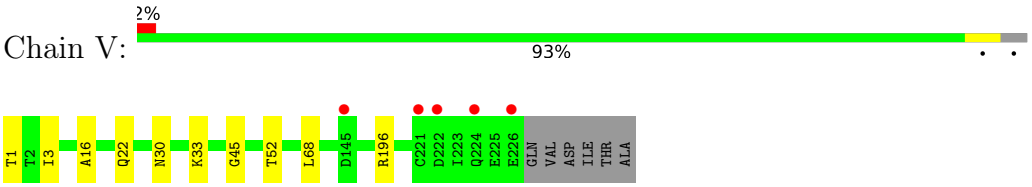
- Molecule 8: Proteasome subunit beta type-2

Chain H:



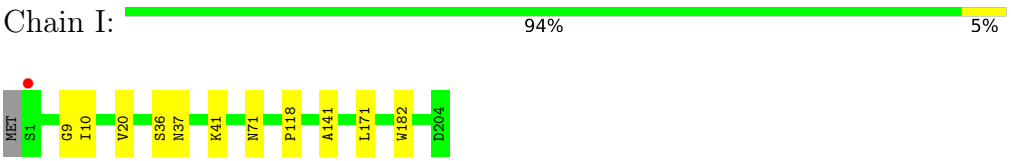
- Molecule 8: Proteasome subunit beta type-2

Chain V:



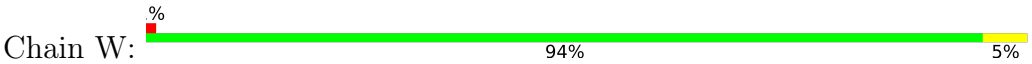
- Molecule 9: Proteasome subunit beta type-3

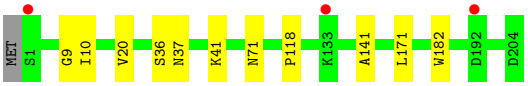
Chain I:



- Molecule 9: Proteasome subunit beta type-3

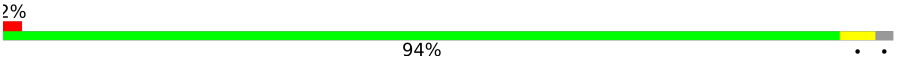
Chain W:

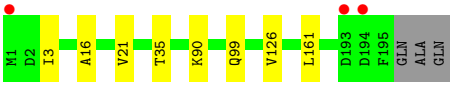




• Molecule 10: Proteasome subunit beta type-4

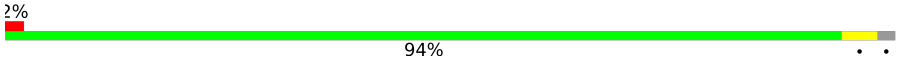
Chain J:

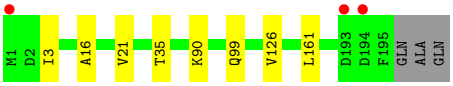




• Molecule 10: Proteasome subunit beta type-4

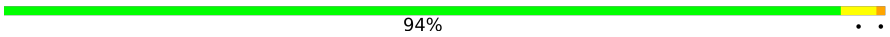
Chain X:

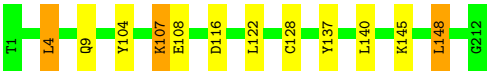




• Molecule 11: Proteasome subunit beta type-5

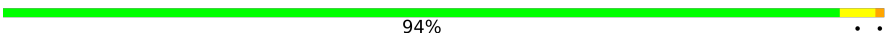
Chain K:

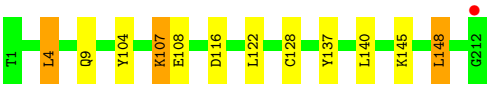




• Molecule 11: Proteasome subunit beta type-5

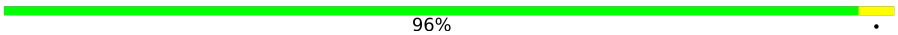
Chain Y:





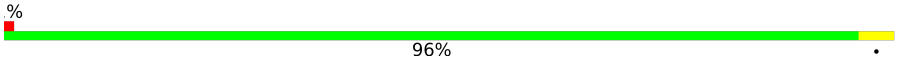
• Molecule 12: Proteasome subunit beta type-6

Chain L:



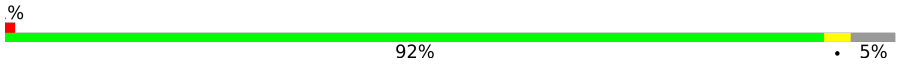
• Molecule 12: Proteasome subunit beta type-6

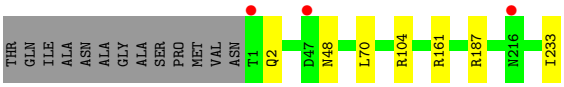
Chain Z:



• Molecule 13: Proteasome subunit beta type-7

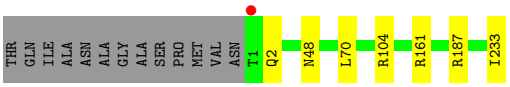
Chain M:





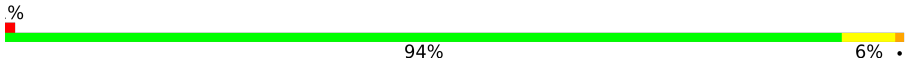
- Molecule 13: Proteasome subunit beta type-7

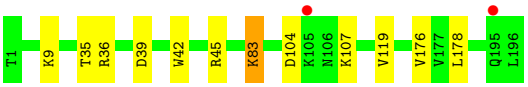
Chain a:



- Molecule 14: Proteasome subunit beta type-1

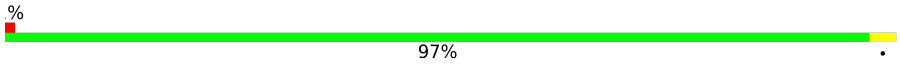
Chain N:

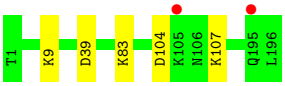




- Molecule 14: Proteasome subunit beta type-1

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	136.63Å 301.80Å 145.57Å 90.00° 113.06° 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) 98.1 (15.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.181 , 0.218 0.187 , 0.222	Depositor DCC
R_{free} test set	14418 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	50142	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: MES, GW2, GVZ, 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	0.35	0/1952	0.55	0/2642
1	O	0.35	0/1952	0.55	0/2642
2	B	0.36	0/1934	0.59	0/2618
2	P	0.36	0/1934	0.59	0/2618
3	C	0.35	0/1910	0.61	0/2586
3	Q	0.35	0/1910	0.60	0/2586
4	D	0.34	0/1837	0.57	0/2475
4	R	0.34	0/1837	0.56	0/2475
5	E	0.35	0/1800	0.56	0/2433
5	S	0.35	0/1800	0.56	0/2433
6	F	0.35	0/1932	0.53	0/2609
6	T	0.35	0/1932	0.53	0/2609
7	G	0.35	0/1945	0.55	0/2634
7	U	0.35	0/1945	0.55	0/2634
8	H	0.32	0/1757	0.57	1/2383 (0.0%)
8	V	0.32	0/1757	0.57	0/2383
9	I	0.34	0/1611	0.58	0/2174
9	W	0.34	0/1611	0.58	0/2174
10	J	0.35	0/1589	0.58	0/2142
10	X	0.34	0/1589	0.58	0/2142
11	K	0.33	0/1681	0.58	1/2274 (0.0%)
11	Y	0.33	0/1681	0.58	1/2274 (0.0%)
12	L	0.35	0/1795	0.58	0/2420
12	Z	0.35	0/1795	0.58	0/2420
13	M	0.35	0/1855	0.61	0/2514
13	a	0.35	0/1855	0.61	0/2514
14	N	0.33	0/1541	0.57	0/2087
14	b	0.33	0/1541	0.57	0/2087
All	All	0.34	0/50278	0.57	3/67982 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Y	4	LEU	CA-CB-CG	5.46	127.86	115.30
11	K	4	LEU	CA-CB-CG	5.44	127.80	115.30
8	H	196	ARG	NE-CZ-NH1	5.22	122.91	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	1	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	4	0
2	P	1904	0	1904	5	0
3	C	1881	0	1895	4	0
3	Q	1881	0	1895	3	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	5	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	2	0
7	U	1907	0	1901	2	0
8	H	1726	0	1722	2	0
8	V	1726	0	1722	3	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	5	0
10	J	1561	0	1569	3	0
10	X	1561	0	1569	3	0
11	K	1644	0	1595	5	0
11	Y	1644	0	1595	5	0
12	L	1757	0	1711	2	0
12	Z	1757	0	1711	2	0
13	M	1824	0	1832	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	a	1824	0	1832	0	0
14	N	1512	0	1481	5	0
14	b	1512	0	1481	0	0
15	G	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	46	0	0	0	0
17	V	46	0	0	0	0
18	H	46	0	0	0	0
18	V	46	0	0	0	0
19	H	12	0	13	0	0
19	V	12	0	13	0	0
20	A	26	0	0	0	0
20	B	16	0	0	0	0
20	C	20	0	0	0	0
20	D	4	0	0	0	0
20	E	9	0	0	0	0
20	F	16	0	0	0	0
20	G	23	0	0	0	0
20	H	28	0	0	0	0
20	I	30	0	0	0	0
20	J	19	0	0	0	0
20	K	21	0	0	0	0
20	L	22	0	0	0	0
20	M	22	0	0	0	0
20	N	19	0	0	0	0
20	O	13	0	0	0	0
20	P	25	0	0	1	0
20	Q	10	0	0	0	0
20	R	20	0	0	0	0
20	S	13	0	0	0	0
20	T	12	0	0	0	0
20	U	22	0	0	0	0
20	V	18	0	0	0	0
20	W	17	0	0	0	0
20	X	24	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	Y	33	0	0	0	0
20	Z	21	0	0	0	0
20	a	25	0	0	0	0
20	b	16	0	0	0	0
All	All	50142	0	49162	65	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 (65) 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)
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.65	0.62
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.65	0.60
5:S:12:PHE:H	6:T:19:GLN:HE22	1.55	0.55
2:B:12:PHE:H	3:C:17:GLN:HE22	1.53	0.55
8:H:45:GLY:HA3	8:H:52:THR:HG21	1.89	0.54
7:G:23:PHE:O	7:G:26:THR:HB	2.09	0.53
5:E:12:PHE:H	6:F:19:GLN:HE22	1.57	0.52
8:V:45:GLY:HA3	8:V:52:THR:HG21	1.89	0.52
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.75	0.52
2:P:93:HIS:HB3	20:P:301:HOH:O	2.09	0.51
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.59	0.50
8:V:1[B]:THR:HG23	8:V:33:LYS:HD3	1.92	0.50
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.76	0.50
7:U:23:PHE:O	7:U:26:THR:HB	2.11	0.49
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.48	0.49
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.61	0.48
1:O:12:PHE:H	2:P:20:GLN:HE22	1.62	0.48
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.96	0.48
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.50	0.47
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.96	0.47
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.97	0.47
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.96	0.47
14:N:35:THR:HG21	14:N:45:ARG:HE	1.80	0.46
6:F:123:ASN:C	6:F:123:ASN:HD22	2.20	0.46
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.51	0.45
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.63	0.45
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.47	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.99	0.45
6:T:123:ASN:HD22	6:T:124:SER:N	2.14	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:201:VAL:O	3:C:202:GLN:CB	2.66	0.44
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.99	0.44
6:F:123:ASN:HD22	6:F:124:SER:N	2.15	0.44
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.98	0.43
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.00	0.43
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.00	0.43
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.53	0.43
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	2.00	0.43
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.54	0.43
6:T:123:ASN:HD22	6:T:123:ASN:C	2.20	0.43
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.54	0.43
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.54	0.43
8:V:3:ILE:HG22	8:V:16:ALA:HB2	2.01	0.43
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.01	0.43
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.01	0.42
8:H:3:ILE:HG22	8:H:16:ALA:HB2	2.01	0.42
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.66	0.42
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.01	0.42
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.02	0.42
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.99	0.42
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.02	0.42
3:C:9:PHE:H	4:D:15:GLN:HE22	1.67	0.42
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.55	0.42
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.02	0.41
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.55	0.41
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.32	0.41
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.56	0.41
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	2.02	0.41
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.32	0.41
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.68	0.41
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.50	0.41
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.92	0.41
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.51	0.41
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.03	0.41
1:A:12:PHE:H	2:B:20:GLN:HE22	1.69	0.40
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.03	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%)	233 (98%)	2 (1%)	3 (1%)	12	30
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	12	30
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	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%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
8	V	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (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%)	224 (97%)	7 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6284/6614 (95%)	6140 (98%)	128 (2%)	16 (0%)	41	66

All (16) 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
1	A	2	THR
2	B	218	GLY
1	O	2	THR
2	P	218	GLY
2	B	220	ASN
2	P	220	ASN
3	C	205	ALA
3	Q	205	ALA
3	C	183	PRO
3	Q	183	PRO

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%)	206 (99%)	3 (1%)	67	86
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	86
2	B	203/216 (94%)	197 (97%)	6 (3%)	41	70
2	P	203/216 (94%)	197 (97%)	6 (3%)	41	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	212/226 (94%)	202 (95%)	10 (5%)	26	54
3	Q	212/226 (94%)	202 (95%)	10 (5%)	26	54
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	54
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	54
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
8	H	186/190 (98%)	183 (98%)	3 (2%)	62	85
8	V	186/190 (98%)	182 (98%)	4 (2%)	52	79
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	84
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	84
10	J	173/175 (99%)	169 (98%)	4 (2%)	50	78
10	X	173/175 (99%)	169 (98%)	4 (2%)	50	78
11	K	169/169 (100%)	162 (96%)	7 (4%)	30	59
11	Y	169/169 (100%)	162 (96%)	7 (4%)	30	59
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%)	192 (96%)	7 (4%)	36	65
13	a	199/208 (96%)	192 (96%)	7 (4%)	36	65
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	69
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	69
All	All	5322/5540 (96%)	5135 (96%)	187 (4%)	36	65

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	79	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	113	ARG
2	B	119	GLN
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
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	8	ASP
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	99	ASN
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	214	TRP
6	F	240	GLN
7	G	75	ASN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	22	GLN
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	3	ILE
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	9	GLN
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	49	ASN
12	L	108	HIS
12	L	130	SER
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
13	M	233	ILE
14	N	9	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	79	LEU
2	P	113	ARG
2	P	119	GLN
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
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	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	8	ASP
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	99	ASN
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	202	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	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	22	GLN
8	V	30	ASN
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	3	ILE
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
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
12	Z	49	ASN
12	Z	108	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	Z	130	SER
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
13	a	233	ILE
14	b	9	LYS
14	b	39	ASP
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 (125) 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	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	100	ASN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
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	30	ASN
8	H	35	HIS
8	H	66	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	158	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
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	30	ASN
8	V	35	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	W	37	ASN
10	X	55	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
18	GW2	H	302[B]	8	49,49,49	1.63	11 (22%)	60,66,66	1.39	7 (11%)
19	MES	H	303	-	12,12,12	2.21	1 (8%)	14,16,16	1.45	2 (14%)
18	GW2	V	302[B]	8	49,49,49	1.36	7 (14%)	60,66,66	1.49	5 (8%)
17	GVZ	V	301[A]	8	49,49,49	1.31	5 (10%)	63,68,68	1.53	9 (14%)
19	MES	V	303	-	12,12,12	2.19	1 (8%)	14,16,16	1.50	2 (14%)
17	GVZ	H	301[A]	8	49,49,49	1.36	4 (8%)	63,68,68	1.54	8 (12%)

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
18	GW2	H	302[B]	8	-	2/44/73/73	0/4/4/4
19	MES	H	303	-	-	5/6/14/14	0/1/1/1
18	GW2	V	302[B]	8	-	3/44/73/73	0/4/4/4
17	GVZ	V	301[A]	8	-	9/44/73/73	0/4/4/4
19	MES	V	303	-	-	2/6/14/14	0/1/1/1
17	GVZ	H	301[A]	8	-	9/44/73/73	0/4/4/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	303	MES	C8-S	-7.37	1.67	1.77
19	V	303	MES	C8-S	-7.25	1.67	1.77
18	H	302[B]	GW2	C40-C41	-6.20	1.36	1.51
17	H	301[A]	GVZ	C40-C41	-4.92	1.39	1.51
18	V	302[B]	GW2	C40-C41	-4.91	1.39	1.51
17	V	301[A]	GVZ	C40-C41	-4.58	1.40	1.51
17	H	301[A]	GVZ	C10-C9	4.26	1.63	1.54
17	V	301[A]	GVZ	C10-C9	4.18	1.62	1.54
18	H	302[B]	GW2	C4-C3	-3.40	1.49	1.54
17	H	301[A]	GVZ	C11-C10	3.15	1.57	1.52
18	H	302[B]	GW2	O21-C9	-3.09	1.35	1.43
18	V	302[B]	GW2	O21-C9	-3.08	1.35	1.43
18	H	302[B]	GW2	C53-C4	-2.92	1.48	1.53
18	H	302[B]	GW2	C4-C5	-2.90	1.50	1.54
17	V	301[A]	GVZ	C11-C10	2.86	1.57	1.52
18	V	302[B]	GW2	C53-C4	-2.77	1.48	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	302[B]	GW2	C2-C3	-2.63	1.46	1.53
18	H	302[B]	GW2	C50-C3	-2.53	1.47	1.53
17	V	301[A]	GVZ	C12-C10	2.45	1.56	1.52
17	H	301[A]	GVZ	C12-C10	2.38	1.56	1.52
18	V	302[B]	GW2	C1-C2	-2.33	1.47	1.53
18	V	302[B]	GW2	C2-C3	-2.33	1.47	1.53
18	H	302[B]	GW2	C6-C5	-2.33	1.47	1.53
17	V	301[A]	GVZ	C6-C5	2.27	1.58	1.53
18	V	302[B]	GW2	C4-C5	-2.13	1.51	1.54
18	H	302[B]	GW2	C1-C2	-2.09	1.47	1.53
18	H	302[B]	GW2	C10-C9	-2.06	1.50	1.53
18	H	302[B]	GW2	C51-C50	-2.02	1.47	1.53
18	V	302[B]	GW2	C51-C50	-2.02	1.47	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	V	302[B]	GW2	C11-C10-C12	-6.68	101.11	109.88
17	H	301[A]	GVZ	C12-C10-C11	-6.57	101.17	110.56
17	V	301[A]	GVZ	C12-C10-C11	-6.47	101.31	110.56
18	H	302[B]	GW2	C11-C10-C12	-5.76	102.31	109.88
19	V	303	MES	O1S-S-C8	4.15	111.91	106.92
19	H	303	MES	O2S-S-C8	3.94	111.66	106.92
18	V	302[B]	GW2	C27-N28-C29	3.35	126.37	121.34
17	V	301[A]	GVZ	C52-C53-C4	-3.23	104.99	111.64
17	V	301[A]	GVZ	C30-N31-C36	3.21	116.07	111.09
17	H	301[A]	GVZ	C30-N31-C36	3.19	116.05	111.09
17	H	301[A]	GVZ	C52-C53-C4	-3.18	105.08	111.64
18	V	302[B]	GW2	C38-C27-N28	-3.12	104.53	110.38
17	V	301[A]	GVZ	C46-O45-C44	2.79	123.57	117.51
17	H	301[A]	GVZ	C46-O45-C44	2.62	123.20	117.51
18	V	302[B]	GW2	O21-C9-C8	-2.52	102.96	108.98
19	V	303	MES	O3S-S-C8	2.50	109.82	105.77
17	V	301[A]	GVZ	C1-C6-C5	-2.49	107.68	111.93
17	V	301[A]	GVZ	C33-C32-N31	-2.44	106.40	110.10
17	H	301[A]	GVZ	C33-C32-N31	-2.44	106.41	110.10
18	H	302[B]	GW2	C29-C30-N31	2.38	118.89	113.36
18	V	302[B]	GW2	C11-C10-C9	-2.37	107.14	111.54
17	H	301[A]	GVZ	C1-C6-C5	-2.36	107.90	111.93
18	H	302[B]	GW2	C38-C27-N28	-2.34	105.99	110.38
17	V	301[A]	GVZ	C12-C10-C9	2.33	115.65	111.28
17	H	301[A]	GVZ	C11-C10-C9	2.33	115.64	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	H	301[A]	GVZ	C12-C10-C9	2.28	115.55	111.28
17	V	301[A]	GVZ	C11-C10-C9	2.27	115.52	111.28
18	H	302[B]	GW2	C7-C5-C4	-2.21	108.59	114.16
18	H	302[B]	GW2	O21-C9-C8	-2.20	103.72	108.98
18	H	302[B]	GW2	C27-N28-C29	2.18	124.61	121.34
18	H	302[B]	GW2	C2-C3-C50	-2.15	107.45	113.08
17	V	301[A]	GVZ	C51-C50-C3	-2.06	108.42	111.93
19	H	303	MES	O3S-S-C8	2.05	109.08	105.77

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301[A]	GVZ	C11-C10-C9-C8
17	H	301[A]	GVZ	C11-C10-C9-O21
17	H	301[A]	GVZ	C12-C10-C9-C8
17	H	301[A]	GVZ	C12-C10-C9-O21
17	H	301[A]	GVZ	O13-C10-C9-C8
17	H	301[A]	GVZ	O13-C10-C9-O21
17	V	301[A]	GVZ	C11-C10-C9-C8
17	V	301[A]	GVZ	C11-C10-C9-O21
17	V	301[A]	GVZ	C12-C10-C9-C8
17	V	301[A]	GVZ	C12-C10-C9-O21
17	V	301[A]	GVZ	O13-C10-C9-C8
17	V	301[A]	GVZ	O13-C10-C9-O21
19	H	303	MES	C7-C8-S-O3S
17	H	301[A]	GVZ	C29-C30-N31-C36
18	H	302[B]	GW2	N28-C29-C30-N31
18	H	302[B]	GW2	O37-C29-C30-N31
17	H	301[A]	GVZ	O37-C29-C30-N31
17	V	301[A]	GVZ	O37-C29-C30-N31
17	H	301[A]	GVZ	N28-C29-C30-N31
17	V	301[A]	GVZ	N28-C29-C30-N31
17	V	301[A]	GVZ	C29-C30-N31-C36
19	H	303	MES	C7-C8-S-O1S
19	H	303	MES	C7-C8-S-O2S
18	V	302[B]	GW2	O37-C29-C30-N31
18	V	302[B]	GW2	C29-C30-N31-C36
18	V	302[B]	GW2	N28-C29-C30-N31
19	H	303	MES	C8-C7-N4-C5
19	H	303	MES	C8-C7-N4-C3
19	V	303	MES	C8-C7-N4-C3

Continued on next page...

Continued from previous page...

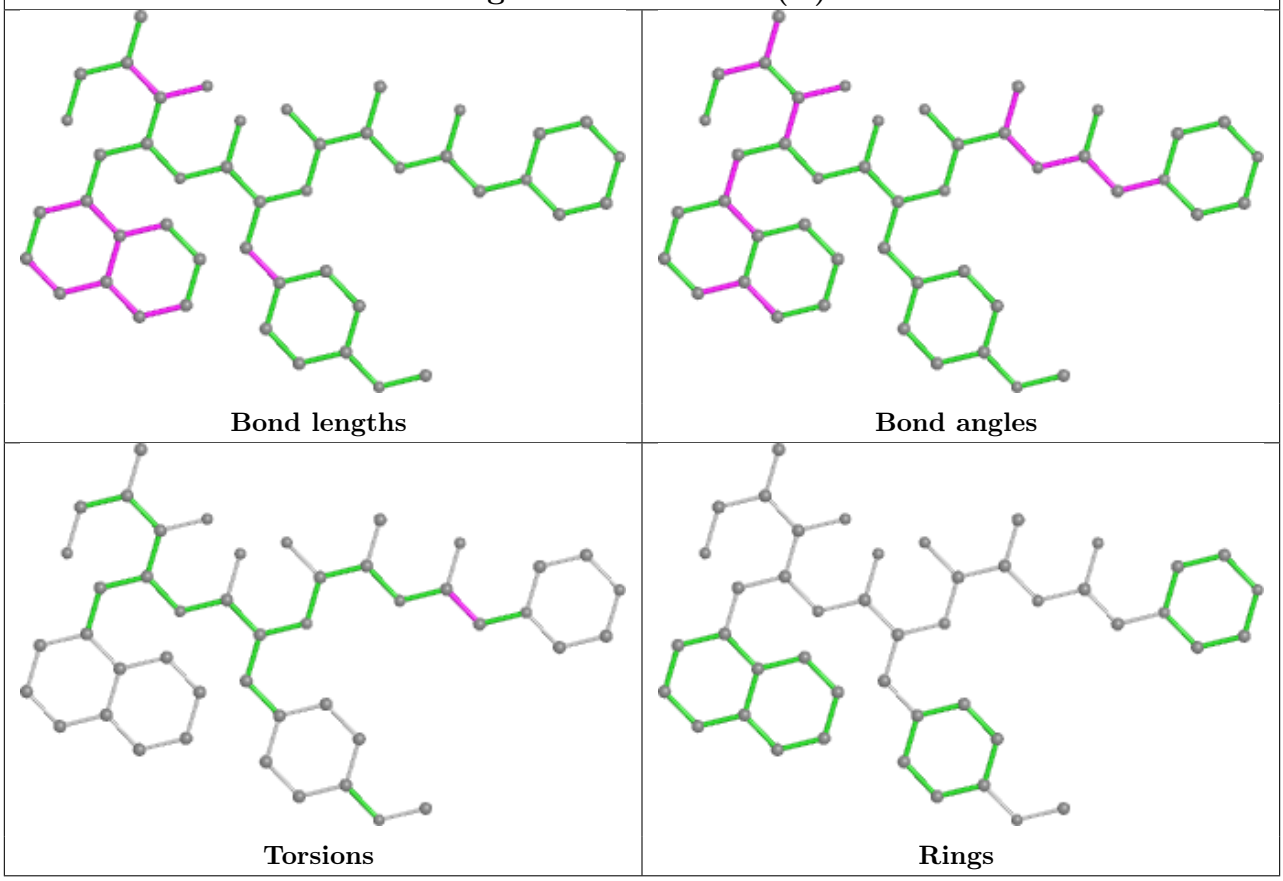
Mol	Chain	Res	Type	Atoms
19	V	303	MES	C8-C7-N4-C5

There are no ring outliers.

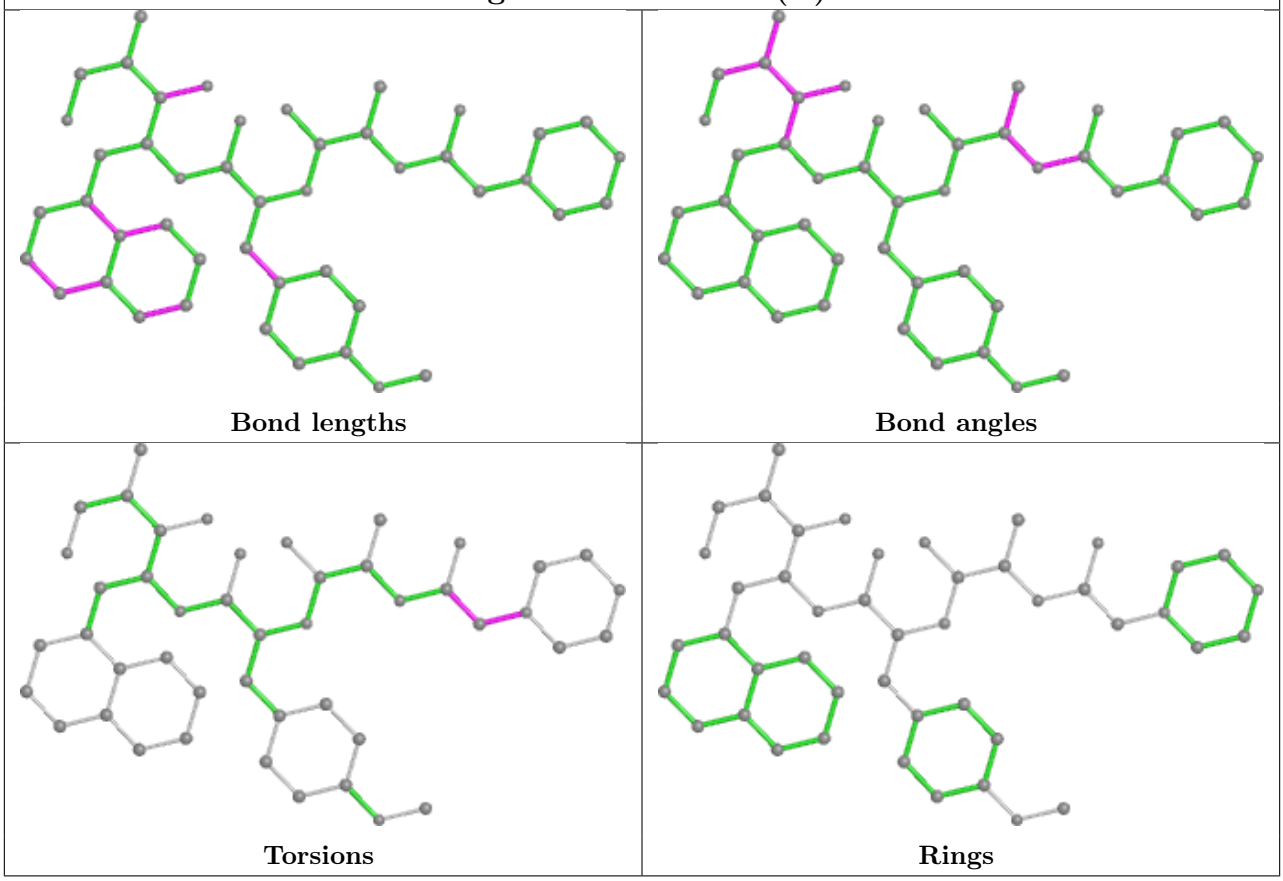
No monomer is involved in short contacts.

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.

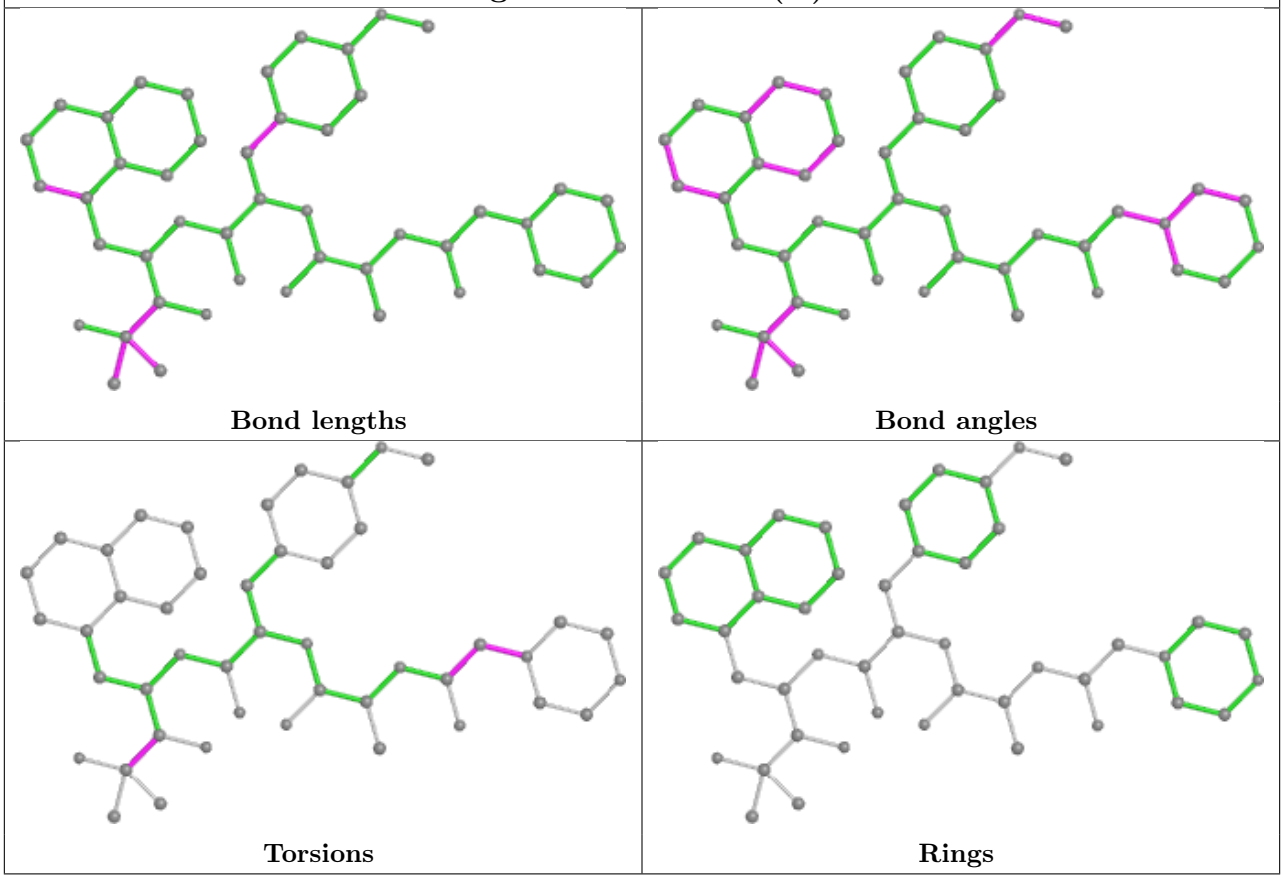
Ligand GW2 H 302 (B)



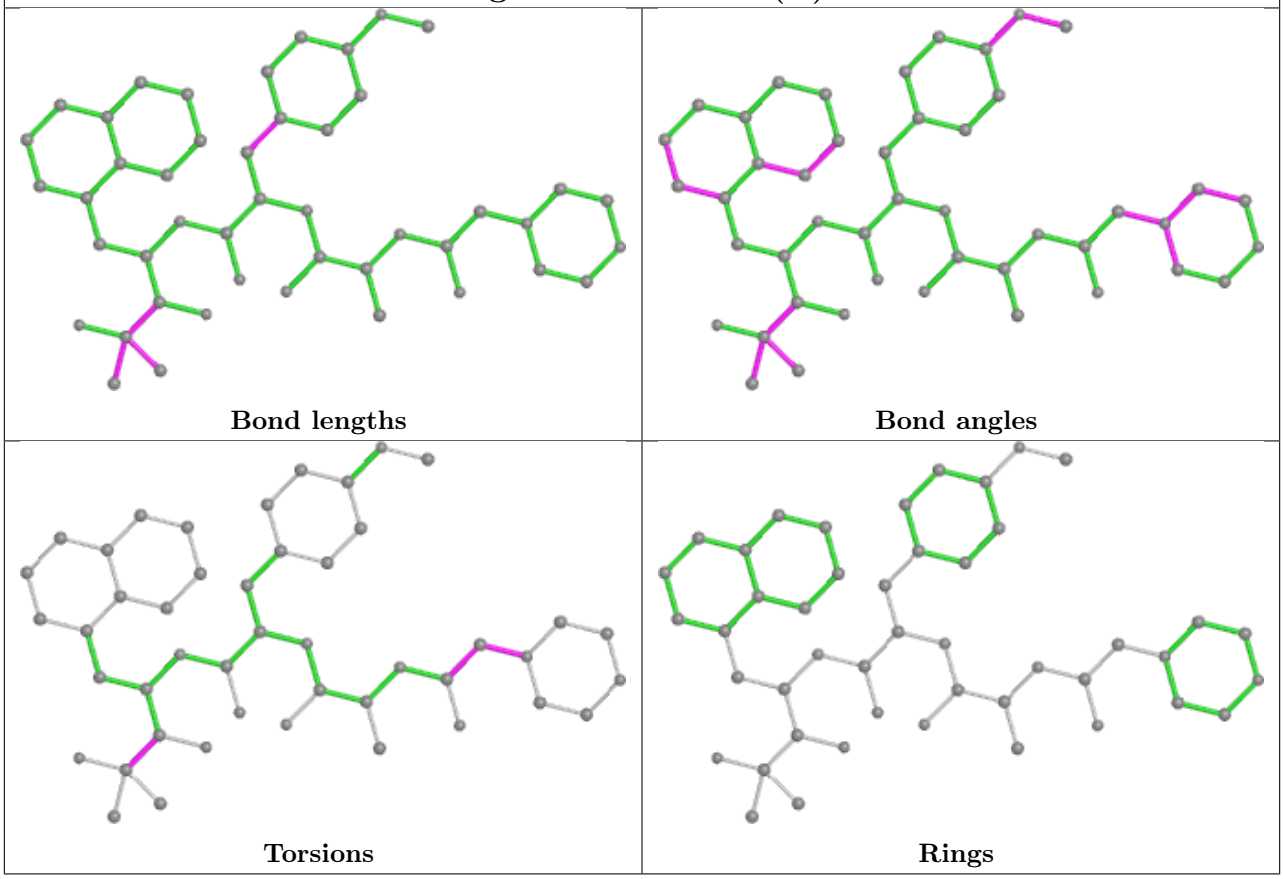
Ligand GW2 V 302 (B)



Ligand GVZ V 301 (A)



Ligand GVZ H 301 (A)



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.39	8 (3%)	47	48	39, 52, 86, 126	0
1	O	250/250 (100%)	-0.31	6 (2%)	59	60	43, 59, 102, 131	0
2	B	244/258 (94%)	-0.27	6 (2%)	57	59	40, 57, 98, 149	0
2	P	244/258 (94%)	-0.18	11 (4%)	33	31	42, 62, 106, 147	0
3	C	240/254 (94%)	-0.11	14 (5%)	23	22	41, 63, 126, 147	0
3	Q	240/254 (94%)	0.10	20 (8%)	11	9	44, 72, 151, 177	0
4	D	235/260 (90%)	-0.38	5 (2%)	63	65	43, 63, 96, 137	0
4	R	235/260 (90%)	-0.28	6 (2%)	56	57	45, 66, 105, 136	0
5	E	231/234 (98%)	-0.18	7 (3%)	50	51	48, 67, 104, 149	0
5	S	231/234 (98%)	-0.07	8 (3%)	44	44	49, 74, 118, 161	0
6	F	243/288 (84%)	-0.34	5 (2%)	63	65	40, 60, 110, 136	0
6	T	243/288 (84%)	-0.25	10 (4%)	37	36	39, 69, 125, 156	0
7	G	241/252 (95%)	-0.43	5 (2%)	63	65	37, 55, 88, 134	0
7	U	241/252 (95%)	-0.34	5 (2%)	63	65	43, 59, 90, 138	0
8	H	226/232 (97%)	-0.45	7 (3%)	49	49	38, 52, 84, 139	0
8	V	226/232 (97%)	-0.37	5 (2%)	62	63	43, 55, 88, 152	0
9	I	204/205 (99%)	-0.66	1 (0%)	91	92	35, 48, 74, 97	0
9	W	204/205 (99%)	-0.65	3 (1%)	73	76	38, 50, 79, 103	0
10	J	195/198 (98%)	-0.49	3 (1%)	73	76	38, 52, 77, 127	0
10	X	195/198 (98%)	-0.49	3 (1%)	73	76	39, 54, 78, 142	0
11	K	212/212 (100%)	-0.54	0	100	100	36, 51, 72, 92	0
11	Y	212/212 (100%)	-0.55	1 (0%)	91	92	39, 51, 73, 94	0
12	L	222/222 (100%)	-0.51	1 (0%)	91	92	40, 55, 83, 121	0
12	Z	222/222 (100%)	-0.52	2 (0%)	84	85	39, 52, 82, 118	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	3 (1%)	77	78	36, 54, 77, 94	0
13	a	233/246 (94%)	-0.54	1 (0%)	92	93	36, 53, 73, 89	0
14	N	196/196 (100%)	-0.58	2 (1%)	82	83	39, 49, 77, 103	0
14	b	196/196 (100%)	-0.52	2 (1%)	82	83	39, 50, 78, 109	0
All	All	6344/6614 (95%)	-0.38	150 (2%)	59	60	35, 57, 101, 177	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	9.6
3	Q	50	LEU	7.3
3	Q	206	LYS	6.3
3	C	206	LYS	6.2
2	B	221	ASP	6.1
2	P	221	ASP	5.7
2	P	51	VAL	5.6
2	B	51	VAL	5.4
10	X	1	MET	5.3
2	P	220	ASN	5.3
2	P	219	ALA	5.2
5	E	202	ASP	5.1
2	P	218	GLY	5.0
3	Q	236	GLN	5.0
5	E	123	GLY	5.0
9	W	1	SER	4.9
10	X	194	ASP	4.9
1	A	249	ALA	4.8
2	B	218	GLY	4.8
1	O	249	ALA	4.7
3	C	205	ALA	4.7
10	J	1	MET	4.7
12	L	174	TYR	4.6
8	V	224	GLN	4.4
2	P	59	ASP	4.4
7	U	242	GLN	4.3
1	A	1	MET	4.1
7	U	206	GLY	4.1
3	Q	239	GLN	4.1
3	C	50	LEU	4.1
5	S	202	ASP	4.0
3	Q	202	GLN	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	R	241	ALA	3.7
3	C	49	THR	3.7
3	C	238	LYS	3.7
8	V	221	CYS	3.6
8	H	226	GLU	3.6
8	V	226	GLU	3.5
3	C	236	GLN	3.5
14	b	105	LYS	3.5
3	Q	205	ALA	3.5
6	T	244	ASN	3.5
2	B	220	ASN	3.4
6	F	181	GLU	3.4
6	T	205	GLU	3.4
6	F	205	GLU	3.3
3	C	202	GLN	3.3
3	Q	204	GLY	3.3
6	T	243	ILE	3.3
2	B	59	ASP	3.2
3	Q	238	LYS	3.2
3	C	240	GLU	3.2
1	O	2	THR	3.1
3	Q	187	GLU	3.1
3	Q	240	GLU	3.1
1	O	1	MET	3.1
9	I	1	SER	3.1
8	V	222	ASP	3.1
14	N	105	LYS	3.1
13	a	1	THR	3.1
4	R	242	GLU	3.1
2	P	52	THR	3.0
5	S	227	GLU	3.0
6	F	244	ASN	3.0
10	J	194	ASP	3.0
5	E	122	TYR	2.9
8	H	222	ASP	2.9
8	H	221	CYS	2.9
1	O	250	LEU	2.9
10	X	193	ASP	2.9
7	U	2	GLY	2.8
12	Z	174	TYR	2.8
2	P	50	LYS	2.8
3	Q	203	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	R	217	GLN	2.7
2	P	182	ASP	2.7
4	R	230	GLU	2.7
1	A	182	GLU	2.7
3	Q	225	GLU	2.7
7	G	240	ALA	2.6
14	b	195	GLN	2.6
6	T	178	HIS	2.6
7	U	222	ASP	2.6
2	P	203	SER	2.6
13	M	47	ASP	2.6
4	D	242	GLU	2.6
5	S	194	GLU	2.5
3	C	239	GLN	2.5
8	H	145	ASP	2.5
6	T	241	LYS	2.5
1	A	2	THR	2.5
1	O	201	GLU	2.5
3	Q	229	GLN	2.5
3	Q	180	LYS	2.4
6	T	204	LYS	2.4
4	R	1	ASP	2.4
1	A	201	GLU	2.4
3	Q	237	GLU	2.4
13	M	1	THR	2.4
8	H	224	GLN	2.4
3	C	203	THR	2.4
6	F	2	THR	2.4
3	Q	48	SER	2.4
3	C	225	GLU	2.4
8	H	198	GLU	2.4
3	Q	60	SER	2.4
9	W	192	ASP	2.4
3	C	180	LYS	2.4
5	S	54	GLU	2.3
5	S	201	ARG	2.3
3	Q	175	LYS	2.3
6	T	230	ASP	2.3
6	T	181	GLU	2.3
14	N	195	GLN	2.3
1	A	203	GLU	2.3
5	S	173	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	P	222	GLY	2.3
1	O	53	SER	2.3
7	G	241	GLU	2.3
4	D	217	GLN	2.3
1	A	248	GLU	2.3
5	S	57	SER	2.2
12	Z	1	GLN	2.2
13	M	216	ASN	2.2
6	F	215	CYS	2.2
10	J	193	ASP	2.2
7	G	68	ARG	2.2
3	Q	55	THR	2.2
11	Y	212	GLY	2.2
5	S	233	ILE	2.2
5	E	217	LYS	2.2
4	D	125	LEU	2.1
2	B	242	GLY	2.1
5	E	173	ARG	2.1
7	G	179	LYS	2.1
3	C	187	GLU	2.1
4	D	1	ASP	2.1
7	G	222	ASP	2.1
6	T	53	LYS	2.1
9	W	133	LYS	2.1
5	E	227	GLU	2.1
7	U	241	GLU	2.1
8	V	145	ASP	2.1
1	A	250	LEU	2.0
6	T	2	THR	2.0
8	H	223	ILE	2.0
3	C	181	GLU	2.0
5	E	203	GLU	2.0
4	R	125	LEU	2.0
4	D	201	GLU	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)

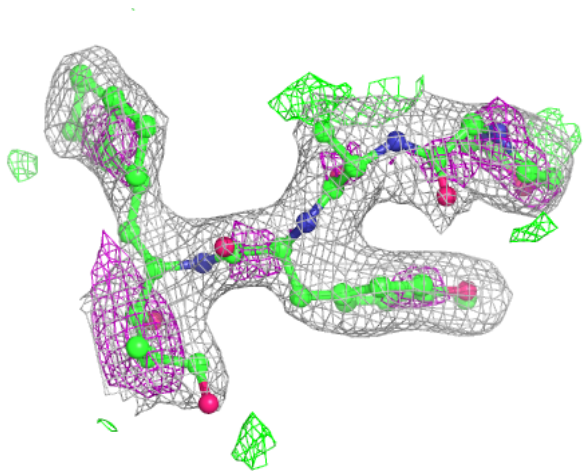
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

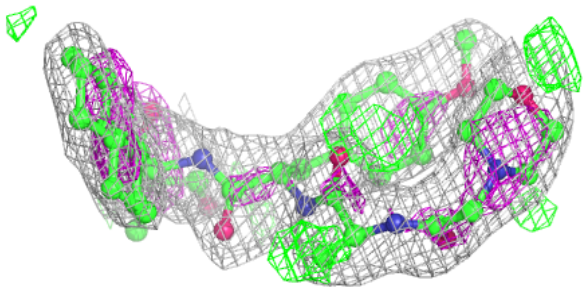
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	MES	V	303	12/12	0.89	0.29	82,87,96,98	0
18	GW2	H	302[B]	46/46	0.91	0.23	49,54,59,63	46
17	GVZ	H	301[A]	46/46	0.91	0.24	50,56,61,64	46
15	MG	Z	301	1/1	0.92	0.20	57,57,57,57	0
18	GW2	V	302[B]	46/46	0.92	0.24	49,55,59,62	46
17	GVZ	V	301[A]	46/46	0.92	0.25	50,57,61,64	46
19	MES	H	303	12/12	0.94	0.22	81,87,93,97	0
15	MG	I	302	1/1	0.95	0.07	57,57,57,57	0
15	MG	I	301	1/1	0.95	0.31	63,63,63,63	0
15	MG	W	301	1/1	0.96	0.26	60,60,60,60	0
15	MG	L	301	1/1	0.96	0.13	76,76,76,76	0
15	MG	N	201	1/1	0.98	0.10	52,52,52,52	0
15	MG	K	301	1/1	0.98	0.09	66,66,66,66	0
15	MG	G	301	1/1	0.98	0.06	49,49,49,49	0
16	CL	G	302	1/1	0.99	0.07	42,42,42,42	0
16	CL	U	301	1/1	0.99	0.18	44,44,44,44	0

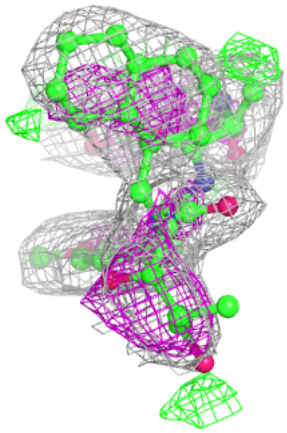
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GW2 H 302 (B):

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

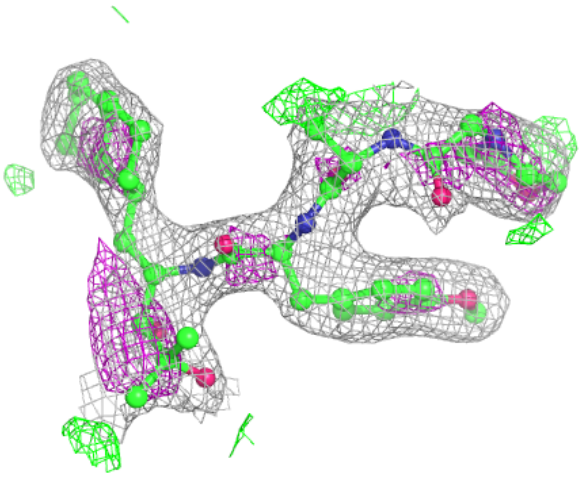


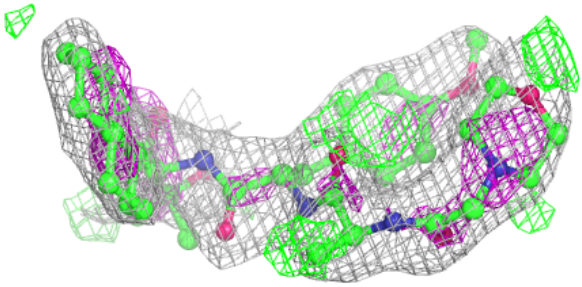


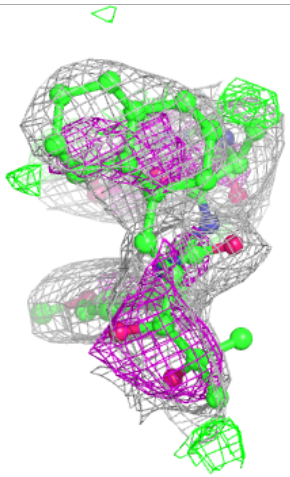


Electron density around GVZ H 301 (A):

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

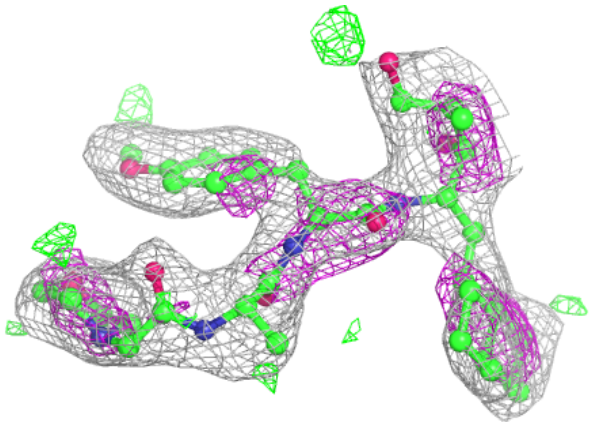


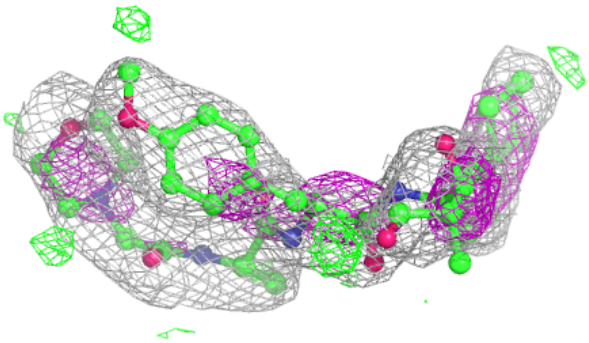


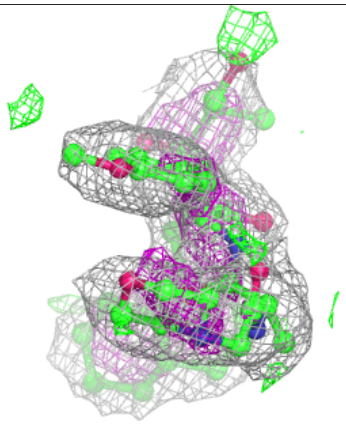


Electron density around GW2 V 302 (B):

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

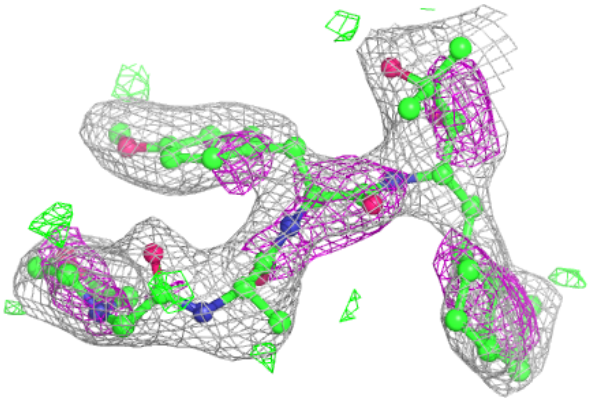


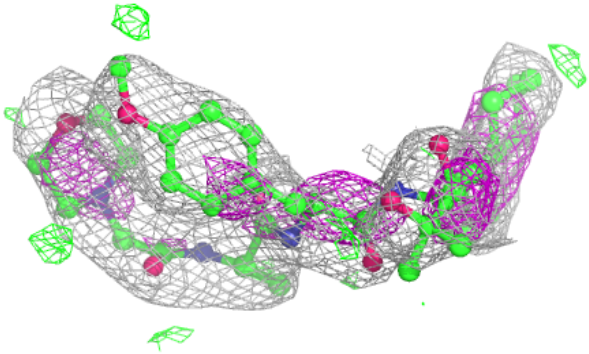


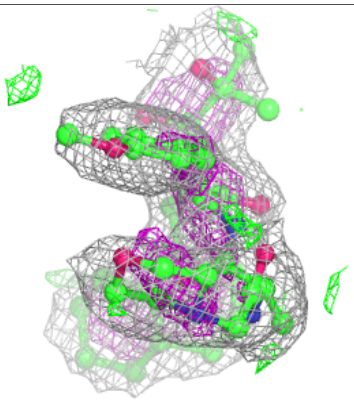


Electron density around GVZ V 301 (A):

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







6.5 Other polymers (i)

There are no such residues in this entry.