



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:43 pm BST

PDB ID : 6HW5
Title : Yeast 20S proteasome in complex with 18
Authors : Huber, E.M.; Groll, M.
Deposited on : 2018-10-11
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

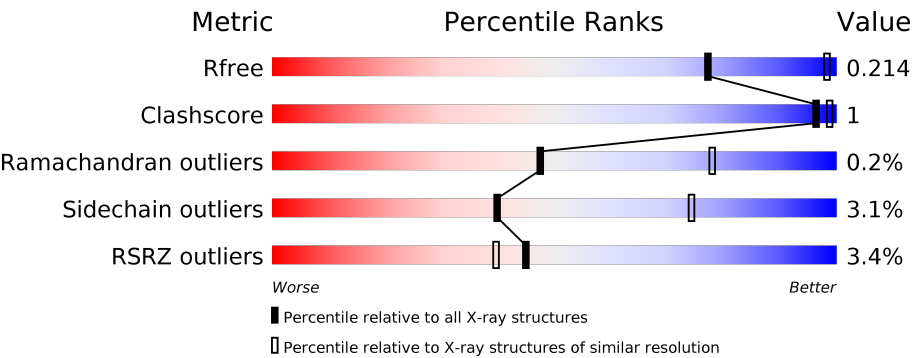
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	<div><div>4%</div><div>98%</div><div></div></div>
1	O	250	<div><div>6%</div><div>97%</div><div></div></div>
2	B	258	<div><div>5%</div><div>88%</div><div>6% 5%</div></div>
2	P	258	<div><div>5%</div><div>89%</div><div>5% 5%</div></div>
3	C	254	<div><div>7%</div><div>89%</div><div>5% 6%</div></div>
3	Q	254	<div><div>10%</div><div>89%</div><div>6%</div></div>

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Mol	Chain	Length	Quality of chain
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

There are 18 unique types of molecules in this entry. The entry contains 49707 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	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	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			

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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
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- 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	0	0
			1	1		
15	K	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	I	2	Total 2 Mg 2	0	0
15	Z	1	Total 1 Mg 1	0	0
15	N	1	Total 1 Mg 1	0	0
15	X	1	Total 1 Mg 1	0	0
15	L	1	Total 1 Mg 1	0	0

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

- # GRT

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	C	N	O	S	0	0
			42	29	7	5	1		



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	K	1	Total	C	N	O	S	0	0
			42	29	7	5	1		
17	V	1	Total	C	N	O	S	0	0
			42	29	7	5	1		
17	Y	1	Total	C	N	O	S	0	0
			42	29	7	5	1		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	9	Total	O	0	0
			9	9		
18	B	8	Total	O	0	0
			8	8		
18	C	8	Total	O	0	0
			8	8		
18	D	4	Total	O	0	0
			4	4		
18	E	4	Total	O	0	0
			4	4		
18	F	13	Total	O	0	0
			13	13		
18	G	9	Total	O	0	0
			9	9		
18	H	9	Total	O	0	0
			9	9		
18	I	6	Total	O	0	0
			6	6		
18	J	9	Total	O	0	0
			9	9		
18	K	9	Total	O	0	0
			9	9		
18	L	11	Total	O	0	0
			11	11		
18	M	12	Total	O	0	0
			12	12		
18	N	4	Total	O	0	0
			4	4		
18	O	5	Total	O	0	0
			5	5		
18	P	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	Q	10	Total 10	O 10	0	0
18	R	6	Total 6	O 6	0	0
18	S	4	Total 4	O 4	0	0
18	T	9	Total 9	O 9	0	0
18	U	11	Total 11	O 11	0	0
18	V	6	Total 6	O 6	0	0
18	W	2	Total 2	O 2	0	0
18	X	16	Total 16	O 16	0	0
18	Y	13	Total 13	O 13	0	0
18	Z	8	Total 8	O 8	0	0
18	a	12	Total 12	O 12	0	0
18	b	9	Total 9	O 9	0	0

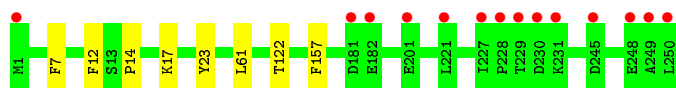
3 Residue-property plots [i](#)

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

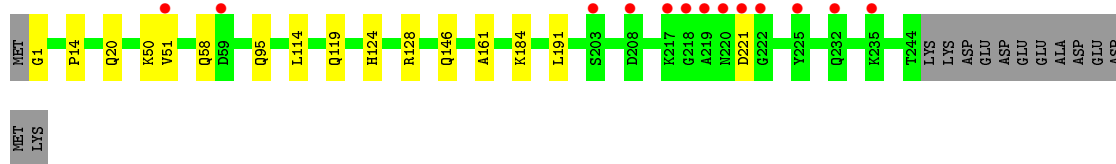
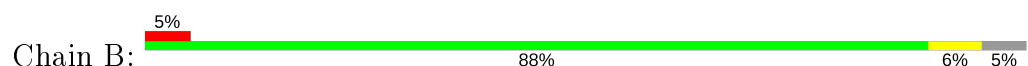
- Molecule 1: Proteasome subunit alpha type-2



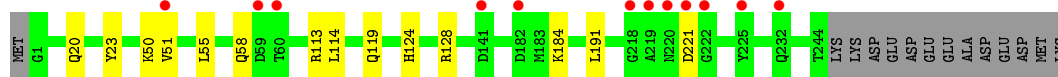
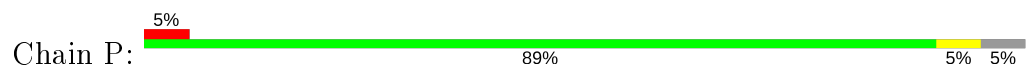
- Molecule 1: Proteasome subunit alpha type-2



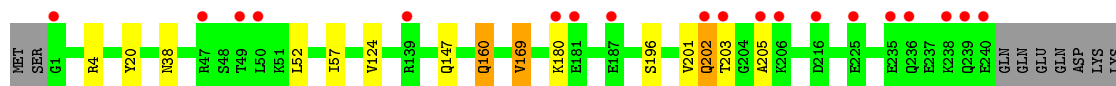
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 2: Proteasome subunit alpha type-3

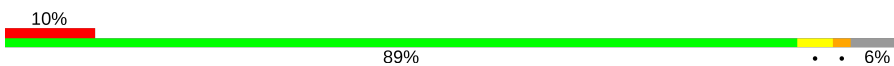


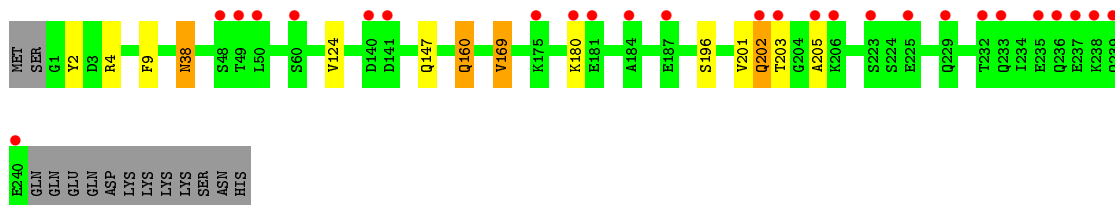
- Molecule 3: Proteasome subunit alpha type-4




LYS
LYS
SER
ASN
HIS

• 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: 




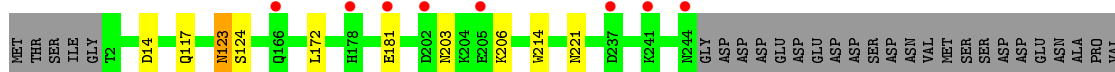
• Molecule 5: Proteasome subunit alpha type-6

Chain S: 

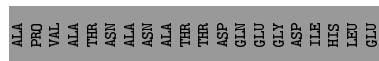
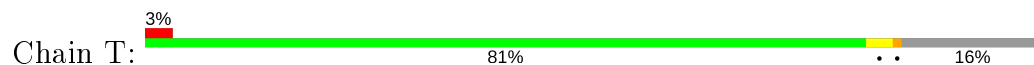


• Molecule 6: Probable proteasome subunit alpha type-7

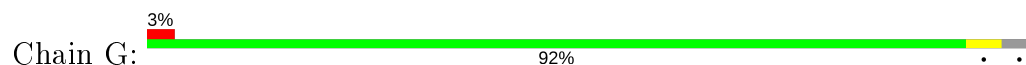
Chain F: 



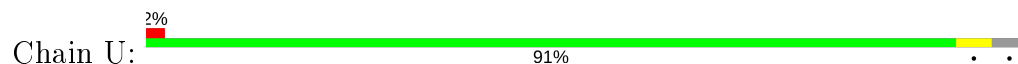
- Molecule 6: Probable proteasome subunit alpha type-7



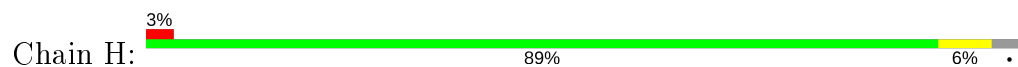
- Molecule 7: Proteasome subunit alpha type-1



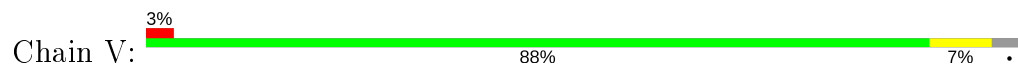
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2



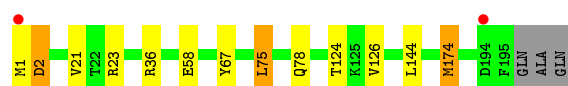
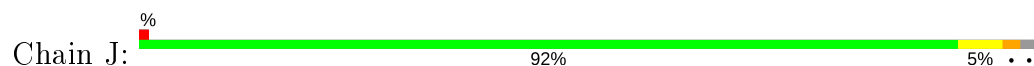
- Molecule 9: Proteasome subunit beta type-3



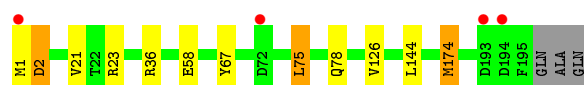
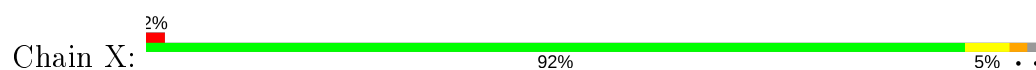
- Molecule 9: Proteasome subunit beta type-3



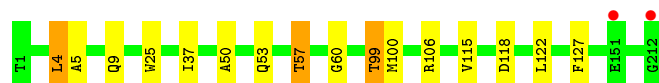
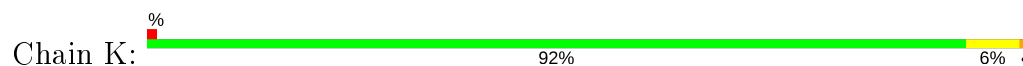
- Molecule 10: Proteasome subunit beta type-4



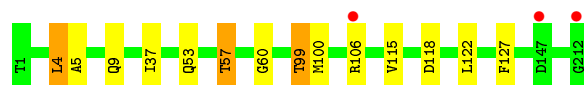
- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5



- Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5



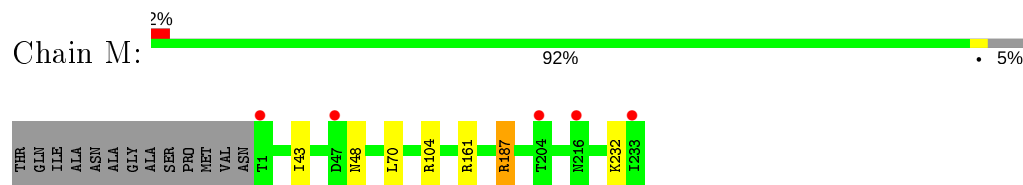
- Molecule 12: Proteasome subunit beta type-6



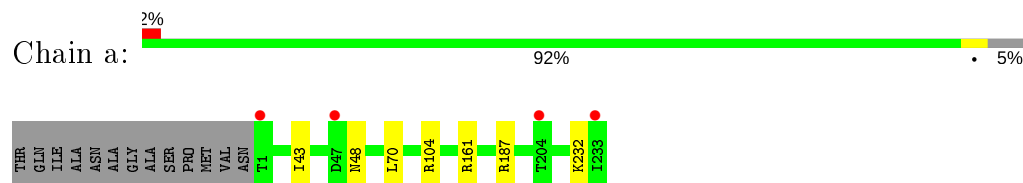
- Molecule 12: Proteasome subunit beta type-6



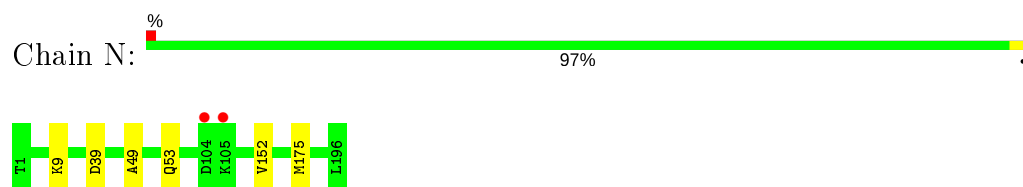
- Molecule 13: Proteasome subunit beta type-7



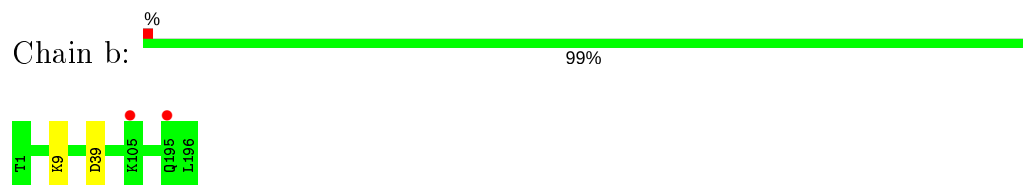
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	138.44Å 299.48Å 147.31Å 90.00° 113.25° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-2.90) 98.5 (15.00-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.180 , 0.211 0.187 , 0.214	Depositor DCC
R_{free} test set	11868 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	77.9	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	49707	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GRT, 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	0.40	0/1952	0.58	0/2642
1	O	0.40	0/1952	0.58	0/2642
2	B	0.40	0/1934	0.60	0/2618
2	P	0.40	0/1934	0.59	0/2618
3	C	0.40	0/1910	0.63	0/2586
3	Q	0.40	0/1910	0.63	0/2586
4	D	0.39	0/1837	0.58	0/2475
4	R	0.38	0/1837	0.58	0/2475
5	E	0.39	0/1800	0.57	0/2433
5	S	0.39	0/1800	0.57	0/2433
6	F	0.39	0/1932	0.55	0/2609
6	T	0.39	0/1932	0.55	0/2609
7	G	0.39	0/1945	0.56	0/2634
7	U	0.39	0/1945	0.56	0/2634
8	H	0.36	0/1715	0.58	0/2326
8	V	0.37	0/1715	0.57	0/2326
9	I	0.39	0/1611	0.60	0/2174
9	W	0.39	0/1611	0.60	0/2174
10	J	0.39	0/1589	0.60	0/2142
10	X	0.39	0/1589	0.60	0/2142
11	K	0.38	0/1681	0.64	2/2274 (0.1%)
11	Y	0.38	0/1681	0.65	2/2274 (0.1%)
12	L	0.39	0/1795	0.59	0/2420
12	Z	0.39	0/1795	0.59	0/2420
13	M	0.39	0/1855	0.64	0/2514
13	a	0.39	0/1855	0.63	0/2514
14	N	0.35	0/1541	0.57	0/2087
14	b	0.35	0/1541	0.57	0/2087
All	All	0.39	0/50194	0.59	4/67868 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	4	LEU	CD1-CG-CD2	-8.76	84.22	110.50
11	K	4	LEU	CD1-CG-CD2	-8.47	85.10	110.50
11	Y	4	LEU	CB-CG-CD1	7.90	124.44	111.00
11	K	4	LEU	CB-CG-CD2	7.14	123.14	111.00

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	3	0
1	O	1915	0	1929	5	0
2	B	1904	0	1904	9	0
2	P	1904	0	1904	5	0
3	C	1881	0	1895	8	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	1	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	1	0
7	U	1907	0	1901	2	0
8	H	1684	0	1687	7	0
8	V	1684	0	1687	8	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	7	0
10	X	1561	0	1569	6	0
11	K	1644	0	1594	8	0
11	Y	1644	0	1594	6	0
12	L	1757	0	1711	6	0
12	Z	1757	0	1711	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1824	0	1832	1	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	2	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	X	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	42	0	0	1	0
17	K	42	0	0	0	0
17	V	42	0	0	1	0
17	Y	42	0	0	0	0
18	A	9	0	0	0	0
18	B	8	0	0	0	0
18	C	8	0	0	0	0
18	D	4	0	0	0	0
18	E	4	0	0	0	0
18	F	13	0	0	0	0
18	G	9	0	0	0	0
18	H	9	0	0	1	0
18	I	6	0	0	0	0
18	J	9	0	0	0	0
18	K	9	0	0	0	0
18	L	11	0	0	0	0
18	M	12	0	0	0	0
18	N	4	0	0	0	0
18	O	5	0	0	0	0
18	P	7	0	0	1	0
18	Q	10	0	0	0	0
18	R	6	0	0	0	0
18	S	4	0	0	0	0
18	T	9	0	0	0	0
18	U	11	0	0	0	0
18	V	6	0	0	0	0
18	W	2	0	0	0	0
18	X	16	0	0	0	0
18	Y	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Z	8	0	0	0	0
18	a	12	0	0	0	0
18	b	9	0	0	0	0
All	All	49707	0	49064	86	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 (86) 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)
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.24	0.67
8:V:50:ALA:CB	9:W:126:ILE:HG23	2.30	0.62
11:Y:53:GLN:O	11:Y:57:THR:OG1	2.21	0.58
11:K:53:GLN:O	11:K:57:THR:OG1	2.22	0.57
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.70	0.56
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.71	0.56
10:X:1:MET:O	10:X:2:ASP:HB2	2.06	0.56
10:J:1:MET:O	10:J:2:ASP:HB2	2.06	0.55
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.71	0.55
10:J:174:MET:HA	10:X:174:MET:HA	1.88	0.55
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.90	0.54
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.90	0.54
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.91	0.53
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.91	0.53
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.91	0.52
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.92	0.52
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.45	0.51
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.74	0.51
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.91	0.51
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.46	0.51
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.45	0.51
14:N:49:ALA:O	14:N:53:GLN:HB2	2.11	0.50
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.94	0.50
1:A:97:TYR:OH	9:I:77:GLU:OE2	2.27	0.50
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.46	0.50
14:N:152:VAL:HA	14:N:175:MET:HE1	1.93	0.50
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.95	0.49
8:H:19:ARG:NH1	8:H:167:LEU:O	2.45	0.49
11:K:99:THR:HG22	11:K:115:VAL:HB	1.95	0.49
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:99:THR:HG22	11:Y:115:VAL:HB	1.95	0.48
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.11	0.48
8:H:50:ALA:CB	9:I:126:ILE:CG2	2.92	0.48
7:U:23:PHE:O	7:U:26:THR:HB	2.14	0.48
8:V:50:ALA:CB	9:W:126:ILE:CG2	2.92	0.47
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.97	0.47
8:V:19:ARG:NH1	8:V:167:LEU:O	2.48	0.47
8:V:3:ILE:HG22	8:V:99:ILE:HD12	1.97	0.47
1:O:12:PHE:H	2:P:20:GLN:HE22	1.63	0.46
8:H:3:ILE:HG22	8:H:99:ILE:HD12	1.97	0.46
2:P:113:ARG:NH1	18:P:301:HOH:O	2.49	0.46
8:H:22:GLN:HG3	17:H:301:GRT:C19	2.46	0.46
2:B:161:ALA:HB3	3:C:52:LEU:HD23	1.99	0.46
6:F:123:ASN:HD22	6:F:124:SER:N	2.14	0.45
6:T:123:ASN:HD22	6:T:124:SER:N	2.14	0.45
4:D:113:LEU:HD12	5:E:78:PRO:HB2	1.98	0.45
8:H:144:GLN:NE2	18:H:401:HOH:O	2.49	0.45
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.48	0.45
8:V:22:GLN:HG3	17:V:301:GRT:C19	2.47	0.44
1:A:12:PHE:H	2:B:20:GLN:HE22	1.66	0.44
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.00	0.43
7:G:23:PHE:O	7:G:26:THR:HB	2.18	0.43
8:V:17:ASP:OD1	8:V:33:LYS:NZ	2.49	0.43
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.00	0.43
8:V:80:LEU:HD12	8:V:113:ILE:HD11	2.00	0.43
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.01	0.43
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.00	0.43
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.00	0.43
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.52	0.43
12:Z:134:GLU:OE1	12:Z:137:ARG:NH2	2.51	0.43
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.00	0.43
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.46	0.42
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.67	0.42
4:R:158:ARG:HB3	5:S:57:SER:HB3	2.01	0.42
11:K:25:TRP:CH2	12:L:144:SER:HA	2.54	0.42
11:K:37:ILE:HG23	11:K:60:GLY:HA2	2.01	0.42
12:L:134:GLU:OE1	12:L:137:ARG:NH2	2.53	0.42
9:I:56:ALA:HB3	10:J:124:THR:HG23	2.02	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.41
1:O:7:PHE:HB3	3:Q:2:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	2.02	0.41
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.56	0.41
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.67	0.41
3:C:201:VAL:O	3:C:202:GLN:CB	2.69	0.41
9:W:98:ARG:O	9:W:126:ILE:HD11	2.20	0.41
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.55	0.41
11:K:50:ALA:CB	12:L:128:VAL:HG23	2.51	0.41
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.69	0.41
3:Q:38:ASN:HD22	3:Q:38:ASN:C	2.25	0.41
8:H:80:LEU:HD12	8:H:113:ILE:HD11	2.02	0.40
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.04	0.40
2:B:1:GLY:HA3	5:E:122:TYR:CD1	2.55	0.40
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.04	0.40
6:T:14:ASP:OD2	6:T:14:ASP:N	2.53	0.40
3:C:169:VAL:HG23	3:C:196:SER:HB2	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%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
2	B	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	19	51
2	P	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	19	51
3	C	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	19	51
3	Q	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	19	51
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	220/232 (95%)	213 (97%)	6 (3%)	1 (0%)	29	61
8	V	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	29	61
10	X	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	29	61
11	K	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
12	Z	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
13	M	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
14	b	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
All	All	6276/6614 (95%)	6107 (97%)	158 (2%)	11 (0%)	47	78

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
10	J	2	ASP
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
3	C	205	ALA
3	Q	205	ALA
2	B	221	ASP
2	P	221	ASP

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Mol	Chain	Res	Type
8	H	9	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	67	89
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	89
2	B	203/216 (94%)	197 (97%)	6 (3%)	41	75
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	71
3	C	212/226 (94%)	205 (97%)	7 (3%)	38	72
3	Q	212/226 (94%)	205 (97%)	7 (3%)	38	72
4	D	194/215 (90%)	187 (96%)	7 (4%)	35	69
4	R	194/215 (90%)	187 (96%)	7 (4%)	35	69
5	E	190/193 (98%)	181 (95%)	9 (5%)	26	59
5	S	190/193 (98%)	181 (95%)	9 (5%)	26	59
6	F	201/239 (84%)	192 (96%)	9 (4%)	27	61
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	61
7	G	206/210 (98%)	199 (97%)	7 (3%)	37	71
7	U	206/210 (98%)	198 (96%)	8 (4%)	32	66
8	H	181/190 (95%)	176 (97%)	5 (3%)	43	76
8	V	181/190 (95%)	175 (97%)	6 (3%)	38	72
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	86
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	86
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	76
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	76
11	K	169/169 (100%)	163 (96%)	6 (4%)	35	69
11	Y	169/169 (100%)	163 (96%)	6 (4%)	35	69
12	L	185/185 (100%)	179 (97%)	6 (3%)	39	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39	73
13	M	199/208 (96%)	192 (96%)	7 (4%)	36	70
13	a	199/208 (96%)	192 (96%)	7 (4%)	36	70
14	N	162/162 (100%)	160 (99%)	2 (1%)	71	91
14	b	162/162 (100%)	160 (99%)	2 (1%)	71	91
All	All	5312/5540 (96%)	5145 (97%)	167 (3%)	40	74

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
2	B	50	LYS
2	B	58	GLN
2	B	114	LEU
2	B	119	GLN
2	B	184	LYS
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	203	THR
4	D	20	LEU
4	D	99	ILE
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	116	GLN
5	E	174	THR
5	E	184	ASN

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Mol	Chain	Res	Type
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP
6	F	117	GLN
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
8	H	30	ASN
8	H	34	LEU
8	H	38	SER
8	H	84	LYS
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	23	ARG
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	57	THR
11	K	99	THR
11	K	106	ARG
11	K	118	ASP
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	126	ASP
12	L	136	CYS

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Mol	Chain	Res	Type
12	L	167	LYS
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	232	LYS
14	N	9	LYS
14	N	39	ASP
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	55	LEU
2	P	58	GLN
2	P	114	LEU
2	P	119	GLN
2	P	184	LYS
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	203	THR
4	R	20	LEU
4	R	99	ILE
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	116	GLN
5	S	174	THR
5	S	184	ASN
5	S	188	LEU

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Mol	Chain	Res	Type
5	S	202	ASP
6	T	14	ASP
6	T	117	GLN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	125	MET
7	U	154	TYR
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
8	V	30	ASN
8	V	34	LEU
8	V	38	SER
8	V	68	LEU
8	V	84	LYS
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	23	ARG
10	X	75	LEU
10	X	78	GLN
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	57	THR
11	Y	99	THR
11	Y	106	ARG
11	Y	118	ASP
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	126	ASP

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Mol	Chain	Res	Type
12	Z	136	CYS
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
13	a	232	LYS
14	b	9	LYS
14	b	39	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	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	91	HIS
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
5	E	184	ASN
6	F	86	ASN
6	F	117	GLN
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN

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Mol	Chain	Res	Type
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
8	H	30	ASN
8	H	66	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
10	J	55	GLN
11	K	85	ASN
11	K	133	GLN
11	K	176	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
14	N	161	GLN
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	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	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN

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Mol	Chain	Res	Type
5	S	120	GLN
5	S	184	ASN
6	T	86	ASN
6	T	117	GLN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	175	ASN
8	V	30	ASN
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
10	X	55	GLN
10	X	86	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	176	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	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
14	b	161	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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	GRT	K	301	11	42,43,43	1.74	8 (19%)	53,57,57	1.28	8 (15%)
17	GRT	V	301	8	42,43,43	1.88	8 (19%)	53,57,57	1.36	6 (11%)
17	GRT	H	301	8	42,43,43	1.83	8 (19%)	53,57,57	1.37	8 (15%)
17	GRT	Y	301	11	42,43,43	1.78	8 (19%)	53,57,57	1.31	8 (15%)

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	GRT	K	301	11	-	3/44/44/44	0/2/2/2
17	GRT	V	301	8	-	5/44/44/44	0/2/2/2
17	GRT	H	301	8	-	6/44/44/44	0/2/2/2
17	GRT	Y	301	11	-	3/44/44/44	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	V	301	GRT	C37-C38	-5.28	1.38	1.51
17	Y	301	GRT	C37-C38	-5.28	1.38	1.51
17	K	301	GRT	C37-C38	-5.28	1.38	1.51
17	H	301	GRT	C37-C38	-5.12	1.39	1.51
17	Y	301	GRT	N10-N9	5.06	1.36	1.23
17	K	301	GRT	N10-N9	4.94	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	V	301	GRT	N10-N9	4.79	1.35	1.23
17	H	301	GRT	N10-N9	4.76	1.35	1.23
17	V	301	GRT	C47-S48	4.32	1.84	1.78
17	K	301	GRT	C7-C3	-4.28	1.41	1.51
17	Y	301	GRT	C7-C3	-4.25	1.41	1.51
17	H	301	GRT	C47-S48	4.02	1.83	1.78
17	K	301	GRT	O50-S48	3.95	1.53	1.44
17	H	301	GRT	O49-S48	3.93	1.53	1.44
17	V	301	GRT	O49-S48	3.92	1.53	1.44
17	V	301	GRT	O50-S48	3.87	1.52	1.44
17	Y	301	GRT	O50-S48	3.83	1.52	1.44
17	K	301	GRT	O49-S48	3.72	1.52	1.44
17	H	301	GRT	O50-S48	3.67	1.52	1.44
17	V	301	GRT	C7-C3	-3.65	1.42	1.51
17	Y	301	GRT	O49-S48	3.60	1.52	1.44
17	H	301	GRT	C7-C3	-3.55	1.42	1.51
17	V	301	GRT	C46-C47	3.17	1.55	1.52
17	H	301	GRT	C44-C41	-3.13	1.40	1.51
17	V	301	GRT	C44-C41	-3.10	1.40	1.51
17	Y	301	GRT	C47-S48	3.05	1.82	1.78
17	K	301	GRT	C44-C41	-2.95	1.41	1.51
17	H	301	GRT	C46-C47	2.94	1.55	1.52
17	Y	301	GRT	C44-C41	-2.88	1.41	1.51
17	Y	301	GRT	C46-C47	2.42	1.55	1.52
17	K	301	GRT	C47-S48	2.09	1.81	1.78
17	K	301	GRT	C46-C47	2.03	1.54	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	301	GRT	O50-S48-O49	-4.29	107.92	117.09
17	V	301	GRT	O50-S48-O49	-4.04	108.47	117.09
17	Y	301	GRT	O50-S48-O49	-3.74	109.10	117.09
17	K	301	GRT	O50-S48-O49	-3.67	109.25	117.09
17	Y	301	GRT	O50-S48-C47	3.26	110.62	108.34
17	H	301	GRT	O50-S48-C47	2.96	110.42	108.34
17	K	301	GRT	O50-S48-C47	2.92	110.39	108.34
17	Y	301	GRT	C33-C28-N27	-2.86	105.13	113.17
17	K	301	GRT	C33-C28-N27	-2.84	105.19	113.17
17	Y	301	GRT	O50-S48-C51	2.76	111.68	108.91
17	V	301	GRT	C37-C38-C39	2.73	126.33	120.91
17	H	301	GRT	C37-C38-C39	2.72	126.31	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	GRT	C37-C38-C39	2.67	126.21	120.91
17	V	301	GRT	C37-C38-C43	-2.62	115.70	120.91
17	Y	301	GRT	C37-C38-C39	2.55	125.97	120.91
17	H	301	GRT	C37-C38-C43	-2.54	115.87	120.91
17	V	301	GRT	C28-C33-N35	-2.50	110.13	116.10
17	Y	301	GRT	C37-C38-C43	-2.49	115.97	120.91
17	K	301	GRT	C37-C38-C43	-2.45	116.05	120.91
17	Y	301	GRT	C8-N9-N10	2.42	117.78	115.24
17	V	301	GRT	C51-S48-C47	2.31	114.10	105.21
17	H	301	GRT	C28-C33-N35	-2.26	110.70	116.10
17	H	301	GRT	C51-S48-C47	2.24	113.84	105.21
17	K	301	GRT	C8-N9-N10	2.21	117.56	115.24
17	V	301	GRT	C16-C15-N14	2.21	115.66	110.58
17	K	301	GRT	O50-S48-C51	2.17	111.08	108.91
17	H	301	GRT	C16-C15-N14	2.16	115.54	110.58
17	Y	301	GRT	C37-C36-N35	-2.15	106.26	110.39
17	K	301	GRT	C37-C36-N35	-2.06	106.42	110.39
17	H	301	GRT	O34-C33-N35	2.04	126.40	122.95

There are no chirality outliers.

All (17) torsion outliers are listed below:

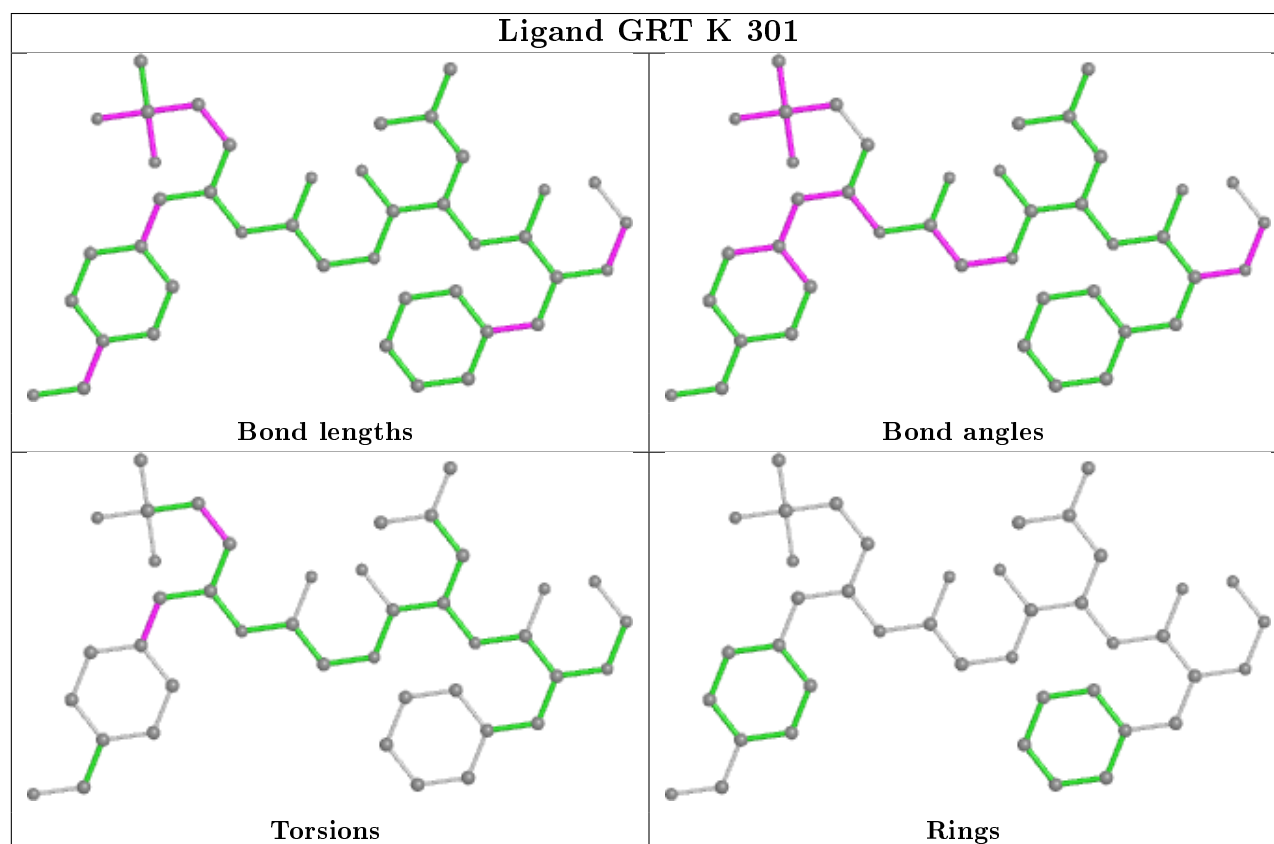
Mol	Chain	Res	Type	Atoms
17	K	301	GRT	C36-C37-C38-C39
17	Y	301	GRT	C36-C37-C38-C39
17	H	301	GRT	C36-C37-C38-C39
17	V	301	GRT	C36-C37-C38-C39
17	K	301	GRT	C36-C37-C38-C43
17	Y	301	GRT	C36-C37-C38-C43
17	H	301	GRT	C36-C37-C38-C43
17	V	301	GRT	C36-C37-C38-C43
17	H	301	GRT	C4-C3-C7-C8
17	H	301	GRT	C2-C3-C7-C8
17	V	301	GRT	C2-C3-C7-C8
17	V	301	GRT	C4-C3-C7-C8
17	H	301	GRT	C46-C47-S48-C51
17	V	301	GRT	C46-C47-S48-C51
17	K	301	GRT	C36-C46-C47-S48
17	Y	301	GRT	C36-C46-C47-S48
17	H	301	GRT	C12-C8-N9-N10

There are no ring outliers.

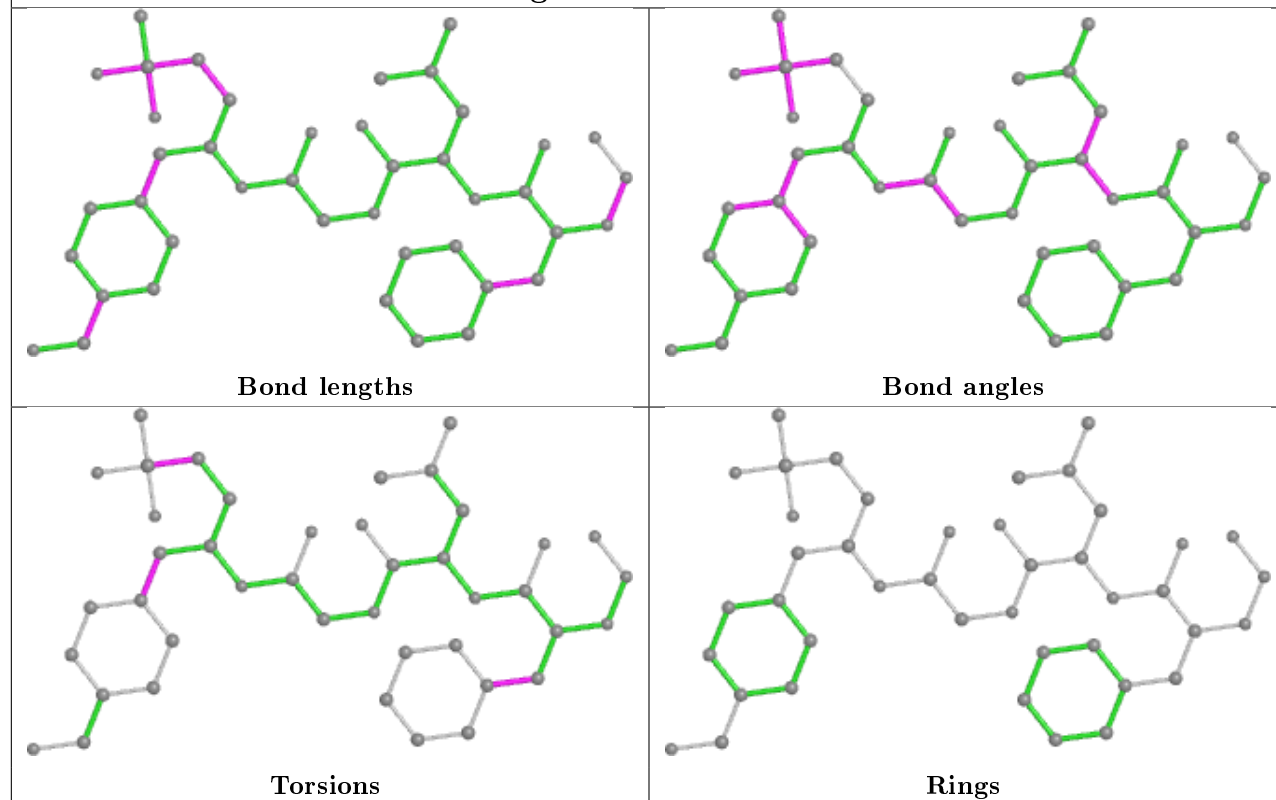
2 monomers are involved in 2 short contacts:

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

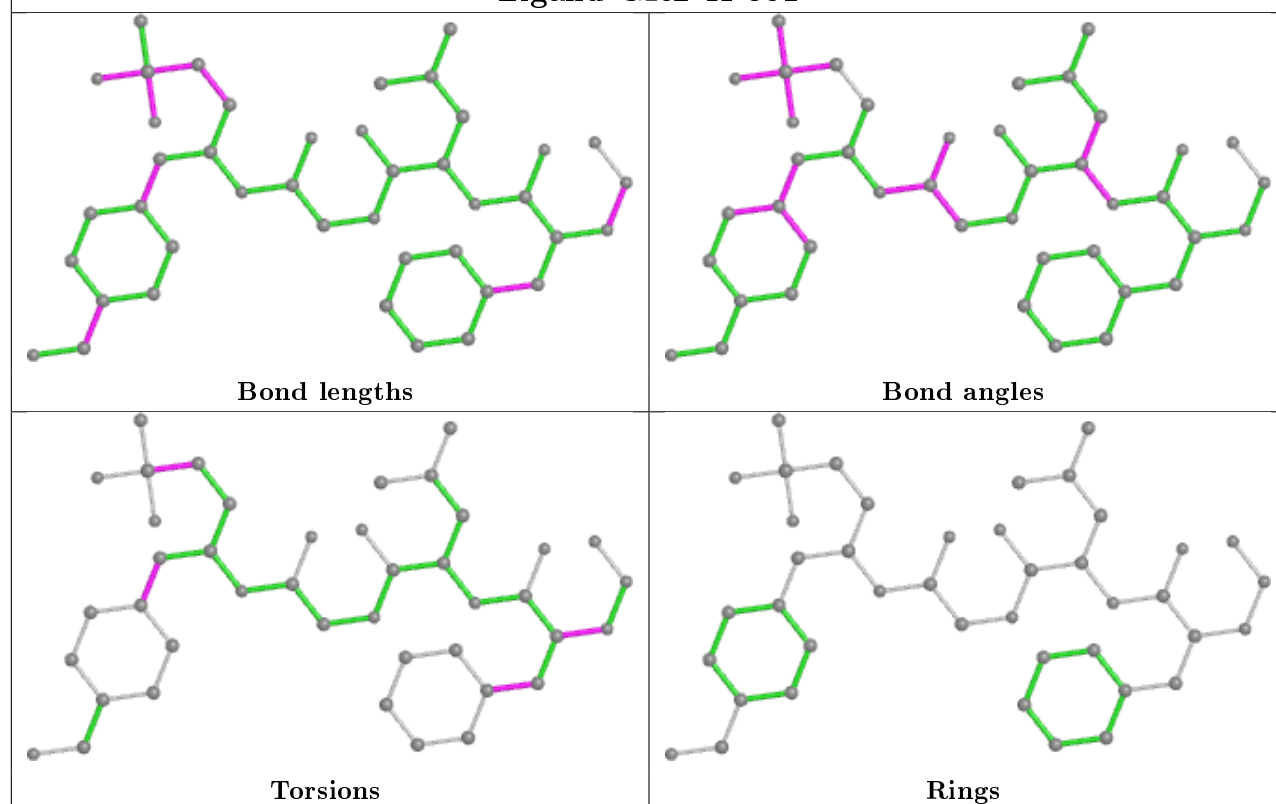
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

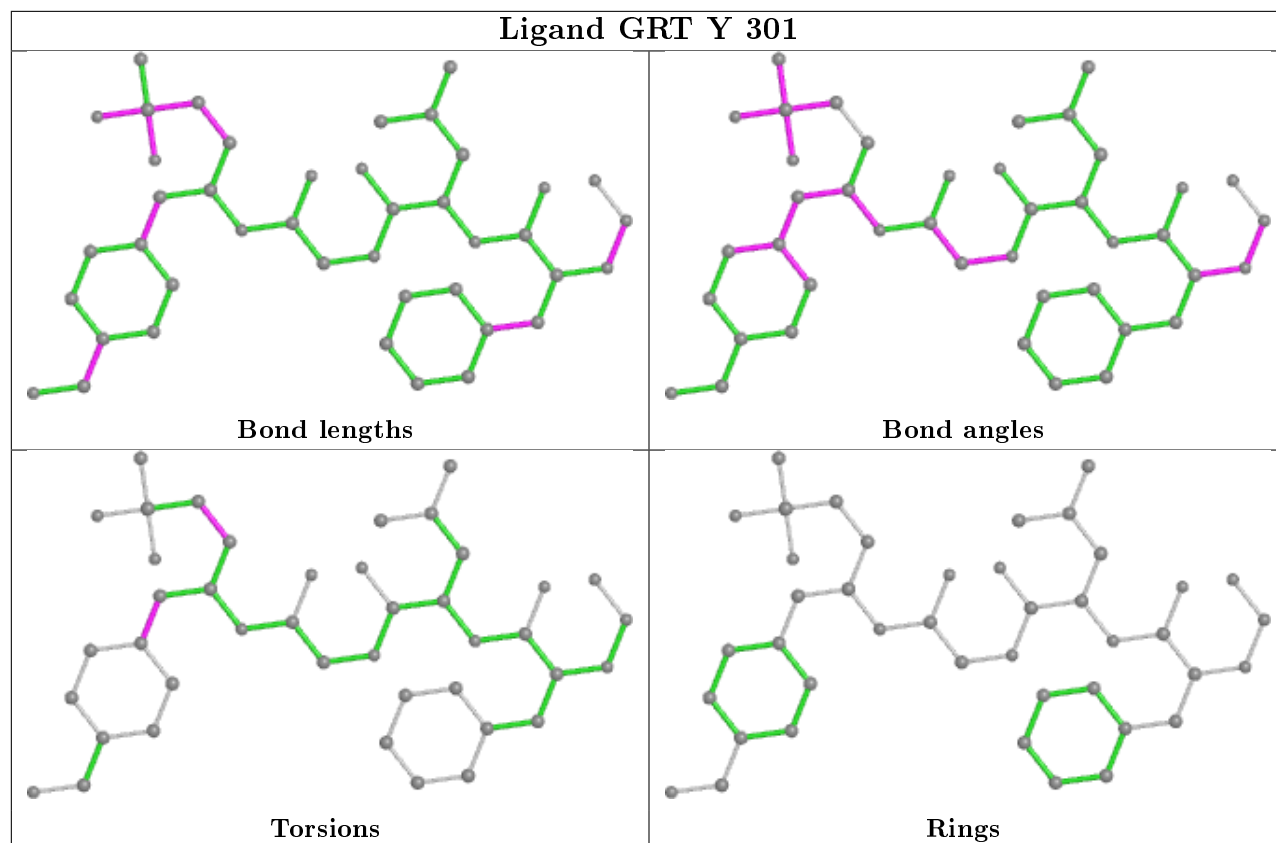


Ligand GRT V 301



Ligand GRT 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, 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%)	-0.20	9 (3%) 42 37	59, 79, 124, 171	0
1	O	250/250 (100%)	-0.05	14 (5%) 24 20	62, 88, 133, 173	0
2	B	244/258 (94%)	-0.10	13 (5%) 26 22	59, 84, 137, 188	0
2	P	244/258 (94%)	-0.10	12 (4%) 29 26	63, 87, 136, 184	0
3	C	240/254 (94%)	-0.04	19 (7%) 12 10	61, 89, 156, 183	0
3	Q	240/254 (94%)	0.16	26 (10%) 5 4	68, 102, 184, 218	0
4	D	235/260 (90%)	-0.22	4 (1%) 70 69	68, 92, 127, 173	0
4	R	235/260 (90%)	-0.16	9 (3%) 40 36	71, 93, 138, 185	0
5	E	231/234 (98%)	-0.10	10 (4%) 35 31	68, 95, 135, 183	0
5	S	231/234 (98%)	-0.03	13 (5%) 24 20	68, 96, 149, 183	0
6	F	243/288 (84%)	-0.29	8 (3%) 46 41	61, 86, 139, 168	0
6	T	243/288 (84%)	-0.19	9 (3%) 41 37	62, 90, 147, 182	0
7	G	241/252 (95%)	-0.27	7 (2%) 51 47	57, 79, 126, 173	0
7	U	241/252 (95%)	-0.27	5 (2%) 63 61	61, 79, 119, 149	0
8	H	222/232 (95%)	-0.13	7 (3%) 47 43	61, 79, 128, 163	0
8	V	222/232 (95%)	-0.08	8 (3%) 42 37	66, 85, 129, 170	0
9	I	204/205 (99%)	-0.50	1 (0%) 91 91	58, 75, 108, 135	0
9	W	204/205 (99%)	-0.46	4 (1%) 65 63	60, 78, 110, 143	0
10	J	195/198 (98%)	-0.36	2 (1%) 82 82	57, 77, 110, 153	0
10	X	195/198 (98%)	-0.35	4 (2%) 63 61	60, 79, 110, 166	0
11	K	212/212 (100%)	-0.41	2 (0%) 84 84	58, 76, 109, 137	0
11	Y	212/212 (100%)	-0.43	3 (1%) 75 75	58, 76, 109, 140	0
12	L	222/222 (100%)	-0.29	4 (1%) 68 67	58, 80, 120, 156	0
12	Z	222/222 (100%)	-0.29	8 (3%) 42 37	53, 78, 120, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.38	5 (2%)	63 61	54, 77, 108, 119	0
13	a	233/246 (94%)	-0.44	4 (1%)	70 69	52, 74, 104, 125	0
14	N	196/196 (100%)	-0.46	2 (1%)	82 82	45, 70, 105, 134	0
14	b	196/196 (100%)	-0.47	2 (1%)	82 82	48, 72, 107, 128	0
All	All	6336/6614 (95%)	-0.24	214 (3%)	45 40	45, 82, 134, 218	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	8.2
3	Q	49	THR	8.1
1	O	249	ALA	7.9
3	Q	236	GLN	7.8
10	X	1	MET	7.8
2	B	218	GLY	7.4
2	B	220	ASN	6.8
8	V	221	CYS	6.7
8	H	221	CYS	6.6
3	C	206	LYS	6.5
5	E	202	ASP	6.1
3	C	49	THR	6.1
2	P	220	ASN	5.9
8	V	222	ASP	5.7
1	O	231	LYS	5.7
8	H	222	ASP	5.4
2	B	219	ALA	5.3
10	X	194	ASP	5.2
10	J	1	MET	5.2
2	B	221	ASP	5.1
1	A	1	MET	5.0
2	P	218	GLY	5.0
2	P	221	ASP	5.0
3	Q	240	GLU	4.9
1	O	1	MET	4.7
3	Q	50	LEU	4.7
2	P	51	VAL	4.7
3	Q	239	GLN	4.7
1	A	231	LYS	4.7
2	P	59	ASP	4.5
3	C	239	GLN	4.5
1	A	229	THR	4.5

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Mol	Chain	Res	Type	RSRZ
3	Q	206	LYS	4.4
5	S	202	ASP	4.4
1	A	248	GLU	4.3
10	J	194	ASP	4.3
3	Q	48	SER	4.2
6	F	202	ASP	4.1
2	B	222	GLY	4.1
3	Q	180	LYS	4.1
9	I	1	SER	4.1
7	U	241	GLU	4.0
1	A	249	ALA	4.0
3	Q	141	ASP	3.9
2	B	217	LYS	3.8
7	G	241	GLU	3.8
8	V	215	GLU	3.7
12	Z	172	LEU	3.7
7	G	179	LYS	3.7
9	W	1	SER	3.7
6	T	230	ASP	3.5
5	S	207	VAL	3.5
4	R	217	GLN	3.4
13	a	1	THR	3.4
3	C	240	GLU	3.4
1	O	201	GLU	3.3
13	M	233	ILE	3.3
8	V	217	ILE	3.3
13	M	47	ASP	3.3
6	T	237	ASP	3.3
2	B	51	VAL	3.3
1	O	248	GLU	3.2
13	a	204	THR	3.2
12	L	172	LEU	3.2
13	M	1	THR	3.2
5	S	52	ALA	3.1
6	T	241	LYS	3.1
14	N	105	LYS	3.1
1	A	230	ASP	3.1
4	D	242	GLU	3.1
8	V	219	ASN	3.1
6	T	244	ASN	3.1
4	R	242	GLU	3.1
3	Q	140	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
10	X	193	ASP	3.0
12	L	167	LYS	3.0
1	A	250	LEU	3.0
7	G	181	LYS	3.0
11	Y	147	ASP	3.0
14	b	105	LYS	2.9
7	G	242	GLN	2.9
3	Q	237	GLU	2.9
12	Z	210	ASP	2.9
2	P	60	THR	2.8
6	F	181	GLU	2.8
3	C	205	ALA	2.8
3	C	238	LYS	2.8
4	R	230	GLU	2.7
5	E	3	ASN	2.7
5	S	194	GLU	2.7
1	A	228	PRO	2.7
3	Q	238	LYS	2.7
3	C	50	LEU	2.7
1	O	182	GLU	2.7
5	E	121	SER	2.7
3	Q	203	THR	2.7
14	b	195	GLN	2.7
12	L	174	TYR	2.7
5	E	227	GLU	2.7
11	Y	106	ARG	2.7
6	F	241	LYS	2.6
5	S	227	GLU	2.6
2	B	203	SER	2.6
3	C	216	ASP	2.6
9	W	131	GLU	2.6
11	K	212	GLY	2.6
5	E	180	LYS	2.6
8	V	206	PRO	2.6
4	R	125	LEU	2.6
5	S	225	ASP	2.6
13	a	47	ASP	2.6
12	Z	165	ASN	2.6
3	Q	233	GLN	2.6
6	F	178	HIS	2.6
2	B	59	ASP	2.6
3	Q	202	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
12	Z	116	GLU	2.6
2	P	225	TYR	2.6
5	S	50	ARG	2.5
7	U	222	ASP	2.5
3	Q	229	GLN	2.5
3	C	181	GLU	2.5
3	Q	187	GLU	2.5
5	S	54	GLU	2.5
7	G	208	GLU	2.5
5	E	233	ILE	2.5
4	D	239	GLU	2.5
4	D	47	THR	2.5
6	F	237	ASP	2.5
4	R	226	GLU	2.5
1	A	220	ASP	2.5
3	Q	181	GLU	2.5
6	F	205	GLU	2.5
3	Q	225	GLU	2.5
3	Q	184	ALA	2.5
11	Y	212	GLY	2.5
5	S	201	ARG	2.4
8	H	217	ILE	2.4
3	Q	232	THR	2.4
7	U	207	THR	2.4
2	P	222	GLY	2.4
8	H	207	ARG	2.4
9	W	192	ASP	2.4
3	C	235	GLU	2.4
6	F	244	ASN	2.4
1	O	250	LEU	2.4
3	C	236	GLN	2.4
6	T	207	ASP	2.4
7	U	181	LYS	2.4
2	P	232	GLN	2.3
12	Z	167	LYS	2.3
12	Z	1	GLN	2.3
6	T	205	GLU	2.3
2	B	225	TYR	2.3
8	H	215	GLU	2.3
3	Q	205	ALA	2.3
5	E	217	LYS	2.3
4	R	47	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	208	ASP	2.3
3	C	180	LYS	2.3
4	R	1	ASP	2.3
5	S	180	LYS	2.3
1	O	221	LEU	2.3
8	H	219	ASN	2.3
2	B	235	LYS	2.3
1	O	245	ASP	2.3
8	V	207	ARG	2.3
1	O	229	THR	2.3
4	R	143	ASP	2.3
13	M	204	THR	2.2
5	E	207	VAL	2.2
1	O	230	ASP	2.2
5	S	51	ASN	2.2
11	K	151	GLU	2.2
13	M	216	ASN	2.2
5	E	225	ASP	2.2
2	B	232	GLN	2.2
5	E	54	GLU	2.2
7	U	203	ASP	2.2
3	C	225	GLU	2.2
12	L	165	ASN	2.2
3	Q	175	LYS	2.2
3	Q	235	GLU	2.1
5	S	218	ASP	2.1
3	Q	223	SER	2.1
3	C	203	THR	2.1
3	C	1	GLY	2.1
1	O	181	ASP	2.1
3	C	47	ARG	2.1
8	V	145	ASP	2.1
14	N	104	ASP	2.1
13	a	233	ILE	2.1
4	R	239	GLU	2.1
12	Z	18	GLU	2.1
6	T	53	LYS	2.1
8	H	213	LEU	2.1
1	O	228	PRO	2.1
3	Q	60	SER	2.1
6	T	215	CYS	2.1
4	D	125	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
6	F	166	GLN	2.1
5	S	30	GLN	2.1
12	Z	174	TYR	2.1
2	P	141	ASP	2.0
3	C	187	GLU	2.0
1	O	227	ILE	2.0
3	C	139	ARG	2.0
10	X	72	ASP	2.0
3	C	202	GLN	2.0
6	T	177	ASP	2.0
7	G	188	GLU	2.0
9	W	133	LYS	2.0
2	P	182	ASP	2.0
7	G	222	ASP	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 carbohydrates 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.

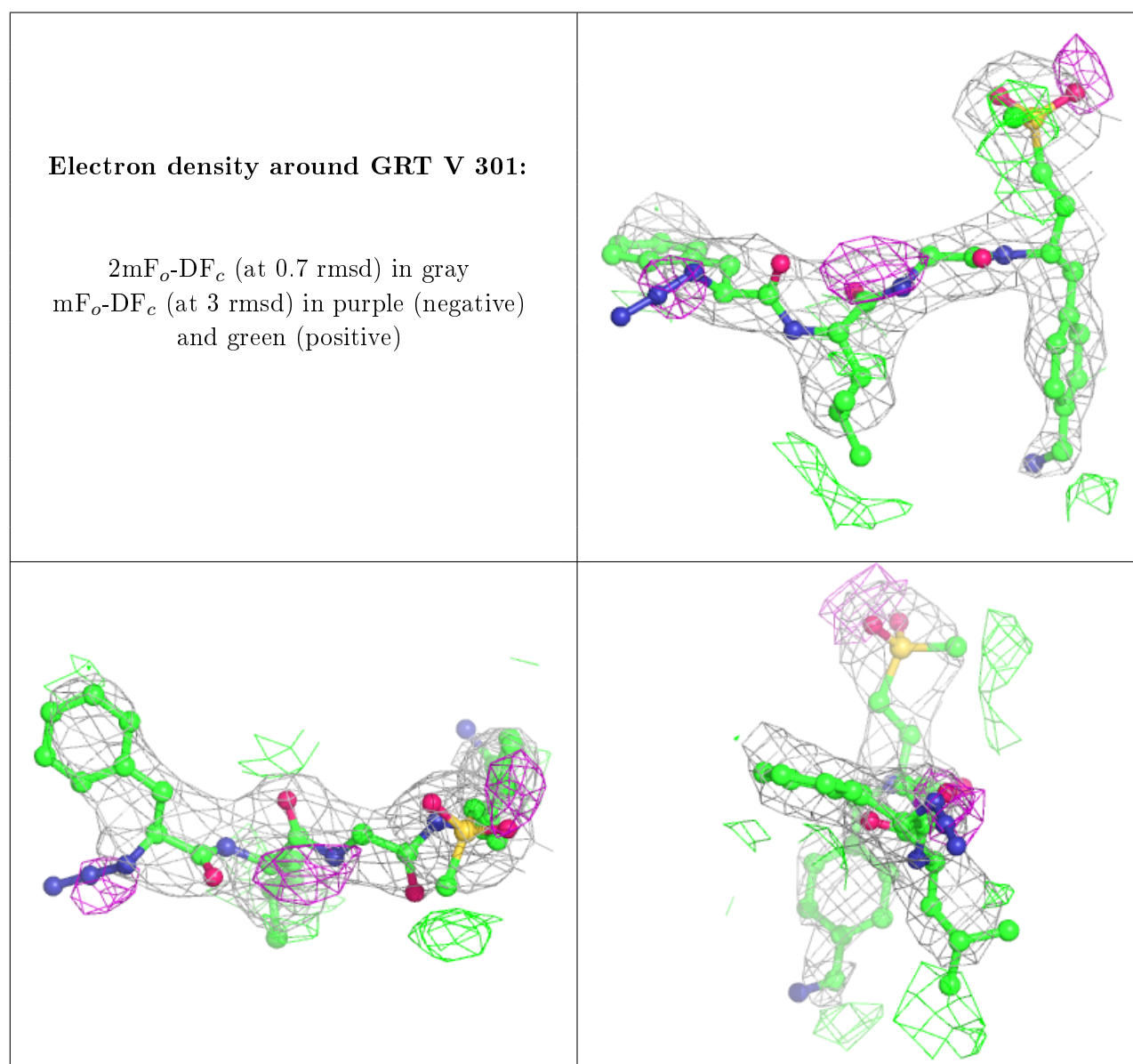
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	GRT	V	301	42/42	0.85	0.29	94,107,121,129	0
17	GRT	H	301	42/42	0.88	0.27	96,104,122,128	0
17	GRT	K	301	42/42	0.91	0.22	77,92,111,120	0
17	GRT	Y	301	42/42	0.91	0.22	81,97,115,117	0
15	MG	I	301	1/1	0.94	0.41	102,102,102,102	0
15	MG	I	302	1/1	0.96	0.09	88,88,88,88	0
15	MG	G	301	1/1	0.96	0.10	74,74,74,74	0
15	MG	K	302	1/1	0.97	0.11	88,88,88,88	0
15	MG	Z	301	1/1	0.98	0.19	78,78,78,78	0

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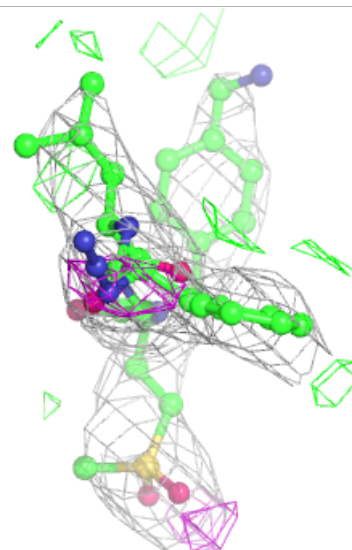
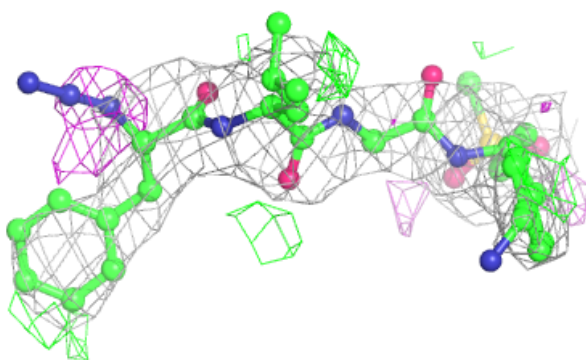
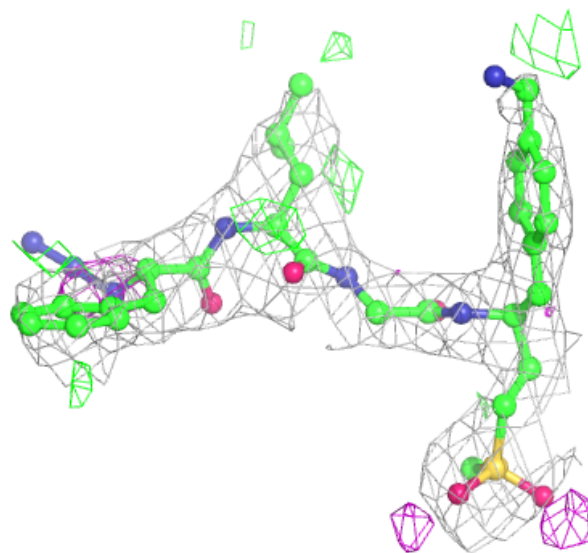
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	CL	G	302	1/1	0.98	0.28	68,68,68,68	0
15	MG	X	201	1/1	0.98	0.23	58,58,58,58	0
15	MG	N	201	1/1	0.99	0.06	55,55,55,55	0
15	MG	L	301	1/1	0.99	0.13	87,87,87,87	0
16	CL	U	301	1/1	0.99	0.30	64,64,64,64	0

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.



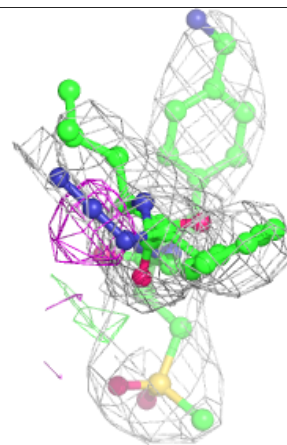
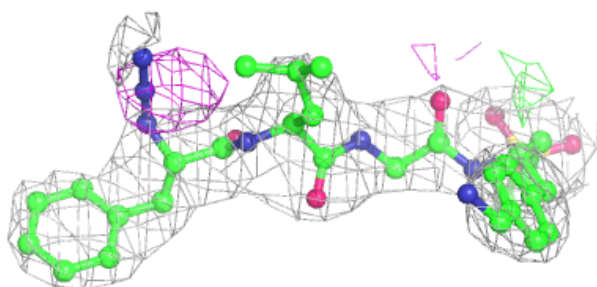
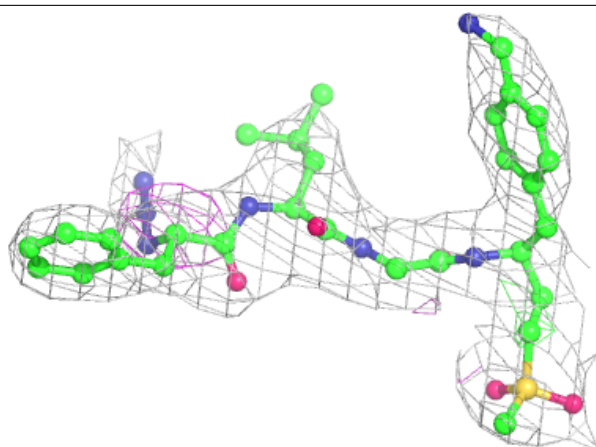
Electron density around GRT H 301:

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



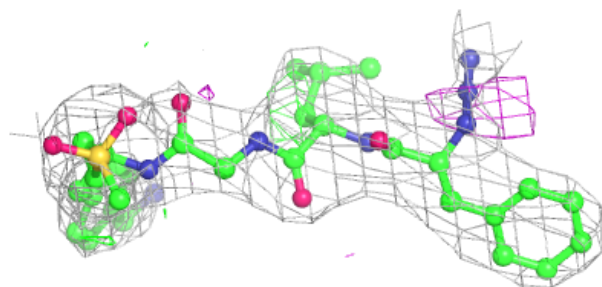
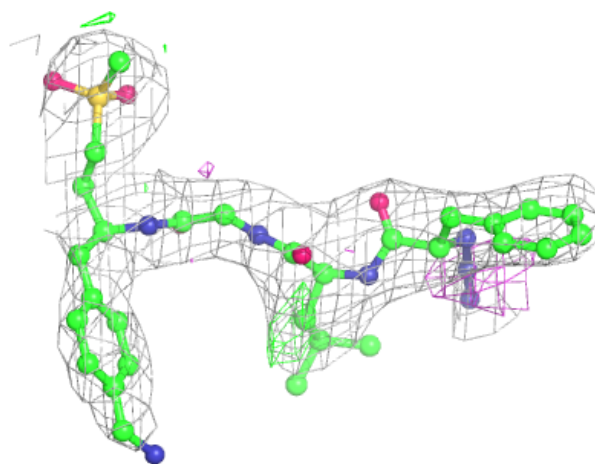
Electron density around GRT K 301:

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



Electron density around GRT Y 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 [i](#)

There are no such residues in this entry.