



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 01:10 pm BST

PDB ID : 6HUB
Title : Yeast 20S proteasome with human beta2c (S171G) in complex with 16
Authors : Huber, E.M.; Groll, M.
Deposited on : 2018-10-05
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

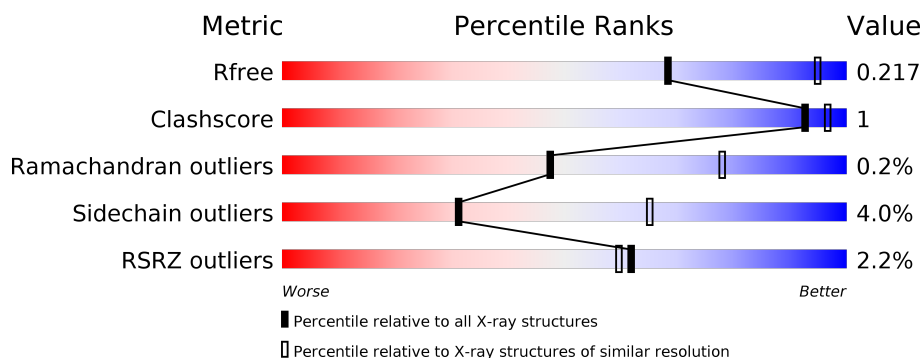
1 Overall quality at a glance

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>2%</div> <div> <div></div> <div>93%</div> <div>• •</div> </div> </div>
1	O	250	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>• •</div> </div> </div>
2	B	258	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>6% • 5%</div> </div> </div>
2	P	258	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>5% • 5%</div> </div> </div>
3	C	254	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>7% • 6%</div> </div> </div>
3	Q	254	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>6% • 6%</div> </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	234	
8	V	234	
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 19 unique types of molecules in this entry. The entry contains 49725 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	240	Total	C	N	O	S	0	0	0
			1842	1171	305	362	4			
1	O	240	Total	C	N	O	S	0	0	0
			1842	1171	305	362	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-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	219	Total	C	N	O	S	0	0	0
			1648	1038	282	316	12			
8	V	219	Total	C	N	O	S	0	0	0
			1648	1038	282	316	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	171	GLY	SER	engineered mutation	UNP Q99436
V	171	GLY	SER	engineered mutation	UNP Q99436

- 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			
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	224	Total	C	N	O	S	0	0	0
			1753	1108	300	338	7			
13	a	224	Total	C	N	O	S	0	0	0
			1753	1108	300	338	7			

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

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

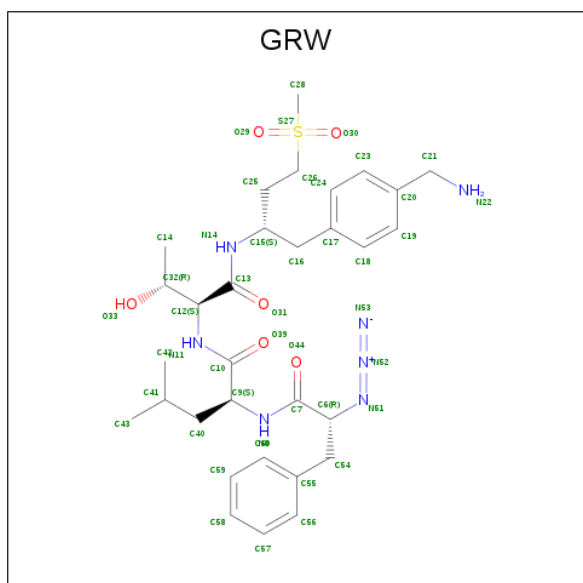
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

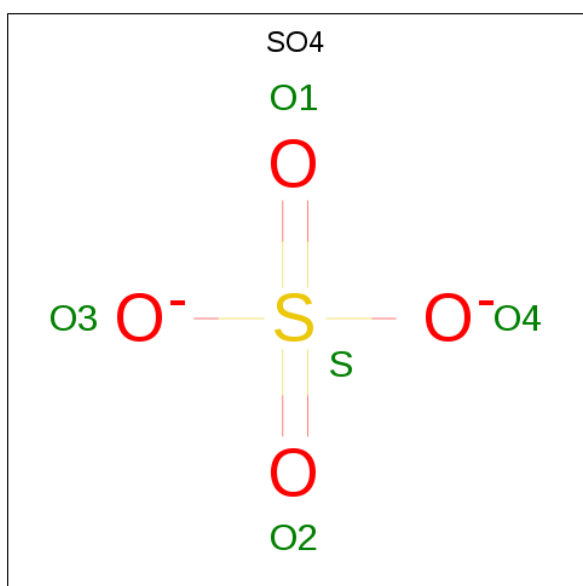
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is (2 {S})- {N}-[(2 {S},3 {R})-1-[(2 {S})-1-[4-(aminomethyl)phenyl]-4-methylsulfonyl-butan-2-yl]amino]-3-oxidanyl-1-oxidanylidene-butan-2-yl]-2-[[{(2 {R})-2-azido-3-phenyl-propanoyl]amino]-4-methyl-pentanamide (three-letter code: GRW) (formula: C₃₁H₄₅N₇O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	C	N	O	S	0	0
			45	31	7	6	1		
17	K	1	Total	C	N	O	S	0	0
			45	31	7	6	1		
17	V	1	Total	C	N	O	S	0	0
			45	31	7	6	1		
17	Y	1	Total	C	N	O	S	0	0
			45	31	7	6	1		

- Molecule 18 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	N	1	Total	O	S	0	0
			5	4	1		
18	b	1	Total	O	S	0	0
			5	4	1		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	18	Total	O	0	0
			18	18		
19	B	23	Total	O	0	0
			23	23		
19	C	16	Total	O	0	0
			16	16		
19	D	23	Total	O	0	0
			23	23		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	E	18	Total O 18 18	0	0
19	F	10	Total O 10 10	0	0
19	G	26	Total O 26 26	0	0
19	H	20	Total O 20 20	0	0
19	I	19	Total O 19 19	0	0
19	J	31	Total O 31 31	0	0
19	K	24	Total O 24 24	0	0
19	L	26	Total O 26 26	0	0
19	M	30	Total O 30 30	0	0
19	N	24	Total O 24 24	0	0
19	O	4	Total O 4 4	0	0
19	P	21	Total O 21 21	0	0
19	Q	16	Total O 16 16	0	0
19	R	19	Total O 19 19	0	0
19	S	15	Total O 15 15	0	0
19	T	15	Total O 15 15	0	0
19	U	24	Total O 24 24	0	0
19	V	16	Total O 16 16	0	0
19	W	19	Total O 19 19	0	0
19	X	33	Total O 33 33	0	0
19	Y	25	Total O 25 25	0	0

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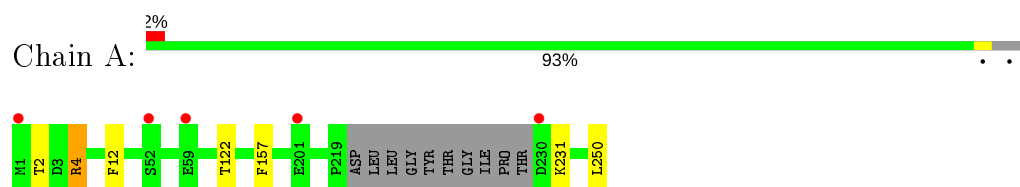
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	Z	20	Total 20	O 20	0	0
19	a	34	Total 34	O 34	0	0
19	b	20	Total 20	O 20	0	0

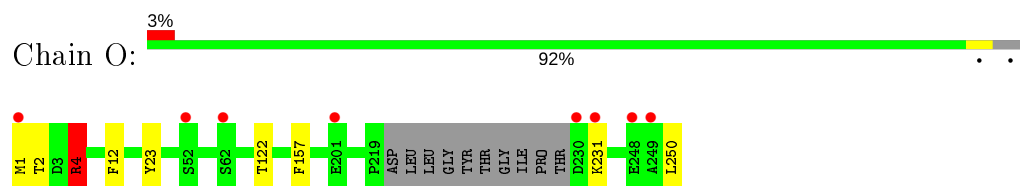
3 Residue-property plots [i](#)

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.

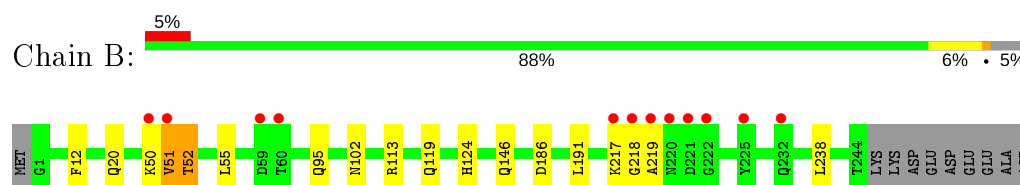
- Molecule 1: Proteasome subunit alpha type-2



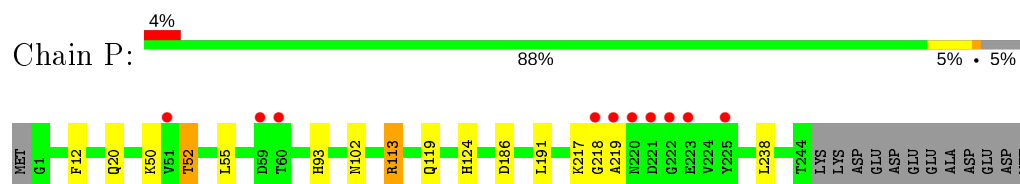
- Molecule 1: Proteasome subunit alpha type-2



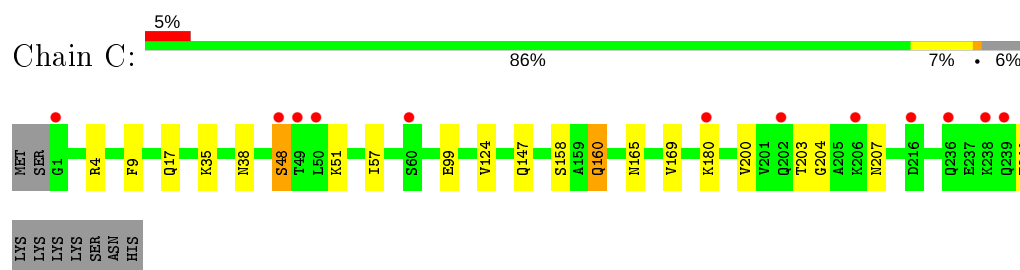
- Molecule 2: Proteasome subunit alpha type-3



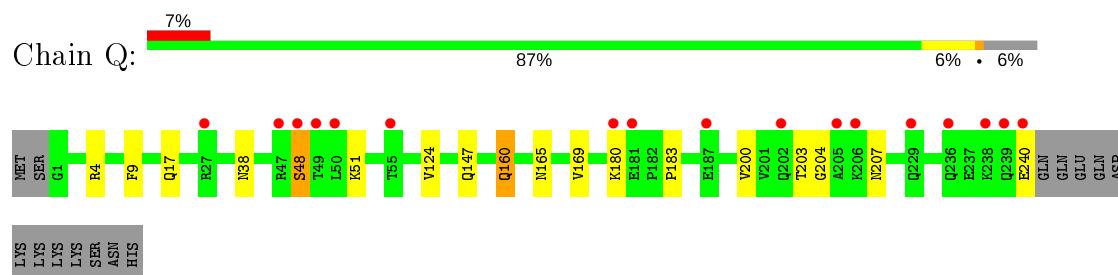
- Molecule 2: Proteasome subunit alpha type-3



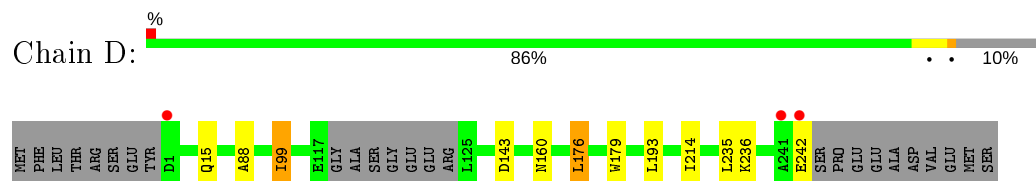
- Molecule 3: Proteasome subunit alpha type-4



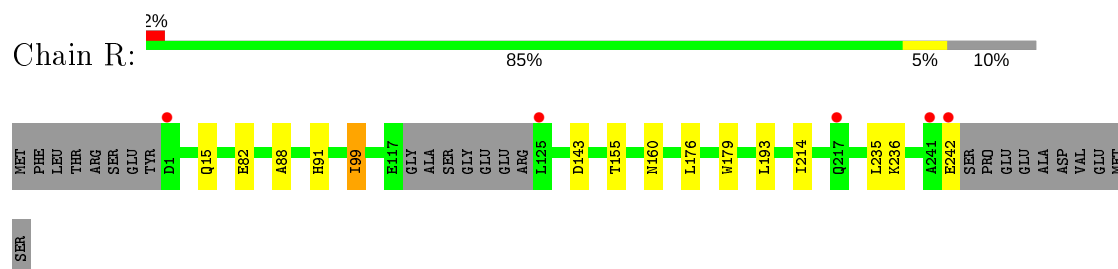
- Molecule 3: Proteasome subunit alpha type-4



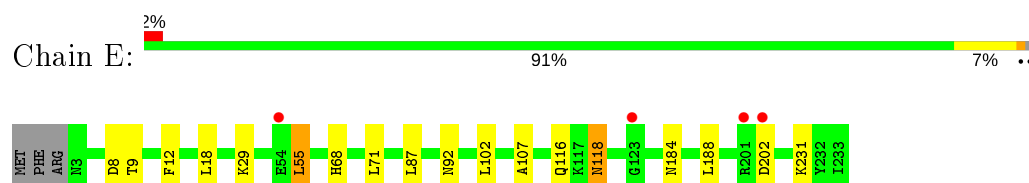
- Molecule 4: Proteasome subunit alpha type-5



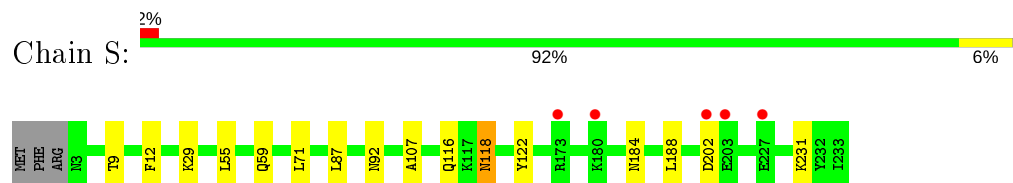
- Molecule 4: Proteasome subunit alpha type-5



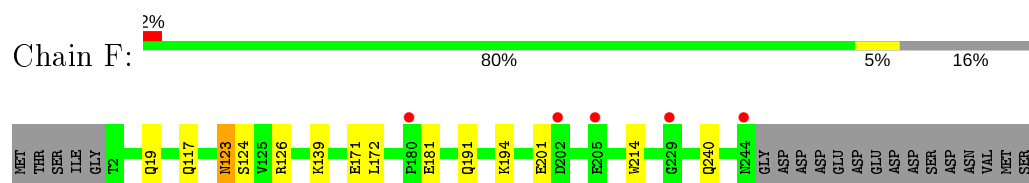
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 5: Proteasome subunit alpha type-6

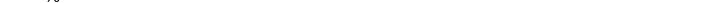


- Molecule 6: Probable proteasome subunit alpha type-7



ALA PRO VAL ALA THR ASN ALA ASN ALA THR THR ASP GLN GLU GLY ASP ILE HIS LEU GLU

- Molecule 6: Probable proteasome subunit alpha type-7

Chain T:  80% 16%

MET	TER	TER	IIE	GLY	T2	Q19	Q117	Y122	M23	S124	K139	G155	E171	L172	E181	E201	W214	Q240	E241	M244	GLY	ASP	ASP	ASP	ASP	GLU	GLU	GLU	GLU	ASP	ASP	ASP	ASP	VAL	MET	TER	TER	ASP	ASP	GLU	GLU	ASP	ASP	ALA	ALA	PRO	VAL	VAL	ALA	TER	TER	ASP	ASP	ALA	ALA
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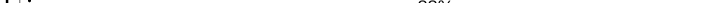
ALA
THR
THR
ASP
GLN
GLU
GLY
ASP
ILE
HIS
LEU
GLU

- Molecule 7: Proteasome subunit alpha type-1

Chain G: 2% 88% 7% .

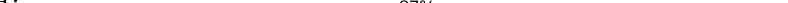
Amino Acid	Count
MET	1
SER	1
GLY	1
ALA	1
ALA	1
ALA	1
SER	1
SER	1
ALA	1
ALA	1
G2	1
E13	1
F23	1
T26	1
P61	1
R68	1
N83	1
Y99	1
D106	1
L115	1
S116	1
Q117	1
R122	1
M125	1
Y146	1
Y154	1
Q167	1
T171	1
E188	1
E208	1
R235	1
L236	1
E241	1
Q242	1
ASP	1

- Molecule 7: Proteasome subunit alpha type-1

Chain U:  88% 8% 4%

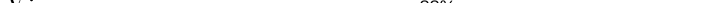
Category	Value	Color
NET	100	Grey
SER	95	Green
GLY	90	Yellow
ALA	85	Yellow
ALA	80	Yellow
ALA	75	Yellow
ALA	70	Yellow
SER	65	Green
ALA	60	Yellow
ALA	55	Yellow
G2	50	Green
P12	45	Yellow
E13	40	Yellow
F23	35	Yellow
T26	30	Yellow
P51	25	Red
T59	20	Yellow
R68	15	Orange
N83	10	Yellow
Y99	5	Yellow
D106	0	Yellow
L115	-5	Yellow
L116	-10	Green
Q117	-15	Green
R122	-20	Yellow
M125	-25	Yellow
Y146	-30	Yellow
Y154	-35	Yellow
Q167	-40	Yellow
T171	-45	Yellow
K181	-50	Red
E208	-55	Yellow
R235	-60	Yellow
L236	-65	Yellow
Q242	-70	Red

- Molecule 8: Proteasome subunit beta type-7

Chain H:  3% 87% 6% 6%

Category	Number of genes
T1	1
L14	1
M24	1
V25	1
S32	1
D61	1
T65	1
T78	1
L98	1
L122	1
L132	1
R143	1
N161	1
K194	1
K195	1
K196	1
T197	1
R201	1
P248	1
L219	1
L19	1
L1E	1
GLU	1
VAL	1
LEU	1
GLU	1
THR	1
VAL	1
GLN	1
THR	1
MET	1
ASP	1
THR	1

- Molecule 8: Proteasome subunit beta type-7

Chain V:  2% 88% 5% 6%

Category	Value
T1	0.00
T2	0.00
L14	0.00
M24	0.00
V25	0.00
A50	0.00
T78	0.00
L98	0.00
L132	0.00
R143	0.00
M181	0.00
D184	0.00
F185	0.00
L186	0.00
K194	0.00
K195	0.00
G196	0.00
T197	0.00
R201	0.00
L219	0.00
GLU	0.00
ILE	0.00
GLU	0.00
VAL	0.00
LEU	0.00
GLU	0.00
GLU	0.00
THR	0.00
VAL	0.00
GLN	0.00
THR	0.00
NET	0.00
ASP	0.00
THR	0.00

- Molecule 9: Proteasome subunit beta type-3


Chain I:  95% .

- Molecule 9: Proteasome subunit beta type-3

Chain W:  95% ..




- Molecule 10: Proteasome subunit beta type-4

Chain J:  90% 8% ...




- Molecule 10: Proteasome subunit beta type-4

Chain X:  90% 7% ...




- Molecule 11: Proteasome subunit beta type-5

Chain K:  90% 9% ..

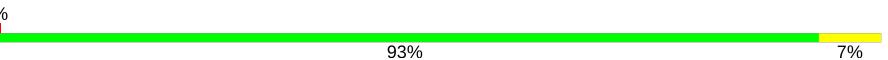


- Molecule 11: Proteasome subunit beta type-5

Chain Y:  87% 12% ..




- Molecule 12: Proteasome subunit beta type-6

Chain L:  93% 7%

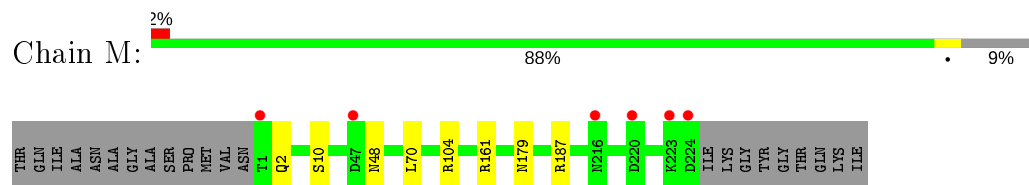


- Molecule 12: Proteasome subunit beta type-6

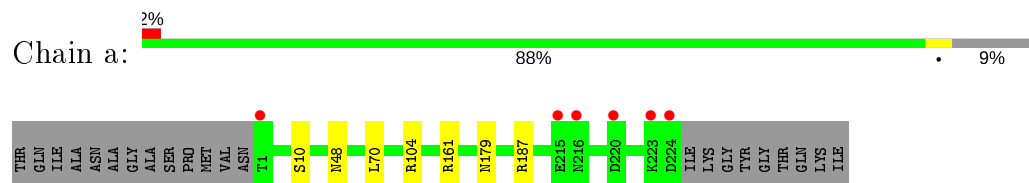
Chain Z:  92% 7%



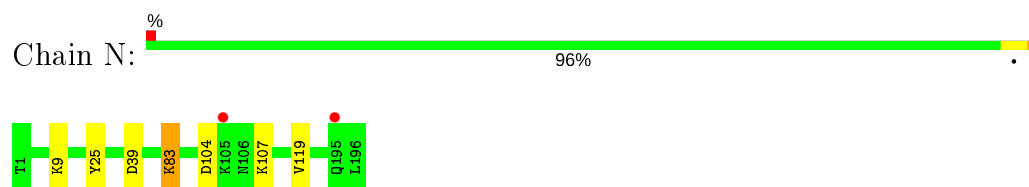
- Molecule 13: Proteasome subunit beta type-7



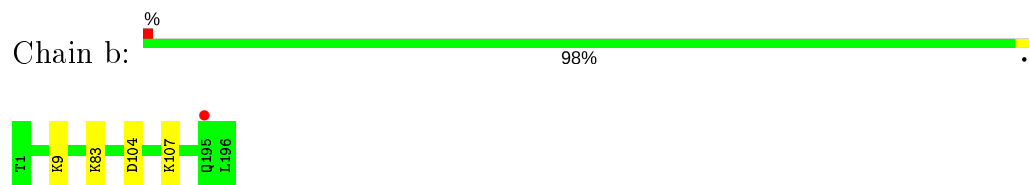
- Molecule 13: Proteasome subunit beta type-7



- 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	135.16Å 299.38Å 144.81Å 90.00° 113.09° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (15.00-2.90) 98.9 (15.00-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.184 , 0.212 0.191 , 0.217	Depositor DCC
R_{free} test set	11445 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	49725	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: GRW, MG, SO4, 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	0.38	0/1876	0.81	3/2535 (0.1%)
1	O	0.38	0/1876	0.82	4/2535 (0.2%)
2	B	0.40	0/1934	0.64	1/2618 (0.0%)
2	P	0.39	0/1934	0.63	0/2618
3	C	0.39	0/1910	0.64	0/2586
3	Q	0.38	0/1910	0.64	0/2586
4	D	0.37	0/1837	0.60	0/2475
4	R	0.37	0/1837	0.60	0/2475
5	E	0.38	0/1800	0.59	0/2433
5	S	0.37	0/1800	0.59	0/2433
6	F	0.38	0/1932	0.56	0/2609
6	T	0.37	0/1932	0.56	0/2609
7	G	0.37	0/1945	0.76	3/2634 (0.1%)
7	U	0.38	0/1945	0.81	3/2634 (0.1%)
8	H	0.37	0/1675	0.88	3/2267 (0.1%)
8	V	0.36	0/1675	0.87	3/2267 (0.1%)
9	I	0.38	0/1611	0.61	0/2174
9	W	0.37	0/1611	0.60	0/2174
10	J	0.38	0/1589	0.66	2/2142 (0.1%)
10	X	0.37	0/1589	0.66	2/2142 (0.1%)
11	K	0.36	0/1681	0.63	0/2274
11	Y	0.36	0/1681	0.63	0/2274
12	L	0.37	0/1795	0.61	0/2420
12	Z	0.37	0/1795	0.60	0/2420
13	M	0.39	0/1783	0.64	0/2420
13	a	0.39	0/1783	0.65	0/2420
14	N	0.36	0/1541	0.59	0/2087
14	b	0.36	0/1541	0.58	0/2087
All	All	0.37	0/49818	0.67	24/67348 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	O	0	1
7	U	0	1
8	V	0	1
All	All	0	4

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	68	ARG	NE-CZ-NH2	-22.56	109.02	120.30
1	A	4	ARG	NE-CZ-NH2	-20.90	109.85	120.30
1	O	4	ARG	NE-CZ-NH1	-20.29	110.16	120.30
8	V	143	ARG	NE-CZ-NH2	-19.96	110.32	120.30
8	H	143	ARG	NE-CZ-NH1	-18.93	110.83	120.30
7	G	68	ARG	NE-CZ-NH1	-17.77	111.42	120.30
8	H	143	ARG	NE-CZ-NH2	16.88	128.74	120.30
7	G	68	ARG	NE-CZ-NH2	15.80	128.20	120.30
1	O	4	ARG	NE-CZ-NH2	15.56	128.08	120.30
1	A	4	ARG	NE-CZ-NH1	14.69	127.64	120.30
8	V	143	ARG	NE-CZ-NH1	13.88	127.24	120.30
7	U	68	ARG	CD-NE-CZ	11.79	140.11	123.60
7	U	68	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	O	4	ARG	CD-NE-CZ	10.05	137.68	123.60
8	V	143	ARG	CD-NE-CZ	10.03	137.64	123.60
1	A	4	ARG	CD-NE-CZ	9.83	137.37	123.60
8	H	143	ARG	CD-NE-CZ	8.14	134.99	123.60
7	G	68	ARG	CD-NE-CZ	7.52	134.13	123.60
1	O	4	ARG	CG-CD-NE	6.25	124.93	111.80
10	J	23	ARG	NE-CZ-NH2	5.80	123.20	120.30
10	X	23	ARG	NE-CZ-NH2	5.70	123.15	120.30
2	B	51	VAL	CG1-CB-CG2	5.55	119.78	110.90
10	J	23	ARG	CG-CD-NE	5.51	123.38	111.80
10	X	23	ARG	CG-CD-NE	5.46	123.26	111.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	ARG	Sidechain
1	O	4	ARG	Sidechain
7	U	68	ARG	Sidechain
8	V	143	ARG	Sidechain

5.2 Too-close contacts

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	1842	0	1855	1	0
1	O	1842	0	1855	4	0
2	B	1904	0	1904	6	0
2	P	1904	0	1904	6	0
3	C	1881	0	1895	11	0
3	Q	1881	0	1895	8	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	6	0
5	E	1773	0	1775	9	0
5	S	1773	0	1775	8	0
6	F	1892	0	1883	5	0
6	T	1892	0	1883	5	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	6	0
8	H	1648	0	1672	7	0
8	V	1648	0	1672	7	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	12	0
10	X	1561	0	1569	11	0
11	K	1644	0	1594	11	0
11	Y	1644	0	1594	14	0
12	L	1757	0	1711	8	0
12	Z	1757	0	1711	9	0
13	M	1753	0	1754	1	0
13	a	1753	0	1754	0	0
14	N	1512	0	1481	3	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	45	0	0	1	0
17	K	45	0	0	0	0
17	V	45	0	0	2	0
17	Y	45	0	0	0	0
18	N	5	0	0	0	0
18	b	5	0	0	0	0
19	A	18	0	0	0	0
19	B	23	0	0	0	0
19	C	16	0	0	0	0
19	D	23	0	0	0	0
19	E	18	0	0	0	0
19	F	10	0	0	0	0
19	G	26	0	0	0	0
19	H	20	0	0	0	0
19	I	19	0	0	0	0
19	J	31	0	0	1	0
19	K	24	0	0	0	0
19	L	26	0	0	0	0
19	M	30	0	0	1	0
19	N	24	0	0	0	0
19	O	4	0	0	0	0
19	P	21	0	0	2	0
19	Q	16	0	0	0	0
19	R	19	0	0	0	0
19	S	15	0	0	0	0
19	T	15	0	0	0	0
19	U	24	0	0	0	0
19	V	16	0	0	0	0
19	W	19	0	0	0	0
19	X	33	0	0	1	0
19	Y	25	0	0	0	0
19	Z	20	0	0	0	0
19	a	34	0	0	0	0
19	b	20	0	0	0	0
All	All	49725	0	48730	132	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 (132) 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)
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.19	0.87
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.22	0.85
2:P:93:HIS:HB3	19:P:301:HOH:O	1.87	0.74
11:Y:77:ALA:O	11:Y:121:ARG:NH1	2.24	0.71
11:K:77:ALA:O	11:K:121:ARG:NH1	2.24	0.70
8:V:1:THR:N	17:V:301:GRW:O30	2.23	0.70
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.56	0.70
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.57	0.69
1:O:12:PHE:H	2:P:20:GLN:HE22	1.43	0.65
5:E:12:PHE:H	6:F:19:GLN:HE22	1.48	0.61
1:A:12:PHE:H	2:B:20:GLN:HE22	1.49	0.61
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.64	0.61
7:G:23:PHE:O	7:G:26:THR:HB	2.01	0.60
7:G:68:ARG:NH1	14:N:39:ASP:OD2	2.34	0.60
2:B:12:PHE:H	3:C:17:GLN:HE22	1.47	0.59
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.67	0.59
5:E:92:ASN:ND2	12:L:70:ASN:HD21	1.96	0.59
5:E:92:ASN:HD21	12:L:70:ASN:ND2	1.99	0.58
10:J:25:ILE:O	10:X:139:TYR:OH	2.21	0.58
11:K:130:GLY:O	11:K:133:GLN:HG2	2.04	0.57
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.17	0.57
11:Y:130:GLY:O	11:Y:133:GLN:HG2	2.05	0.57
7:U:23:PHE:O	7:U:26:THR:HB	2.04	0.56
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	1.99	0.55
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.20	0.55
5:S:12:PHE:H	6:T:19:GLN:HE22	1.54	0.54
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	1.97	0.53
10:J:139:TYR:OH	10:X:25:ILE:O	2.25	0.53
3:C:48:SER:HB2	3:C:207:ASN:HD21	1.74	0.53
10:X:174:MET:HB2	19:X:218:HOH:O	2.10	0.52
7:G:99:TYR:O	8:H:78:THR:HB	2.10	0.52
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.75	0.52
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.74	0.51
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.92	0.51
11:Y:145:LYS:HG3	11:Y:148:LEU:HD12	1.93	0.51
3:Q:48:SER:HB2	3:Q:207:ASN:HD21	1.75	0.51
11:K:210:VAL:HA	9:W:37:ASN:OD1	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.93	0.50
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.76	0.50
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.93	0.50
11:K:145:LYS:HG3	11:K:148:LEU:HD12	1.94	0.50
6:T:123:ASN:HD22	6:T:124:SER:N	2.09	0.50
6:F:123:ASN:HD22	6:F:124:SER:N	2.10	0.50
2:P:113:ARG:NE	19:P:301:HOH:O	2.33	0.49
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.94	0.49
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.45	0.49
8:H:51:ASP:O	8:H:55:THR:OG1	2.23	0.49
10:J:139:TYR:CE1	11:Y:134:THR:HG22	2.47	0.49
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.95	0.48
11:K:176:ASN:ND2	11:K:190:ASN:HD22	2.11	0.48
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.95	0.48
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.78	0.48
10:X:23:ARG:HG2	10:X:23:ARG:HH21	1.78	0.48
11:Y:51:ASP:HB3	11:Y:97:MET:HE2	1.95	0.48
11:Y:105:THR:OG1	11:Y:108:GLU:HG3	2.14	0.47
11:K:105:THR:OG1	11:K:108:GLU:HG3	2.14	0.47
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.95	0.47
13:M:2:GLN:NE2	19:M:301:HOH:O	2.47	0.47
8:H:132:LEU:HD22	14:N:25:TYR:CE1	2.50	0.47
8:V:219:LEU:HD21	9:W:194:VAL:HG23	1.97	0.47
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.45	0.46
11:K:51:ASP:HB3	11:K:97:MET:HE2	1.96	0.46
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.97	0.46
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.64	0.46
17:V:301:GRW:C14	17:V:301:GRW:C10	2.93	0.46
10:J:23:ARG:CG	10:J:23:ARG:HH21	2.29	0.46
9:W:37:ASN:HB3	9:W:182:TRP:CE3	2.50	0.46
5:E:118:ASN:N	5:E:118:ASN:HD22	2.14	0.46
10:X:23:ARG:CG	10:X:23:ARG:HH21	2.29	0.46
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.97	0.46
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.80	0.46
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.65	0.45
10:J:23:ARG:HH21	10:J:23:ARG:HG2	1.81	0.45
9:I:37:ASN:OD1	11:Y:210:VAL:HA	2.16	0.45
3:Q:48:SER:HB2	3:Q:207:ASN:ND2	2.32	0.45
3:C:48:SER:HB2	3:C:207:ASN:ND2	2.32	0.45
6:T:123:ASN:C	6:T:123:ASN:HD22	2.19	0.45
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:219:LEU:HD11	9:I:194:VAL:HG23	1.99	0.45
8:H:25:VAL:HG11	9:I:146:PHE:CD2	2.51	0.45
9:I:37:ASN:HB3	9:I:182:TRP:CE3	2.51	0.45
8:V:25:VAL:HG11	9:W:146:PHE:CD2	2.52	0.45
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.51	0.44
11:Y:50:ALA:CB	12:Z:128:VAL:HG23	2.48	0.44
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.00	0.44
6:F:123:ASN:C	6:F:123:ASN:HD22	2.21	0.44
11:K:134:THR:HG22	10:X:139:TYR:CE1	2.53	0.44
12:L:8:ASN:HA	12:L:30:ILE:O	2.17	0.44
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.00	0.43
8:V:1:THR:HG22	8:V:2:THR:N	2.33	0.43
4:R:82:GLU:OE2	11:Y:69:ARG:NH1	2.51	0.43
8:H:184:ASP:HB3	8:H:186:LEU:CD1	2.49	0.43
3:Q:203:THR:HG22	3:Q:204:GLY:H	1.84	0.43
1:O:4:ARG:HD3	5:S:122:TYR:CD2	2.53	0.43
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.54	0.43
5:S:118:ASN:HD22	5:S:118:ASN:N	2.17	0.42
10:J:177:LYS:NZ	10:X:169:GLU:O	2.52	0.42
3:C:203:THR:HG22	3:C:204:GLY:H	1.84	0.42
8:V:184:ASP:HB3	8:V:186:LEU:CD1	2.49	0.42
8:V:50:ALA:HB2	9:W:128:CYS:HB2	2.01	0.42
10:J:145:ASP:OD1	11:Y:209:ASN:ND2	2.52	0.42
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.00	0.42
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.83	0.42
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.02	0.42
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.02	0.42
7:U:99:TYR:O	8:V:78:THR:HB	2.20	0.42
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.02	0.42
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.66	0.42
2:B:217:LYS:O	2:B:219:ALA:N	2.53	0.42
3:C:165:ASN:HB2	3:C:200:VAL:HG11	2.01	0.42
3:Q:165:ASN:HB2	3:Q:200:VAL:HG11	2.02	0.42
11:Y:176:ASN:ND2	11:Y:190:ASN:HD22	2.18	0.42
11:K:176:ASN:HD21	11:K:190:ASN:HD22	1.68	0.41
1:O:1:MET:HG3	6:T:122:TYR:CE1	2.56	0.41
10:J:174:MET:HB2	19:J:216:HOH:O	2.20	0.41
2:P:217:LYS:O	2:P:219:ALA:N	2.54	0.41
6:T:155:GLY:HA3	7:U:59:THR:HG21	2.03	0.41
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.51	0.41
4:R:155:THR:HG23	5:S:59:GLN:HE22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.56	0.41
3:C:35:LYS:HG2	3:C:158:SER:O	2.21	0.41
6:F:191:GLN:HE22	6:F:194:LYS:HE2	1.86	0.41
5:E:18:LEU:HD21	6:F:126:ARG:HD2	2.03	0.40
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.56	0.40
3:C:9:PHE:H	4:D:15:GLN:HE22	1.70	0.40
3:C:99:GLU:CD	11:K:121:ARG:HH22	2.25	0.40
8:H:1:THR:HB	17:H:301:GRW:O30	2.21	0.40
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.52	0.40
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.57	0.40
5:E:68:HIS:HE1	5:E:102:LEU:O	2.05	0.40
9:I:37:ASN:N	9:I:37:ASN:HD22	2.20	0.40
10:J:146:HIS:CE1	11:Y:204:GLU:OE1	2.74	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	236/250 (94%)	226 (96%)	9 (4%)	1 (0%)	34	66
1	O	236/250 (94%)	227 (96%)	8 (3%)	1 (0%)	34	66
2	B	242/258 (94%)	236 (98%)	4 (2%)	2 (1%)	19	51
2	P	242/258 (94%)	236 (98%)	4 (2%)	2 (1%)	19	51
3	C	238/254 (94%)	236 (99%)	2 (1%)	0	100	100
3	Q	238/254 (94%)	236 (99%)	1 (0%)	1 (0%)	34	66
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	219 (96%)	10 (4%)	0	100	100
5	S	229/234 (98%)	220 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	239 (100%)	0	0	100	100
8	H	217/234 (93%)	215 (99%)	2 (1%)	0	100	100
8	V	217/234 (93%)	215 (99%)	2 (1%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	210/212 (99%)	201 (96%)	7 (3%)	2 (1%)	15	45
11	Y	210/212 (99%)	200 (95%)	8 (4%)	2 (1%)	15	45
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	222/246 (90%)	213 (96%)	9 (4%)	0	100	100
13	a	222/246 (90%)	212 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6228/6618 (94%)	6078 (98%)	139 (2%)	11 (0%)	47	78

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	LYS
2	B	52	THR
2	B	218	GLY
1	O	231	LYS
2	P	52	THR
2	P	218	GLY
11	K	147	ASP
11	Y	147	ASP
11	K	148	LEU
11	Y	148	LEU
3	Q	183	PRO

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	201/209 (96%)	197 (98%)	4 (2%)	55	82
1	O	201/209 (96%)	197 (98%)	4 (2%)	55	82
2	B	203/216 (94%)	193 (95%)	10 (5%)	25	57
2	P	203/216 (94%)	194 (96%)	9 (4%)	28	61
3	C	212/226 (94%)	203 (96%)	9 (4%)	30	63
3	Q	212/226 (94%)	203 (96%)	9 (4%)	30	63
4	D	194/215 (90%)	186 (96%)	8 (4%)	30	64
4	R	194/215 (90%)	186 (96%)	8 (4%)	30	64
5	E	190/193 (98%)	179 (94%)	11 (6%)	20	50
5	S	190/193 (98%)	180 (95%)	10 (5%)	22	54
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%)	196 (95%)	10 (5%)	25	57
7	U	206/210 (98%)	196 (95%)	10 (5%)	25	57
8	H	179/194 (92%)	171 (96%)	8 (4%)	27	61
8	V	179/194 (92%)	172 (96%)	7 (4%)	32	66
9	I	172/173 (99%)	166 (96%)	6 (4%)	36	70
9	W	172/173 (99%)	166 (96%)	6 (4%)	36	70
10	J	173/175 (99%)	166 (96%)	7 (4%)	31	65
10	X	173/175 (99%)	166 (96%)	7 (4%)	31	65
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%)	177 (96%)	8 (4%)	29	62
12	Z	185/185 (100%)	177 (96%)	8 (4%)	29	62
13	M	192/208 (92%)	185 (96%)	7 (4%)	35	69
13	a	192/208 (92%)	185 (96%)	7 (4%)	35	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	158 (98%)	4 (2%)	47	78
14	b	162/162 (100%)	158 (98%)	4 (2%)	47	78
All	All	5278/5548 (95%)	5067 (96%)	211 (4%)	31	65

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	51	VAL
2	B	52	THR
2	B	55	LEU
2	B	102	ASN
2	B	113	ARG
2	B	119	GLN
2	B	186	ASP
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	48	SER
3	C	51	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	240	GLU
4	D	99	ILE
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

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Mol	Chain	Res	Type
5	E	55	LEU
5	E	71	LEU
5	E	116	GLN
5	E	118	ASN
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	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	214	TRP
6	F	240	GLN
7	G	13	GLU
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	154	TYR
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	14	LEU
8	H	24	MET
8	H	32	SER
8	H	78	THR
8	H	98	LEU
8	H	122	LEU
8	H	143	ARG
8	H	201	ARG
9	I	37	ASN
9	I	123	PHE
9	I	151	SER
9	I	160	GLU
9	I	171	LEU
9	I	182	TRP
10	J	2	ASP

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Mol	Chain	Res	Type
10	J	3	ILE
10	J	23	ARG
10	J	35	THR
10	J	78	GLN
10	J	90	LYS
10	J	99	GLN
11	K	9	GLN
11	K	18	SER
11	K	35	ILE
11	K	73	ARG
11	K	100	MET
11	K	108	GLU
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	108	HIS
12	L	130	SER
12	L	136	CYS
12	L	150	LEU
12	L	161	GLU
13	M	10	SER
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	179	ASN
13	M	187	ARG
14	N	9	LYS
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	2	THR
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	52	THR
2	P	55	LEU
2	P	102	ASN
2	P	113	ARG
2	P	119	GLN
2	P	186	ASP

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Mol	Chain	Res	Type
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	48	SER
3	Q	51	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	116	GLN
5	S	118	ASN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	214	TRP
6	T	240	GLN
7	U	13	GLU
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN

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Mol	Chain	Res	Type
7	U	122	ARG
7	U	125	MET
7	U	154	TYR
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	14	LEU
8	V	24	MET
8	V	78	THR
8	V	98	LEU
8	V	132	LEU
8	V	143	ARG
8	V	201	ARG
9	W	37	ASN
9	W	123	PHE
9	W	151	SER
9	W	160	GLU
9	W	171	LEU
9	W	182	TRP
10	X	2	ASP
10	X	3	ILE
10	X	23	ARG
10	X	35	THR
10	X	78	GLN
10	X	90	LYS
10	X	99	GLN
11	Y	9	GLN
11	Y	18	SER
11	Y	35	ILE
11	Y	73	ARG
11	Y	100	MET
11	Y	108	GLU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	108	HIS
12	Z	130	SER
12	Z	136	CYS
12	Z	150	LEU
12	Z	161	GLU
13	a	10	SER
13	a	48	ASN

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Mol	Chain	Res	Type
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	179	ASN
13	a	187	ARG
14	b	9	LYS
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	207	ASN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	146	GLN
4	D	160	ASN
4	D	210	GLN
4	D	225	ASN
5	E	59	GLN
5	E	68	HIS
5	E	90	GLN
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN

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Mol	Chain	Res	Type
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	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
7	G	184	HIS
7	G	186	ASN
8	H	153	ASN
9	I	71	ASN
10	J	55	GLN
10	J	118	GLN
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	176	ASN
12	L	3	ASN
12	L	55	ASN
12	L	80	ASN
12	L	152	ASN
12	L	153	GLN
12	L	158	ASN
13	M	2	GLN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN

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Mol	Chain	Res	Type
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
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
3	Q	207	ASN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	146	GLN
4	R	210	GLN
4	R	225	ASN
5	S	59	GLN
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	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	153	ASN
9	W	71	ASN

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Mol	Chain	Res	Type
10	X	55	GLN
10	X	86	GLN
10	X	118	GLN
11	Y	9	GLN
11	Y	62	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	55	ASN
12	Z	152	ASN
12	Z	153	GLN
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 carbohydrates 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	SO4	N	202	-	4,4,4	0.28	0	6,6,6	0.10	0
18	SO4	b	201	-	4,4,4	0.31	0	6,6,6	0.17	0
17	GRW	H	301	8	45,46,46	1.97	7 (15%)	58,62,62	7.85	8 (13%)
17	GRW	K	301	11	45,46,46	1.57	7 (15%)	58,62,62	8.01	12 (20%)
17	GRW	V	301	8	45,46,46	1.73	6 (13%)	58,62,62	7.77	15 (25%)
17	GRW	Y	301	11	45,46,46	1.67	8 (17%)	58,62,62	7.99	12 (20%)

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	GRW	H	301	8	-	13/51/51/51	0/2/2/2
17	GRW	K	301	11	-	14/51/51/51	0/2/2/2
17	GRW	V	301	8	-	13/51/51/51	0/2/2/2
17	GRW	Y	301	11	-	14/51/51/51	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	GRW	C54-C55	-6.11	1.36	1.51
17	H	301	GRW	N52-N51	-5.94	1.07	1.23
17	V	301	GRW	C54-C55	-5.38	1.38	1.51
17	Y	301	GRW	C16-C17	-5.29	1.38	1.51
17	H	301	GRW	C16-C17	-5.26	1.38	1.51
17	K	301	GRW	C16-C17	-5.11	1.39	1.51
17	V	301	GRW	C16-C17	-4.77	1.39	1.51
17	V	301	GRW	N52-N51	-4.61	1.11	1.23
17	Y	301	GRW	N52-N51	-4.17	1.12	1.23
17	K	301	GRW	N52-N51	-4.07	1.12	1.23
17	H	301	GRW	C21-C20	-3.99	1.37	1.51
17	Y	301	GRW	O30-S27	3.88	1.52	1.44
17	Y	301	GRW	O29-S27	3.86	1.52	1.44
17	K	301	GRW	O29-S27	3.82	1.52	1.44
17	K	301	GRW	O30-S27	3.80	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	V	301	GRW	O30-S27	3.68	1.52	1.44
17	V	301	GRW	C21-C20	-3.54	1.39	1.51
17	Y	301	GRW	C21-C20	-3.38	1.39	1.51
17	K	301	GRW	C54-C55	-3.37	1.43	1.51
17	H	301	GRW	C54-C6	-3.31	1.48	1.53
17	K	301	GRW	C21-C20	-3.26	1.40	1.51
17	Y	301	GRW	C54-C55	-3.23	1.43	1.51
17	Y	301	GRW	C26-S27	3.22	1.82	1.78
17	H	301	GRW	O29-S27	3.00	1.51	1.44
17	H	301	GRW	O30-S27	2.89	1.50	1.44
17	V	301	GRW	O29-S27	2.55	1.50	1.44
17	Y	301	GRW	C25-C26	2.13	1.54	1.52
17	K	301	GRW	C26-S27	2.11	1.81	1.78

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	GRW	C6-N51-N52	60.04	178.40	115.24
17	Y	301	GRW	C6-N51-N52	59.93	178.28	115.24
17	H	301	GRW	C6-N51-N52	58.82	177.12	115.24
17	V	301	GRW	C6-N51-N52	57.14	175.35	115.24
17	V	301	GRW	C54-C55-C56	-6.94	107.12	120.91
17	V	301	GRW	C54-C55-C60	6.59	134.00	120.91
17	H	301	GRW	O29-S27-C26	-4.79	104.99	108.34
17	V	301	GRW	C16-C15-N14	-4.41	101.92	110.39
17	H	301	GRW	C28-S27-C26	3.56	118.94	105.21
17	V	301	GRW	C25-C15-C16	3.55	116.93	111.14
17	Y	301	GRW	O29-S27-O30	-3.55	109.50	117.09
17	V	301	GRW	C54-C6-C7	3.40	116.78	109.55
17	K	301	GRW	O29-S27-C26	-3.26	106.06	108.34
17	K	301	GRW	O29-S27-O30	-3.24	110.17	117.09
17	K	301	GRW	C28-S27-C26	3.18	117.46	105.21
17	K	301	GRW	C16-C17-C24	3.10	127.05	120.91
17	Y	301	GRW	C16-C17-C24	3.05	126.95	120.91
17	K	301	GRW	C16-C17-C18	-3.03	114.88	120.91
17	K	301	GRW	O29-S27-C28	-3.01	105.88	108.91
17	Y	301	GRW	C16-C17-C18	-3.00	114.95	120.91
17	V	301	GRW	O29-S27-C26	-2.99	106.25	108.34
17	H	301	GRW	O29-S27-O30	-2.95	110.80	117.09
17	Y	301	GRW	C28-S27-C26	2.89	116.36	105.21
17	V	301	GRW	O30-S27-C28	-2.88	106.01	108.91
17	H	301	GRW	O30-S27-C26	-2.82	106.37	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	301	GRW	C55-C54-C6	2.72	118.87	113.40
17	V	301	GRW	C41-C40-C9	-2.71	107.97	115.43
17	H	301	GRW	O30-S27-C28	-2.62	106.27	108.91
17	H	301	GRW	C54-C55-C60	-2.61	115.72	120.91
17	V	301	GRW	O29-S27-O30	-2.55	111.64	117.09
17	Y	301	GRW	C54-C55-C60	2.52	125.90	120.91
17	H	301	GRW	C54-C6-N51	-2.51	105.16	109.30
17	K	301	GRW	C54-C55-C60	2.42	125.70	120.91
17	Y	301	GRW	C40-C9-C10	-2.42	104.82	110.57
17	V	301	GRW	O29-S27-C28	2.41	111.33	108.91
17	K	301	GRW	C40-C9-C10	-2.38	104.91	110.57
17	Y	301	GRW	O29-S27-C28	-2.27	106.63	108.91
17	K	301	GRW	C32-C12-C13	-2.27	106.29	111.28
17	K	301	GRW	C54-C6-C7	2.24	114.31	109.55
17	V	301	GRW	C32-C12-C13	-2.21	106.42	111.28
17	Y	301	GRW	C32-C12-C13	-2.20	106.44	111.28
17	Y	301	GRW	C54-C6-C7	2.18	114.17	109.55
17	V	301	GRW	C54-C6-N51	2.16	112.86	109.30
17	Y	301	GRW	O29-S27-C26	-2.13	106.85	108.34
17	Y	301	GRW	C54-C55-C56	-2.11	116.72	120.91
17	K	301	GRW	C54-C55-C56	-2.07	116.79	120.91
17	V	301	GRW	C15-N14-C13	2.02	126.42	123.20

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	GRW	N51-C6-C7-N8
17	H	301	GRW	C54-C6-N51-N52
17	H	301	GRW	C55-C54-C6-C7
17	H	301	GRW	C55-C54-C6-N51
17	H	301	GRW	C25-C26-S27-O30
17	H	301	GRW	C25-C26-S27-O29
17	H	301	GRW	C6-N51-N52-N53
17	V	301	GRW	N51-C6-C7-N8
17	V	301	GRW	N51-C6-C7-O44
17	V	301	GRW	C25-C26-S27-O30
17	V	301	GRW	C25-C26-S27-O29
17	K	301	GRW	N51-C6-C7-N8
17	K	301	GRW	N51-C6-C7-O44
17	K	301	GRW	C7-C6-N51-N52
17	K	301	GRW	C25-C26-S27-C28

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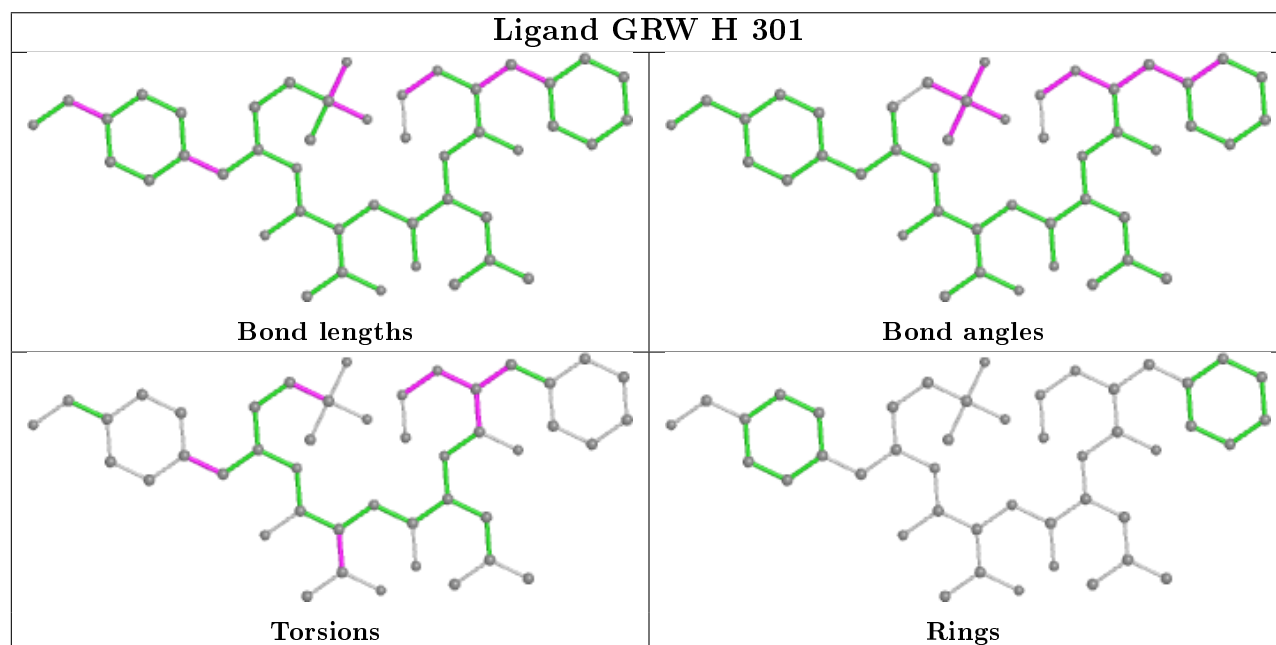
Mol	Chain	Res	Type	Atoms
17	K	301	GRW	C25-C26-S27-O30
17	K	301	GRW	C25-C26-S27-O29
17	Y	301	GRW	N51-C6-C7-N8
17	Y	301	GRW	N51-C6-C7-O44
17	Y	301	GRW	C25-C26-S27-C28
17	Y	301	GRW	C25-C26-S27-O30
17	Y	301	GRW	C25-C26-S27-O29
17	Y	301	GRW	C6-N51-N52-N53
17	Y	301	GRW	C6-C54-C55-C60
17	K	301	GRW	C6-C54-C55-C60
17	Y	301	GRW	C6-C54-C55-C56
17	K	301	GRW	C6-C54-C55-C56
17	Y	301	GRW	C15-C16-C17-C24
17	K	301	GRW	C15-C16-C17-C24
17	K	301	GRW	C15-C16-C17-C18
17	Y	301	GRW	C15-C16-C17-C18
17	H	301	GRW	C15-C16-C17-C24
17	H	301	GRW	C15-C16-C17-C18
17	Y	301	GRW	C54-C6-C7-O44
17	V	301	GRW	C15-C16-C17-C18
17	V	301	GRW	C15-C16-C17-C24
17	H	301	GRW	C54-C6-C7-O44
17	K	301	GRW	C54-C6-C7-O44
17	V	301	GRW	C6-N51-N52-N53
17	K	301	GRW	C6-N51-N52-N53
17	H	301	GRW	C54-C6-C7-N8
17	H	301	GRW	C7-C6-N51-N52
17	V	301	GRW	C7-C6-N51-N52
17	Y	301	GRW	C7-C6-N51-N52
17	K	301	GRW	C15-C25-C26-S27
17	Y	301	GRW	C15-C25-C26-S27
17	V	301	GRW	C55-C54-C6-N51
17	V	301	GRW	C13-C12-N11-C10
17	V	301	GRW	C54-C6-C7-O44
17	K	301	GRW	C54-C6-C7-N8
17	Y	301	GRW	C54-C6-C7-N8
17	H	301	GRW	N11-C12-C32-O33
17	V	301	GRW	C54-C6-N51-N52
17	V	301	GRW	C25-C26-S27-C28

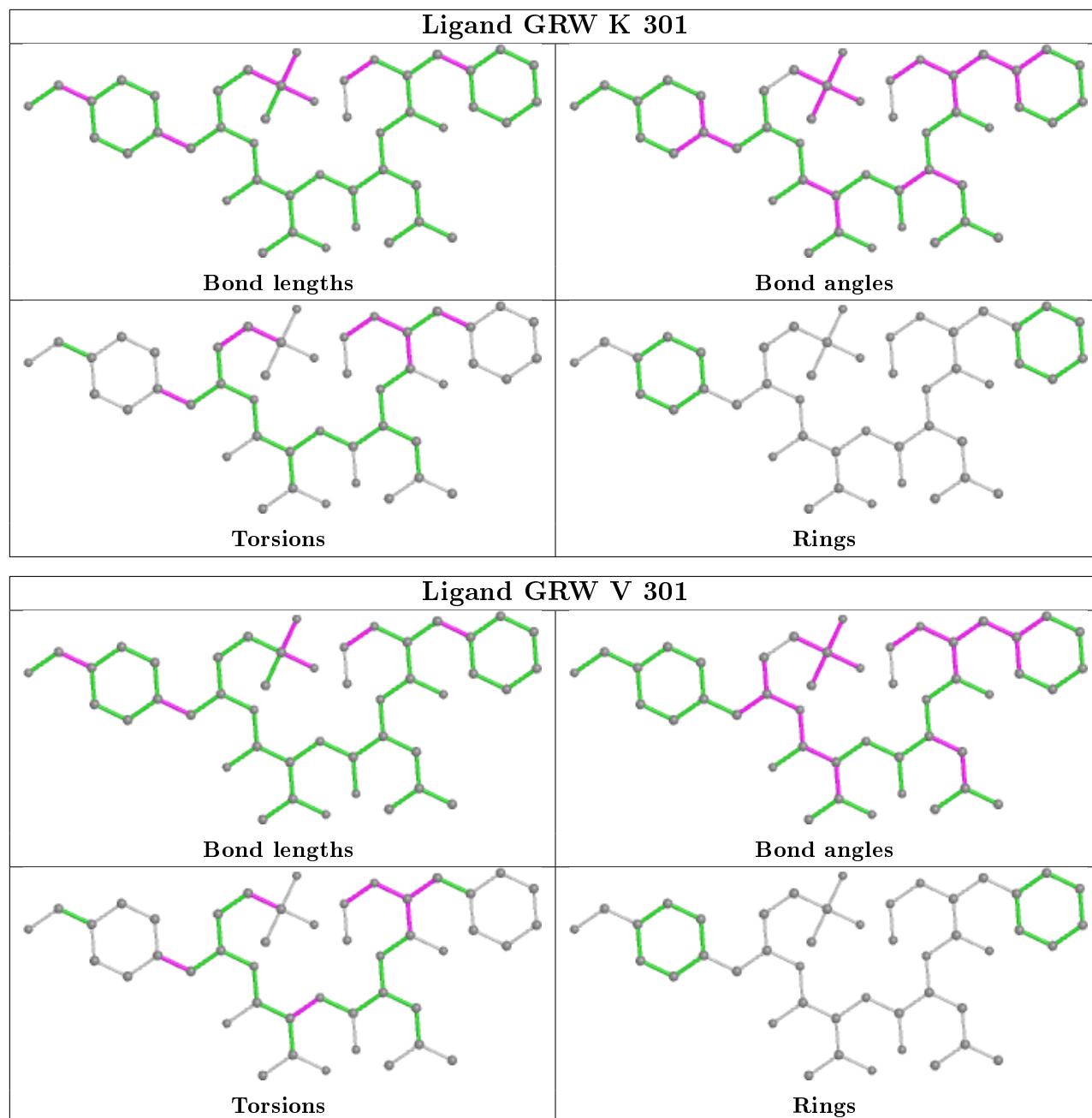
There are no ring outliers.

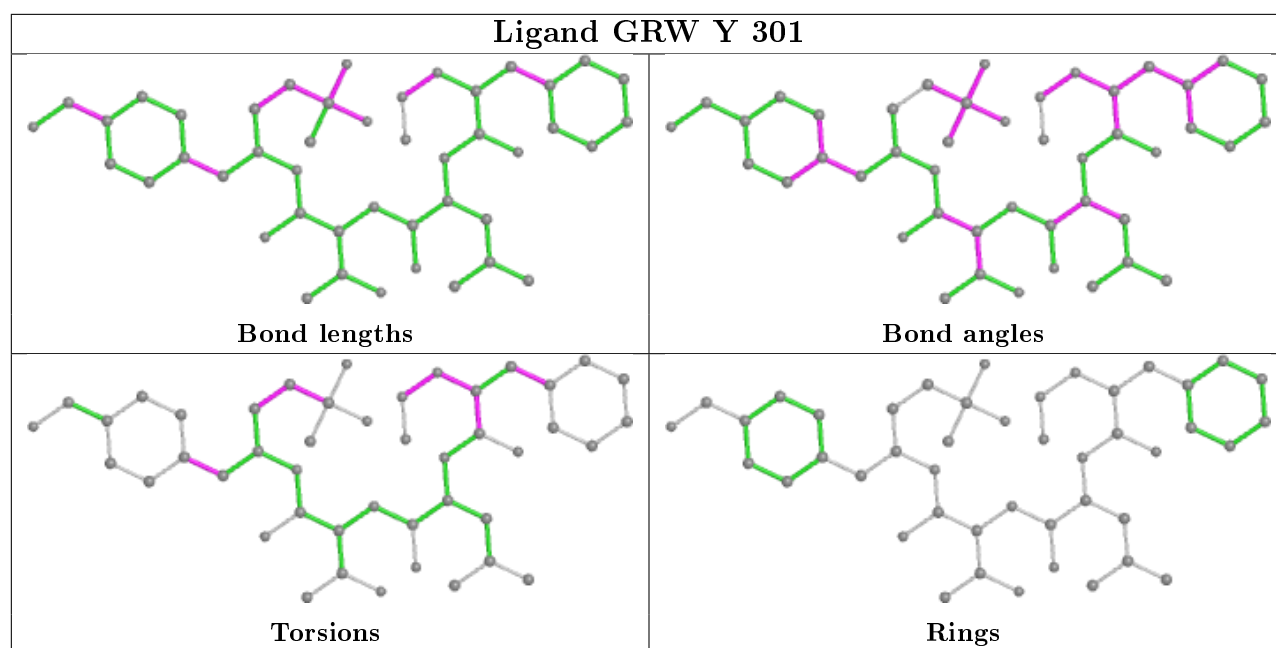
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	301	GRW	1	0
17	V	301	GRW	2	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.







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	240/250 (96%)	-0.27	5 (2%) 63 61	41, 59, 100, 133	0
1	O	240/250 (96%)	-0.22	8 (3%) 46 41	46, 68, 113, 149	0
2	B	244/258 (94%)	-0.17	12 (4%) 29 26	41, 63, 111, 166	0
2	P	244/258 (94%)	-0.19	10 (4%) 37 32	45, 63, 113, 163	0
3	C	240/254 (94%)	-0.19	12 (5%) 28 25	42, 65, 126, 160	0
3	Q	240/254 (94%)	0.11	17 (7%) 16 12	56, 85, 161, 182	0
4	D	235/260 (90%)	-0.39	3 (1%) 77 77	44, 65, 97, 141	0
4	R	235/260 (90%)	-0.23	5 (2%) 63 61	52, 73, 114, 147	0
5	E	231/234 (98%)	-0.26	4 (1%) 70 69	47, 67, 104, 144	0
5	S	231/234 (98%)	-0.21	5 (2%) 62 59	49, 74, 117, 150	0
6	F	243/288 (84%)	-0.42	5 (2%) 63 61	40, 60, 107, 140	0
6	T	243/288 (84%)	-0.30	3 (1%) 79 79	42, 72, 120, 153	0
7	G	241/252 (95%)	-0.41	5 (2%) 63 61	40, 58, 97, 153	0
7	U	241/252 (95%)	-0.35	3 (1%) 79 79	45, 60, 94, 136	0
8	H	219/234 (93%)	-0.34	6 (2%) 54 50	37, 56, 111, 124	0
8	V	219/234 (93%)	-0.34	5 (2%) 60 58	40, 58, 114, 144	0
9	I	204/205 (99%)	-0.66	1 (0%) 91 91	35, 52, 78, 107	0
9	W	204/205 (99%)	-0.64	1 (0%) 91 91	38, 53, 82, 104	0
10	J	195/198 (98%)	-0.50	2 (1%) 82 82	36, 56, 82, 126	0
10	X	195/198 (98%)	-0.45	2 (1%) 82 82	39, 58, 84, 146	0
11	K	212/212 (100%)	-0.49	1 (0%) 91 91	38, 55, 87, 110	0
11	Y	212/212 (100%)	-0.46	3 (1%) 75 75	40, 58, 91, 120	0
12	L	222/222 (100%)	-0.49	3 (1%) 75 75	35, 55, 100, 128	0
12	Z	222/222 (100%)	-0.46	4 (1%) 68 67	35, 54, 96, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	224/246 (91%)	-0.40	6 (2%) 54 50	37, 57, 86, 131	0
13	a	224/246 (91%)	-0.39	6 (2%) 54 50	36, 57, 86, 130	0
14	N	196/196 (100%)	-0.53	2 (1%) 82 82	34, 50, 83, 108	0
14	b	196/196 (100%)	-0.56	1 (0%) 91 91	36, 53, 83, 114	0
All	All	6292/6618 (95%)	-0.36	140 (2%) 62 59	34, 61, 109, 182	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	220	ASN	8.0
2	B	221	ASP	7.7
2	P	221	ASP	7.1
3	Q	50	LEU	6.7
3	Q	49	THR	6.2
13	M	216	ASN	6.0
13	a	216	ASN	5.9
2	B	51	VAL	5.7
2	P	220	ASN	5.6
1	O	230	ASP	5.2
5	E	202	ASP	5.2
13	a	1	THR	5.1
2	P	219	ALA	5.0
10	X	1	MET	5.0
2	P	59	ASP	4.9
2	P	222	GLY	4.8
1	O	1	MET	4.6
1	O	249	ALA	4.6
3	Q	206	LYS	4.5
3	C	49	THR	4.5
2	P	51	VAL	4.5
10	X	194	ASP	4.4
3	Q	238	LYS	4.4
1	A	230	ASP	4.4
2	B	218	GLY	4.4
8	V	196	GLY	4.3
3	Q	239	GLN	4.3
11	Y	147	ASP	4.3
13	a	224	ASP	4.2
12	Z	174	TYR	4.1
14	b	195	GLN	4.0
3	Q	240	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
13	a	215	GLU	4.0
10	J	1	MET	4.0
1	A	1	MET	3.9
3	Q	236	GLN	3.9
3	Q	48	SER	3.9
3	C	238	LYS	3.9
13	M	1	THR	3.8
2	B	219	ALA	3.7
7	U	181	LYS	3.7
3	C	206	LYS	3.7
3	Q	187	GLU	3.7
8	H	196	GLY	3.6
12	L	174	TYR	3.6
13	a	220	ASP	3.6
3	Q	202	GLN	3.6
2	P	218	GLY	3.6
5	S	180	LYS	3.6
14	N	195	GLN	3.6
3	C	50	LEU	3.5
2	B	59	ASP	3.5
5	E	123	GLY	3.4
7	G	241	GLU	3.3
12	Z	173	LYS	3.3
2	B	222	GLY	3.3
2	B	225	TYR	3.2
3	Q	205	ALA	3.2
1	O	231	LYS	3.2
8	V	194	LYS	3.2
6	T	181	GLU	3.1
7	G	2	GLY	3.1
13	M	47	ASP	3.1
8	V	219	LEU	3.1
4	D	241	ALA	3.1
4	R	242	GLU	3.0
3	C	202	GLN	2.9
9	I	1	SER	2.9
5	S	202	ASP	2.9
3	C	239	GLN	2.8
3	C	60	SER	2.8
8	V	181	ASN	2.8
2	P	225	TYR	2.8
4	D	242	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	232	GLN	2.8
1	O	201	GLU	2.7
6	T	241	LYS	2.7
12	Z	163	GLY	2.7
2	P	223	GLU	2.7
4	D	1	ASP	2.7
9	W	1	SER	2.7
3	C	1	GLY	2.7
11	K	147	ASP	2.7
1	O	52	SER	2.7
4	R	125	LEU	2.7
3	Q	27	ARG	2.6
3	Q	47	ARG	2.6
13	M	220	ASP	2.6
6	F	202	ASP	2.6
3	C	236	GLN	2.6
1	A	201	GLU	2.6
4	R	241	ALA	2.6
11	Y	106	ARG	2.6
2	B	217	LYS	2.6
8	H	219	LEU	2.5
6	F	244	ASN	2.5
5	S	173	ARG	2.5
2	P	60	THR	2.5
3	C	48	SER	2.5
3	Q	181	GLU	2.4
12	L	173	LYS	2.4
10	J	194	ASP	2.4
11	Y	202	GLU	2.4
13	a	223	LYS	2.4
3	Q	229	GLN	2.4
6	F	180	PRO	2.3
6	T	244	ASN	2.3
4	R	1	ASP	2.3
5	E	54	GLU	2.3
5	S	227	GLU	2.3
8	H	218	PRO	2.3
7	G	242	GLN	2.3
1	O	62	SER	2.3
3	C	180	LYS	2.3
4	R	217	GLN	2.3
6	F	205	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
8	H	181	ASN	2.2
7	G	51	PRO	2.2
3	C	216	ASP	2.2
6	F	229	GLY	2.2
8	H	197	THR	2.2
8	H	194	LYS	2.2
2	B	50	LYS	2.2
1	O	248	GLU	2.2
3	Q	180	LYS	2.2
14	N	105	LYS	2.2
5	E	201	ARG	2.2
7	U	242	GLN	2.1
7	U	51	PRO	2.1
8	V	197	THR	2.1
1	A	59	GLU	2.1
3	Q	55	THR	2.1
13	M	224	ASP	2.1
12	L	1	GLN	2.0
1	A	52	SER	2.0
5	S	203	GLU	2.0
2	B	60	THR	2.0
12	Z	162	PRO	2.0
13	M	223	LYS	2.0
7	G	188	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 carbohydrates in this entry.

6.4 Ligands [i](#)

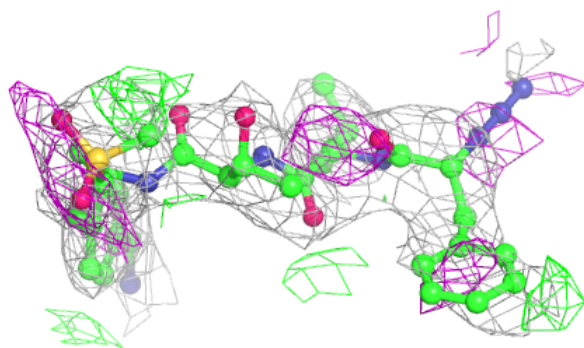
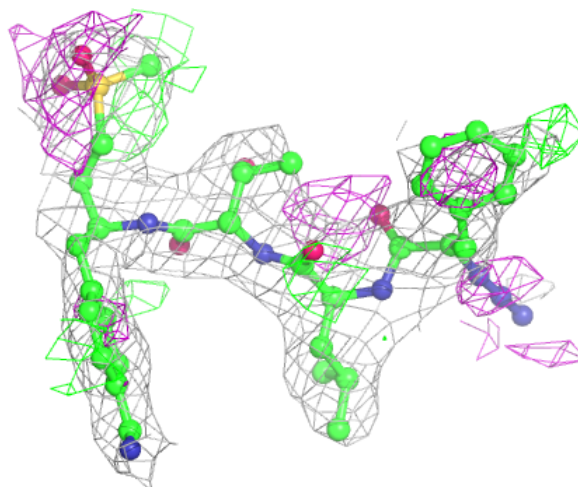
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	MG	W	301	1/1	0.87	0.42	81,81,81,81	0
15	MG	Z	301	1/1	0.89	0.45	64,64,64,64	0
17	GRW	V	301	45/45	0.89	0.27	50,64,89,101	0
17	GRW	H	301	45/45	0.89	0.27	48,60,90,95	0
15	MG	I	302	1/1	0.90	0.27	82,82,82,82	0
17	GRW	K	301	45/45	0.93	0.19	41,51,70,84	0
17	GRW	Y	301	45/45	0.93	0.19	37,49,63,81	0
16	CL	G	302	1/1	0.94	0.32	63,63,63,63	0
15	MG	I	301	1/1	0.95	0.37	64,64,64,64	0
15	MG	K	302	1/1	0.95	0.12	68,68,68,68	0
15	MG	L	301	1/1	0.95	0.21	65,65,65,65	0
18	SO4	N	202	5/5	0.96	0.14	44,49,55,58	5
18	SO4	b	201	5/5	0.96	0.16	45,51,59,59	5
15	MG	N	201	1/1	0.96	0.11	40,40,40,40	0
15	MG	G	301	1/1	0.98	0.09	60,60,60,60	0
16	CL	U	301	1/1	0.99	0.34	79,79,79,79	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.

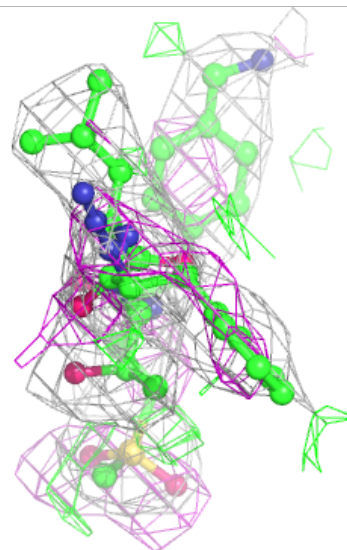
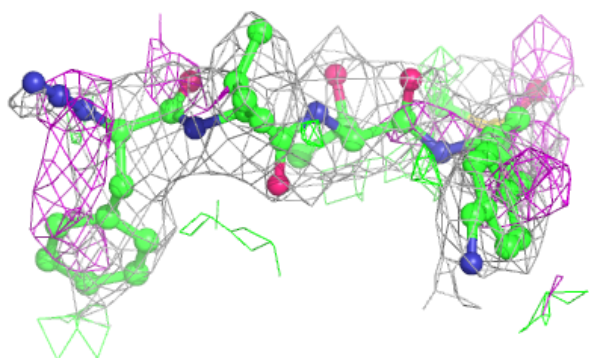
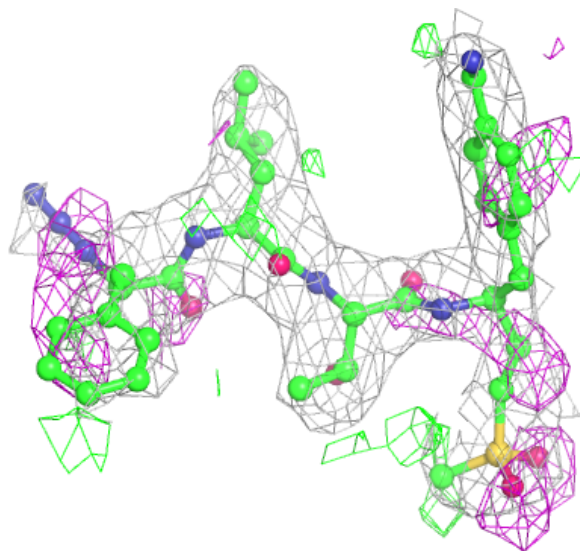
Electron density around GRW V 301:

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



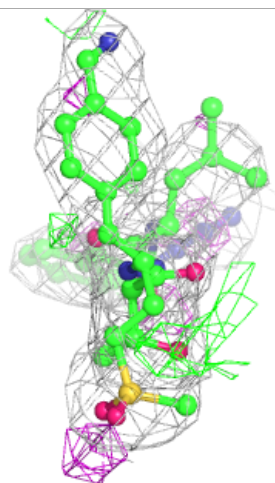
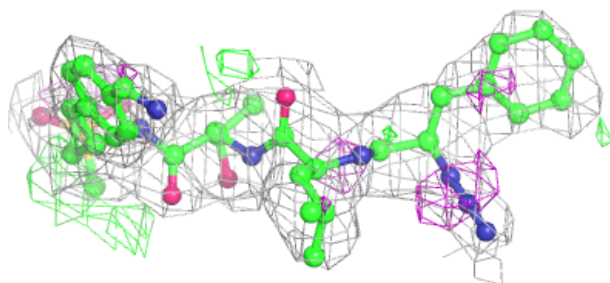
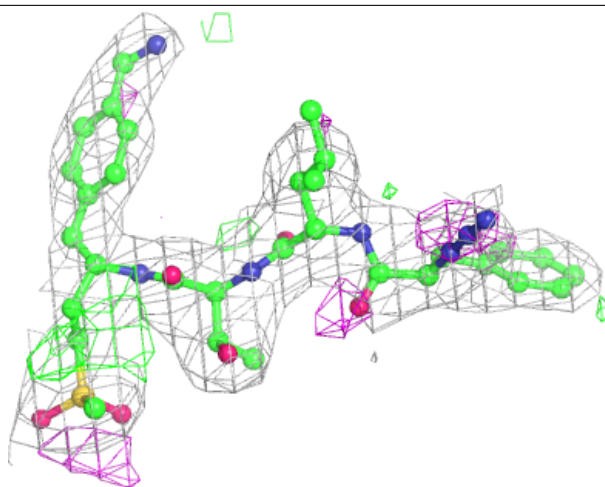
Electron density around GRW H 301:

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



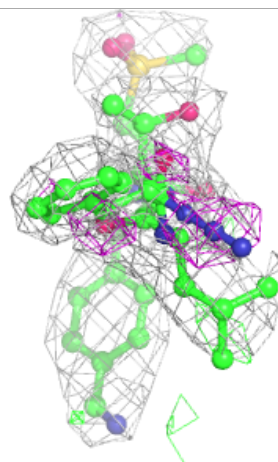
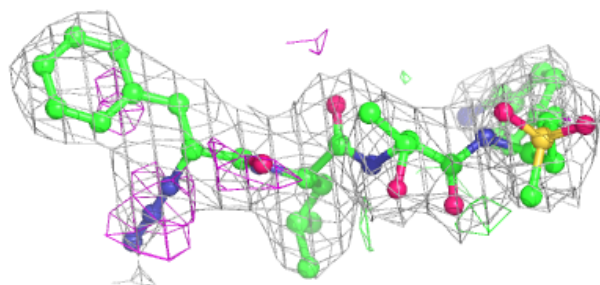
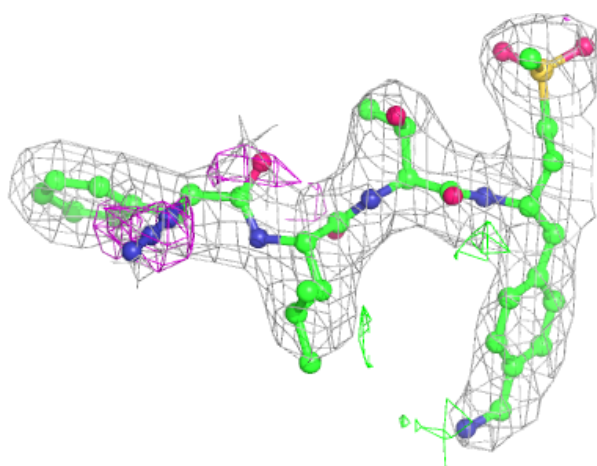
Electron density around GRW K 301:

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



Electron density around GRW 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.