Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 07:21 pm GMT

PDB ID	:	6HUC
Title	:	Yeast 20S proteasome with human beta2c (S171G) in complex with 18
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2018-10-05
Resolution	:	3.00 Å(reported)

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

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

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

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

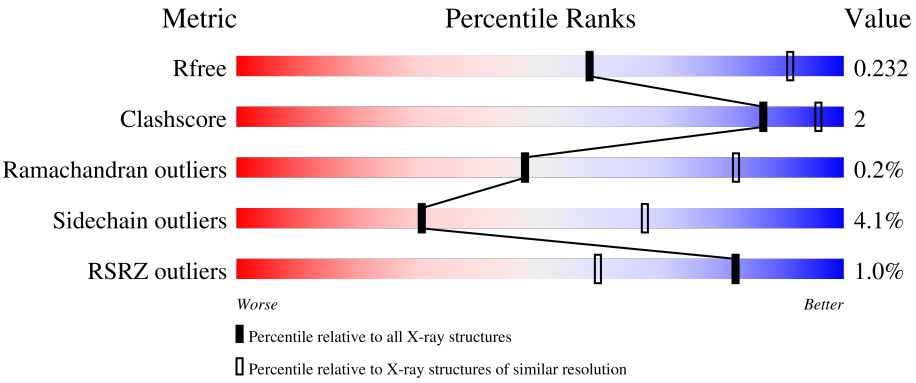
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	93%
1	O	250	93%
2	B	258	85% 8% 5%
2	P	258	86% 8% 5%
3	C	254	87% 7% 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	3% 87% 7% 6%
4	D	260	84% 6% 10%
4	R	260	84% 6% 10%
5	E	234	91% 8%
5	S	234	2% 91% 7%
6	F	288	79% 5% 16%
6	T	288	79% 5% 16%
7	G	252	88% 7%
7	U	252	88% 7%
8	H	234	83% 8% 6%
8	V	234	2% 82% 10% 6%
9	I	205	92% 7%
9	W	205	94% 6%
10	J	198	89% 9%
10	X	198	88% 10%
11	K	212	77% 20%
11	Y	212	77% 20%
12	L	222	91% 9%
12	Z	222	90% 9%
13	M	246	88% 9%
13	a	246	2% 88% 9%
14	N	196	95% 5%
14	b	196	98%

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 49480 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			

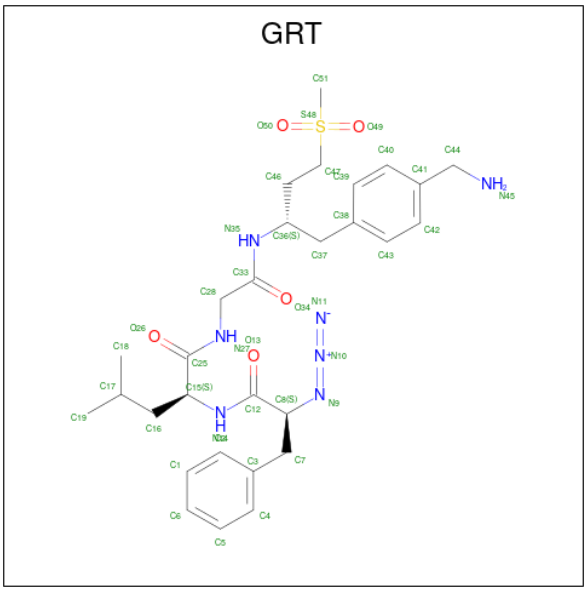
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

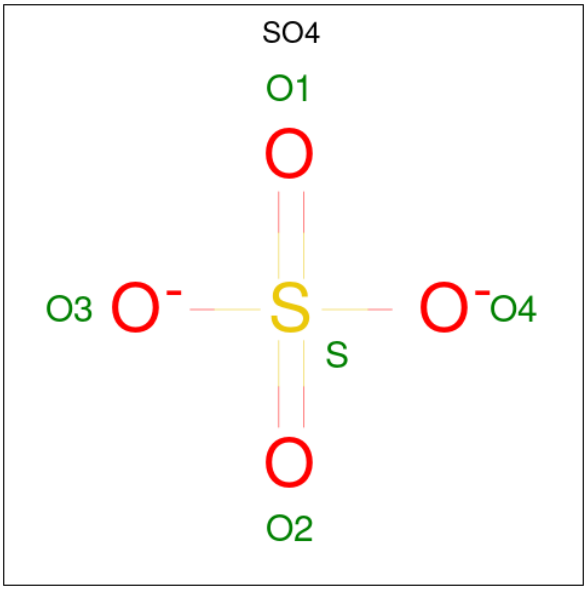
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is (2 {S})- {N}-[2-[[(2 {S})-1-[4-(aminomethyl)phenyl]-4-methylsulfonyl-butan-2-yl]amino]-2-oxidanylidene-ethyl]-2-[[(2 {S})-2-azido-3-phenyl-propanoyl]amino]-4-methyl-pentanamide (three-letter code: GRT) (formula: $C_{29}H_{41}N_7O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	C	N	O	S	0	0
			42	29	7	5	1		
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 SULFATE ION (three-letter code: SO4) (formula: O_4S).



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	6	Total	O	0	0
			6	6		
19	B	14	Total	O	0	0
			14	14		
19	C	8	Total	O	0	0
			8	8		
19	D	13	Total	O	0	0
			13	13		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	E	11	Total O 11 11	0	0
19	F	9	Total O 9 9	0	0
19	G	14	Total O 14 14	0	0
19	H	12	Total O 12 12	0	0
19	I	19	Total O 19 19	0	0
19	J	17	Total O 17 17	0	0
19	K	24	Total O 24 24	0	0
19	L	15	Total O 15 15	0	0
19	M	16	Total O 16 16	0	0
19	N	13	Total O 13 13	0	0
19	O	7	Total O 7 7	0	0
19	P	14	Total O 14 14	0	0
19	Q	12	Total O 12 12	0	0
19	R	7	Total O 7 7	0	0
19	S	12	Total O 12 12	0	0
19	T	7	Total O 7 7	0	0
19	U	12	Total O 12 12	0	0
19	V	14	Total O 14 14	0	0
19	W	7	Total O 7 7	0	0
19	X	13	Total O 13 13	0	0
19	Y	18	Total O 18 18	0	0

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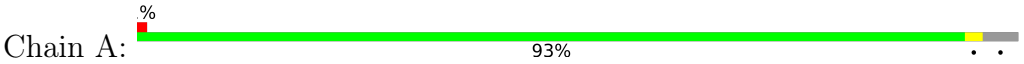
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	Z	12	Total O 12 12	0	0
19	a	11	Total O 11 11	0	0
19	b	19	Total O 19 19	0	0

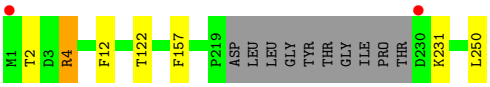
3 Residue-property plots (i)

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

• Molecule 1: Proteasome subunit alpha type-2

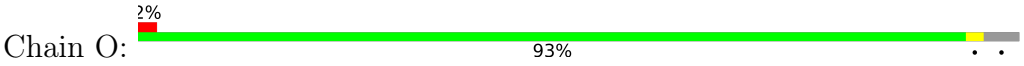
Chain A:

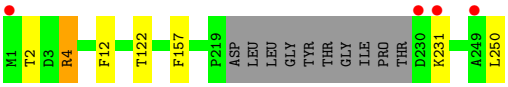




• Molecule 1: Proteasome subunit alpha type-2

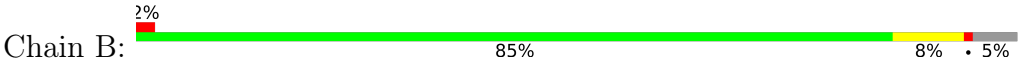
Chain O:

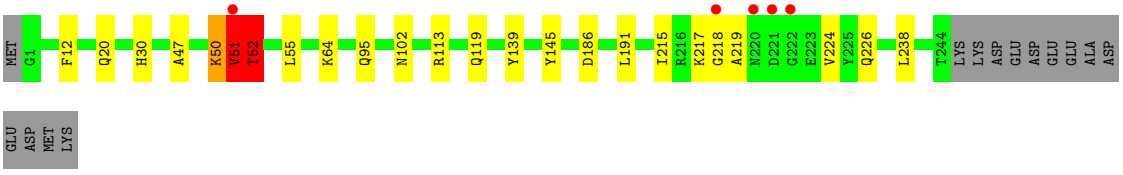




• Molecule 2: Proteasome subunit alpha type-3

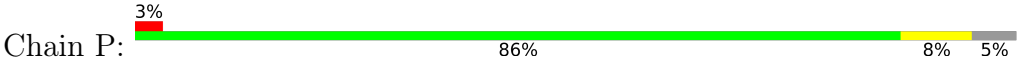
Chain B:

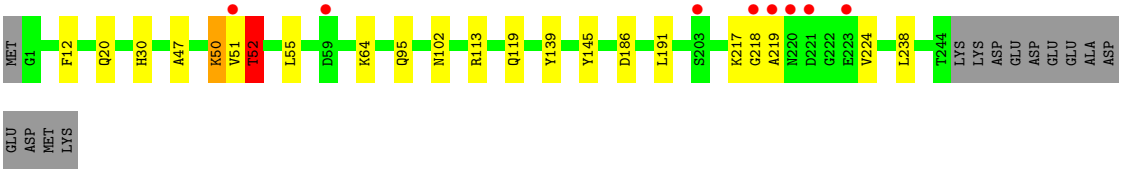




• Molecule 2: Proteasome subunit alpha type-3

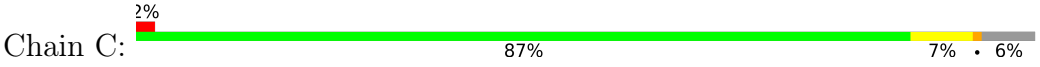
Chain P:



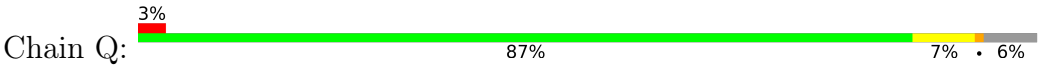


• Molecule 3: Proteasome subunit alpha type-4

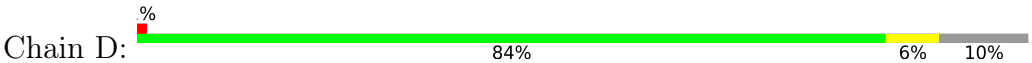
Chain C:

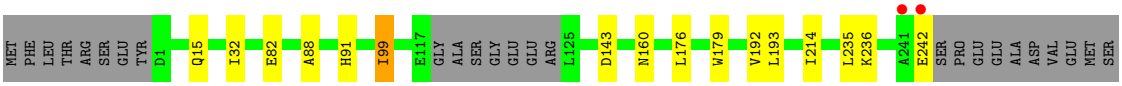


• Molecule 3: Proteasome subunit alpha type-4

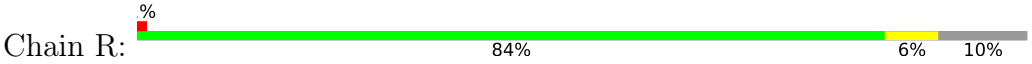


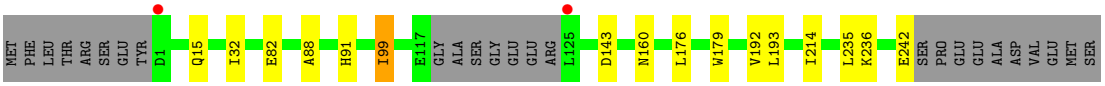
• Molecule 4: Proteasome subunit alpha type-5



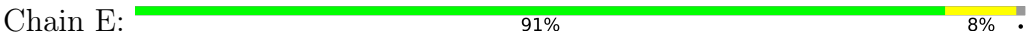


• Molecule 4: Proteasome subunit alpha type-5

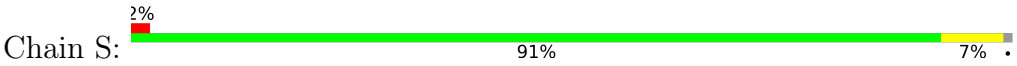




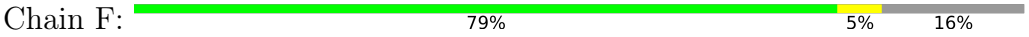
• Molecule 5: Proteasome subunit alpha type-6

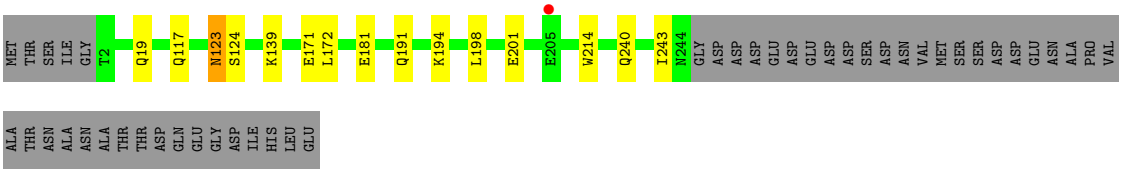


• Molecule 5: Proteasome subunit alpha type-6



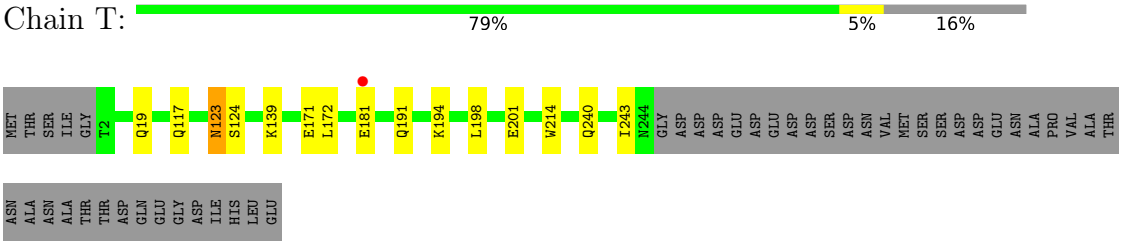
• Molecule 6: Probable proteasome subunit alpha type-7





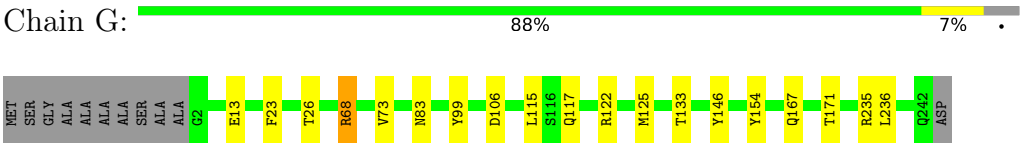
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



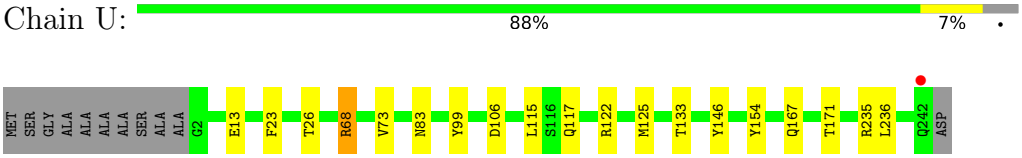
• Molecule 7: Proteasome subunit alpha type-1

Chain G:



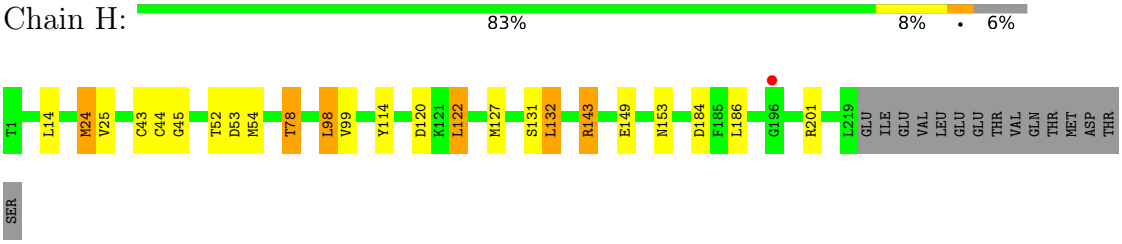
• Molecule 7: Proteasome subunit alpha type-1

Chain U:



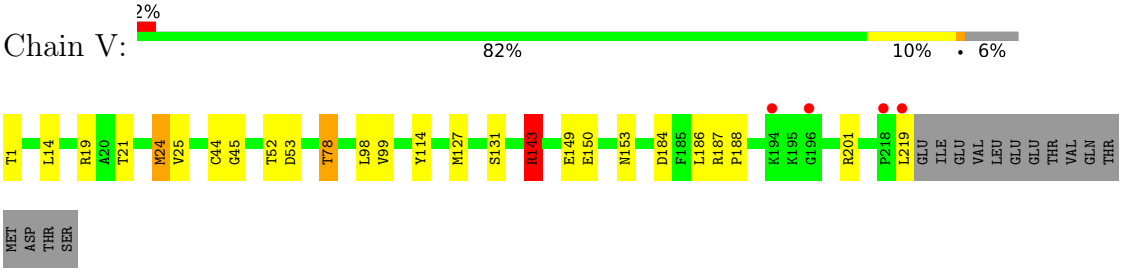
• Molecule 8: Proteasome subunit beta type-7

Chain H:



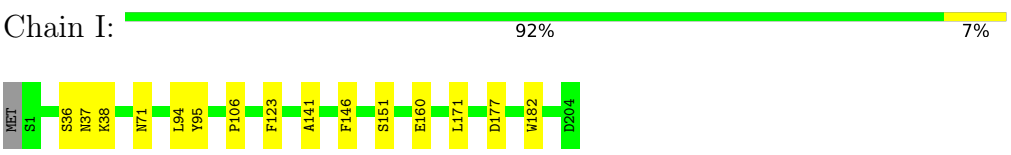
• Molecule 8: Proteasome subunit beta type-7

Chain V:



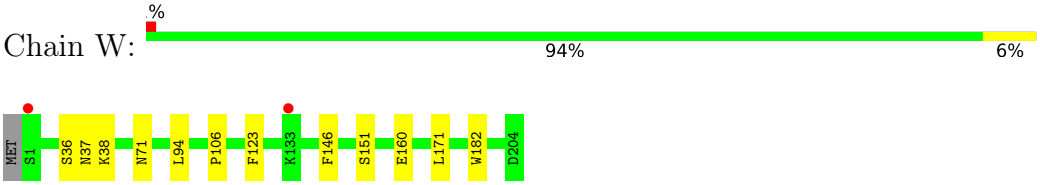
• Molecule 9: Proteasome subunit beta type-3

Chain I:



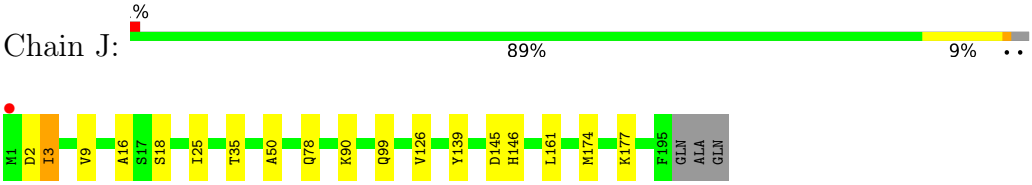
• Molecule 9: Proteasome subunit beta type-3

Chain W:



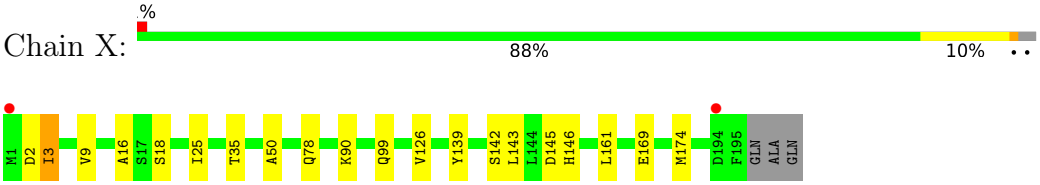
• Molecule 10: Proteasome subunit beta type-4

Chain J:



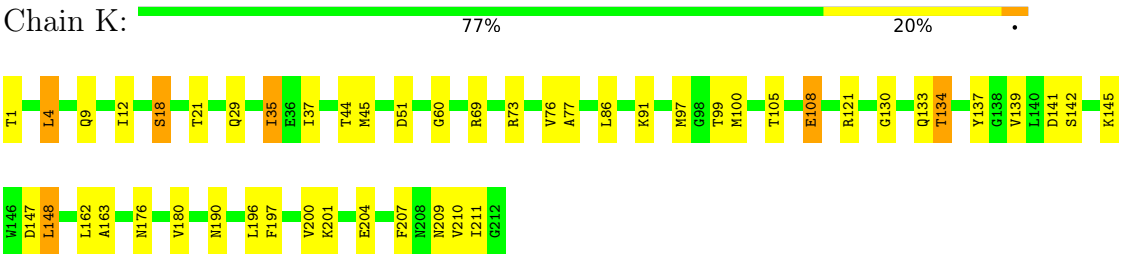
• Molecule 10: Proteasome subunit beta type-4

Chain X:



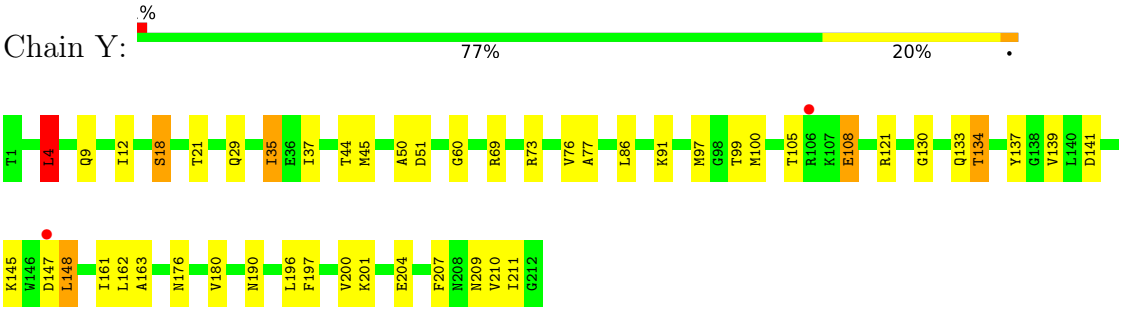
• Molecule 11: Proteasome subunit beta type-5

Chain K:



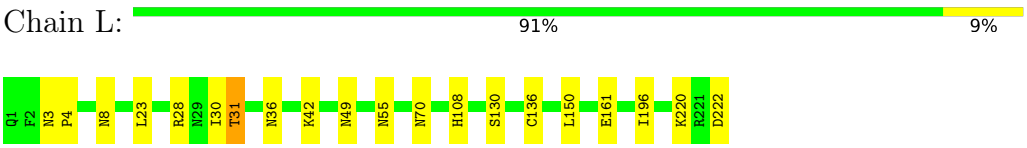
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



• Molecule 12: Proteasome subunit beta type-6

Chain L:



• Molecule 12: Proteasome subunit beta type-6

Chain Z:

• Molecule 13: Proteasome subunit beta type-7

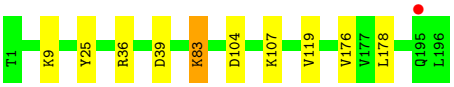
Chain M:

• Molecule 13: Proteasome subunit beta type-7

Chain a:

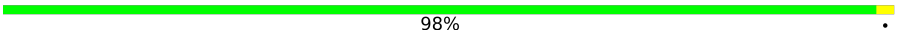
• Molecule 14: Proteasome subunit beta type-1

Chain N:



• Molecule 14: Proteasome subunit beta type-1

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	133.87Å 299.99Å 143.69Å 90.00° 112.65° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-3.00) 98.6 (15.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.181 , 0.218 0.193 , 0.232	Depositor DCC
R_{free} test set	10174 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	55.8	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	49480	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GRT, CL, MG, SO4

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	0.37	0/1876	0.82	3/2535 (0.1%)
1	O	0.37	0/1876	0.83	4/2535 (0.2%)
2	B	0.39	0/1934	0.66	1/2618 (0.0%)
2	P	0.38	0/1934	0.65	0/2618
3	C	0.38	0/1910	0.65	0/2586
3	Q	0.37	0/1910	0.65	0/2586
4	D	0.36	0/1837	0.61	0/2475
4	R	0.36	0/1837	0.60	0/2475
5	E	0.36	0/1800	0.61	0/2433
5	S	0.36	0/1800	0.60	0/2433
6	F	0.37	0/1932	0.58	0/2609
6	T	0.37	0/1932	0.58	0/2609
7	G	0.38	0/1945	0.77	3/2634 (0.1%)
7	U	0.39	0/1945	0.82	3/2634 (0.1%)
8	H	0.37	0/1675	0.89	3/2267 (0.1%)
8	V	0.36	0/1675	0.87	3/2267 (0.1%)
9	I	0.39	0/1611	0.61	0/2174
9	W	0.39	0/1611	0.62	0/2174
10	J	0.37	0/1589	0.65	0/2142
10	X	0.37	0/1589	0.64	0/2142
11	K	0.37	0/1681	0.68	1/2274 (0.0%)
11	Y	0.38	0/1681	0.68	1/2274 (0.0%)
12	L	0.38	0/1795	0.62	0/2420
12	Z	0.38	0/1795	0.62	0/2420
13	M	0.39	0/1783	0.66	0/2420
13	a	0.39	0/1783	0.66	0/2420
14	N	0.35	0/1541	0.60	0/2087
14	b	0.35	0/1541	0.60	0/2087
All	All	0.37	0/49818	0.68	22/67348 (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 (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	U	68	ARG	NE-CZ-NH2	-22.82	108.89	120.30
1	A	4	ARG	NE-CZ-NH2	-20.28	110.16	120.30
1	O	4	ARG	NE-CZ-NH1	-20.04	110.28	120.30
8	V	143	ARG	NE-CZ-NH2	-19.71	110.45	120.30
8	H	143	ARG	NE-CZ-NH1	-19.65	110.48	120.30
7	G	68	ARG	NE-CZ-NH1	-17.89	111.35	120.30
8	H	143	ARG	NE-CZ-NH2	17.35	128.98	120.30
1	O	4	ARG	NE-CZ-NH2	15.92	128.26	120.30
7	G	68	ARG	NE-CZ-NH2	15.47	128.03	120.30
1	A	4	ARG	NE-CZ-NH1	14.72	127.66	120.30
8	V	143	ARG	NE-CZ-NH1	13.83	127.22	120.30
7	U	68	ARG	NE-CZ-NH1	11.98	126.29	120.30
7	U	68	ARG	CD-NE-CZ	11.87	140.21	123.60
1	O	4	ARG	CD-NE-CZ	9.93	137.50	123.60
8	V	143	ARG	CD-NE-CZ	9.56	136.98	123.60
1	A	4	ARG	CD-NE-CZ	9.41	136.78	123.60
8	H	143	ARG	CD-NE-CZ	8.35	135.28	123.60
7	G	68	ARG	CD-NE-CZ	7.67	134.33	123.60
1	O	4	ARG	CG-CD-NE	6.26	124.95	111.80
11	K	4	LEU	CA-CB-CG	5.83	128.71	115.30
11	Y	4	LEU	CA-CB-CG	5.73	128.47	115.30
2	B	51	VAL	CG1-CB-CG2	5.57	119.81	110.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	ARG	Sidechain

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

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	1842	0	1855	1	0
1	O	1842	0	1855	1	0
2	B	1904	0	1904	10	0
2	P	1904	0	1904	11	0
3	C	1881	0	1895	9	0
3	Q	1881	0	1895	8	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	6	0
5	E	1773	0	1775	8	0
5	S	1773	0	1775	7	0
6	F	1892	0	1883	5	0
6	T	1892	0	1883	5	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	5	0
8	H	1648	0	1672	15	0
8	V	1648	0	1672	15	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	11	0
10	X	1561	0	1569	13	0
11	K	1644	0	1594	34	0
11	Y	1644	0	1594	30	0
12	L	1757	0	1711	11	0
12	Z	1757	0	1711	13	0
13	M	1753	0	1754	0	0
13	a	1753	0	1754	0	0
14	N	1512	0	1481	5	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	1	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	N	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	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	2	0
17	K	42	0	0	1	0
17	V	42	0	0	3	0
17	Y	42	0	0	0	0
18	N	5	0	0	0	0
18	b	5	0	0	0	0
19	A	6	0	0	0	0
19	B	14	0	0	0	0
19	C	8	0	0	0	0
19	D	13	0	0	0	0
19	E	11	0	0	1	0
19	F	9	0	0	0	0
19	G	14	0	0	0	0
19	H	12	0	0	0	0
19	I	19	0	0	0	0
19	J	17	0	0	1	0
19	K	24	0	0	0	0
19	L	15	0	0	0	0
19	M	16	0	0	0	0
19	N	13	0	0	1	0
19	O	7	0	0	0	0
19	P	14	0	0	0	0
19	Q	12	0	0	0	0
19	R	7	0	0	0	0
19	S	12	0	0	0	0
19	T	7	0	0	0	0
19	U	12	0	0	0	0
19	V	14	0	0	0	0
19	W	7	0	0	0	0
19	X	13	0	0	1	0
19	Y	18	0	0	0	0
19	Z	12	0	0	0	0
19	a	11	0	0	0	0
19	b	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	49480	0	48730	201	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 2.

All (201) 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)
11:K:77:ALA:O	11:K:121:ARG:NH1	2.00	0.93
11:Y:77:ALA:O	11:Y:121:ARG:NH1	2.02	0.92
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.21	0.87
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.16	0.87
4:R:82:GLU:OE2	11:Y:69:ARG:NH1	2.17	0.77
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.52	0.74
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.53	0.73
1:O:12:PHE:H	2:P:20:GLN:HE22	1.39	0.71
7:G:68:ARG:NH1	14:N:39:ASP:OD2	2.25	0.68
11:Y:145:LYS:HG3	11:Y:148:LEU:HD12	1.76	0.68
11:K:145:LYS:HG3	11:K:148:LEU:HD12	1.75	0.68
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	1.91	0.66
7:G:23:PHE:O	7:G:26:THR:HB	1.95	0.66
11:Y:105:THR:OG1	11:Y:108:GLU:HG3	1.97	0.65
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	1.93	0.65
7:U:23:PHE:O	7:U:26:THR:HB	1.98	0.63
11:K:105:THR:OG1	11:K:108:GLU:HG3	1.98	0.63
11:K:130:GLY:O	11:K:133:GLN:HG2	1.99	0.62
11:Y:130:GLY:O	11:Y:133:GLN:HG2	1.98	0.62
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.13	0.62
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.14	0.61
5:E:92:ASN:HD21	12:L:70:ASN:ND2	1.96	0.61
2:B:12:PHE:H	3:C:17:GLN:HE22	1.48	0.61
5:E:92:ASN:ND2	12:L:70:ASN:HD21	1.94	0.61
4:D:82:GLU:OE2	11:K:69:ARG:NH1	2.34	0.60
11:Y:137:TYR:O	11:Y:141:ASP:HB2	2.02	0.59
11:K:137:TYR:O	11:K:141:ASP:HB2	2.03	0.59
10:J:145:ASP:OD1	11:Y:209:ASN:ND2	2.35	0.59
9:I:38:LYS:HG2	11:Y:211:ILE:HD11	1.84	0.59
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.67	0.58
10:J:139:TYR:CE1	11:Y:134:THR:HG22	2.38	0.58
7:G:99:TYR:O	8:H:78:THR:HB	2.04	0.58
1:A:12:PHE:H	2:B:20:GLN:HE22	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:35:ILE:HB	11:K:45:MET:CE	2.34	0.57
5:S:12:PHE:H	6:T:19:GLN:HE22	1.50	0.57
11:K:209:ASN:ND2	10:X:145:ASP:OD1	2.37	0.56
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.70	0.56
3:Q:165:ASN:HB2	3:Q:200:VAL:HG11	1.87	0.56
11:K:18:SER:OG	11:K:29:GLN:O	2.23	0.56
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.87	0.56
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.88	0.56
11:Y:35:ILE:HB	11:Y:45:MET:CE	2.36	0.56
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.88	0.55
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.88	0.55
3:C:165:ASN:HB2	3:C:200:VAL:HG11	1.88	0.54
5:E:12:PHE:H	6:F:19:GLN:HE22	1.53	0.54
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.87	0.54
3:Q:203:THR:HG22	3:Q:204:GLY:H	1.72	0.54
3:C:203:THR:HG22	3:C:204:GLY:H	1.72	0.54
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.90	0.54
11:K:176:ASN:ND2	11:K:190:ASN:HD22	2.06	0.53
11:Y:196:LEU:O	11:Y:200:VAL:HG23	2.07	0.53
11:K:196:LEU:O	11:K:200:VAL:HG23	2.09	0.53
11:K:211:ILE:HD11	9:W:38:LYS:HG2	1.91	0.53
3:C:48:SER:HB2	3:C:207:ASN:HD21	1.74	0.52
11:Y:51:ASP:HB3	11:Y:97:MET:CE	2.40	0.52
11:K:51:ASP:HB3	11:K:97:MET:CE	2.40	0.52
11:K:1:THR:N	17:K:301:GRT:O49	2.31	0.52
6:T:123:ASN:HD22	6:T:124:SER:N	2.08	0.52
11:K:134:THR:HG22	10:X:139:TYR:CE1	2.45	0.51
11:K:51:ASP:HB3	11:K:97:MET:HE2	1.91	0.51
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.76	0.51
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.75	0.51
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.41	0.51
11:Y:51:ASP:HB3	11:Y:97:MET:HE2	1.92	0.51
11:K:209:ASN:O	9:W:37:ASN:OD1	2.28	0.50
6:F:123:ASN:HD22	6:F:124:SER:N	2.10	0.50
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.76	0.50
3:Q:48:SER:HB2	3:Q:207:ASN:HD21	1.75	0.50
11:K:204:GLU:OE1	10:X:146:HIS:CE1	2.65	0.49
7:U:99:TYR:O	8:V:78:THR:HB	2.13	0.49
11:Y:139:VAL:HG21	11:Y:163:ALA:CB	2.42	0.49
8:H:45:GLY:HA3	8:H:52:THR:HG21	1.92	0.49
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:18:SER:OG	11:Y:29:GLN:O	2.29	0.49
8:V:1:THR:N	17:V:301:GRT:O50	2.35	0.49
8:V:45:GLY:HA3	8:V:52:THR:HG21	1.93	0.49
12:L:220:LYS:HE3	12:L:222:ASP:OD1	2.13	0.49
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.77	0.49
2:B:51:VAL:O	2:B:52:THR:O	2.31	0.49
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.94	0.49
10:J:146:HIS:CE1	11:Y:204:GLU:OE1	2.66	0.49
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.95	0.49
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.95	0.48
5:E:68:HIS:HE1	5:E:102:LEU:O	1.97	0.48
11:K:139:VAL:HG21	11:K:163:ALA:CB	2.43	0.48
12:Z:220:LYS:HE3	12:Z:222:ASP:OD1	2.14	0.48
8:H:120:ASP:HB3	8:H:122:LEU:HD22	1.96	0.48
11:K:76:VAL:N	11:K:108:GLU:OE2	2.44	0.48
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.46	0.47
11:Y:44:THR:O	11:Y:99:THR:OG1	2.32	0.47
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.79	0.47
8:V:184:ASP:HB3	8:V:186:LEU:CD1	2.44	0.47
8:H:184:ASP:HB3	8:H:186:LEU:CD1	2.44	0.47
10:J:174:MET:HB2	19:J:207:HOH:O	2.14	0.47
11:K:44:THR:O	11:K:99:THR:OG1	2.32	0.47
11:Y:139:VAL:HG21	11:Y:163:ALA:HB2	1.96	0.47
11:K:139:VAL:HG23	10:X:142:SER:HB2	1.97	0.47
8:H:114:TYR:CE2	8:H:127:MET:CE	2.97	0.47
5:S:68:HIS:HE1	5:S:102:LEU:O	1.98	0.47
8:V:114:TYR:CE2	8:V:127:MET:CE	2.98	0.47
11:Y:176:ASN:ND2	11:Y:190:ASN:HD22	2.13	0.47
11:K:201:LYS:NZ	11:K:207:PHE:O	2.47	0.47
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.63	0.47
3:C:48:SER:HB2	3:C:207:ASN:ND2	2.30	0.46
11:K:139:VAL:HG21	11:K:163:ALA:HB2	1.97	0.46
11:Y:35:ILE:HB	11:Y:45:MET:HE2	1.97	0.46
8:V:143:ARG:NH1	8:V:150:GLU:OE1	2.49	0.46
10:J:139:TYR:OH	10:X:25:ILE:O	2.34	0.46
3:Q:48:SER:HB2	3:Q:207:ASN:ND2	2.31	0.46
8:V:25:VAL:HG11	9:W:146:PHE:CD2	2.51	0.46
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.81	0.45
8:H:132:LEU:HD22	14:N:25:TYR:CE1	2.50	0.45
2:P:30:HIS:O	2:P:50:LYS:NZ	2.35	0.45
8:H:25:VAL:HG11	9:I:146:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:51:VAL:O	2:P:52:THR:O	2.34	0.45
11:Y:50:ALA:CB	12:Z:128:VAL:HG23	2.46	0.45
2:B:145:TYR:OH	2:B:217:LYS:N	2.46	0.45
8:H:184:ASP:HB3	8:H:186:LEU:HD11	1.98	0.45
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.52	0.45
11:K:35:ILE:HB	11:K:45:MET:HE1	1.97	0.45
2:B:217:LYS:O	2:B:219:ALA:N	2.49	0.45
7:G:73:VAL:HG12	7:G:133:THR:HB	1.98	0.45
8:V:184:ASP:HB3	8:V:186:LEU:HD11	1.99	0.45
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.64	0.45
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.52	0.44
10:J:50:ALA:O	11:K:91:LYS:NZ	2.50	0.44
6:F:123:ASN:HD22	6:F:123:ASN:C	2.20	0.44
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.53	0.44
11:Y:76:VAL:N	11:Y:108:GLU:OE2	2.45	0.44
12:L:8:ASN:HA	12:L:30:ILE:O	2.17	0.44
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.17	0.44
8:H:149:GLU:O	8:H:153:ASN:ND2	2.51	0.44
8:V:53:ASP:OD2	17:V:301:GRT:N45	2.51	0.44
3:C:99:GLU:CD	11:K:121:ARG:HH22	2.21	0.44
11:K:142:SER:HB3	10:X:143:LEU:HD21	2.00	0.44
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.99	0.44
11:Y:201:LYS:NZ	11:Y:207:PHE:O	2.48	0.44
11:K:86:LEU:C	11:K:86:LEU:HD13	2.38	0.43
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.00	0.43
6:T:123:ASN:HD22	6:T:123:ASN:C	2.21	0.43
7:U:73:VAL:HG12	7:U:133:THR:HB	1.99	0.43
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.99	0.43
2:P:217:LYS:O	2:P:219:ALA:N	2.51	0.43
9:I:94:LEU:HD11	9:I:106:PRO:HG2	2.01	0.43
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.39	0.43
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.53	0.43
8:H:43:CYS:SG	8:H:98:LEU:HB3	2.58	0.43
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.67	0.43
9:W:94:LEU:HD11	9:W:106:PRO:HG2	2.00	0.43
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.54	0.42
8:H:54:MET:HG3	9:I:95:TYR:CG	2.54	0.42
11:K:162:LEU:HD22	11:K:200:VAL:HG21	2.01	0.42
8:V:149:GLU:O	8:V:153:ASN:ND2	2.51	0.42
10:J:25:ILE:O	10:X:139:TYR:OH	2.37	0.42
6:F:191:GLN:HE22	6:F:194:LYS:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.01	0.42
11:Y:162:LEU:HD22	11:Y:200:VAL:HG21	2.01	0.42
8:H:24:MET:HE2	12:Z:196:ILE:HD11	2.02	0.42
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.49	0.42
10:J:177:LYS:NZ	10:X:169:GLU:O	2.52	0.42
2:P:145:TYR:OH	2:P:217:LYS:N	2.45	0.42
5:E:147:GLN:HG2	19:E:310:HOH:O	2.19	0.42
12:L:196:ILE:HD11	8:V:24:MET:HE1	2.02	0.41
10:X:174:MET:HB2	19:X:207:HOH:O	2.19	0.41
11:K:12:ILE:HB	11:K:180:VAL:HB	2.02	0.41
8:H:44:CYS:HB2	8:H:99:VAL:HB	2.01	0.41
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.02	0.41
11:K:197:PHE:HZ	11:K:210:VAL:HG21	1.86	0.41
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.56	0.41
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.02	0.41
8:V:187:ARG:HA	8:V:188:PRO:HA	1.86	0.41
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.02	0.41
3:C:203:THR:HB	3:C:207:ASN:HD22	1.85	0.41
2:B:215:ILE:HG12	2:B:226:GLN:HG2	2.03	0.41
6:T:191:GLN:HE22	6:T:194:LYS:HE2	1.85	0.41
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.01	0.41
12:L:28:ARG:HG2	12:L:30:ILE:HG23	2.03	0.41
14:N:36:ARG:HD2	19:N:306:HOH:O	2.20	0.41
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.68	0.41
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.03	0.41
2:B:30:HIS:O	2:B:50:LYS:NZ	2.36	0.41
5:E:9:THR:HG21	5:E:119:THR:HA	2.03	0.40
8:H:53:ASP:OD1	17:H:301:GRT:N45	2.55	0.40
8:H:53:ASP:OD2	17:H:301:GRT:N45	2.54	0.40
11:K:176:ASN:HD21	11:K:190:ASN:HD22	1.67	0.40
3:Q:203:THR:HB	3:Q:207:ASN:HD22	1.86	0.40
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.51	0.40
8:V:44:CYS:HB2	8:V:99:VAL:HB	2.02	0.40
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.20	0.40
12:Z:28:ARG:HG2	12:Z:30:ILE:HG23	2.03	0.40
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.04	0.40
3:C:9:PHE:H	4:D:15:GLN:HE22	1.70	0.40
8:V:53:ASP:OD1	17:V:301:GRT:N45	2.55	0.40
11:Y:197:PHE:HZ	11:Y:210:VAL:HG21	1.84	0.40
6:F:198:LEU:HD12	6:F:243:ILE:HG22	2.03	0.40
2:P:145:TYR:OH	2:P:217:LYS:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:9:THR:HG21	5:S:119:THR:HA	2.03	0.40
6:T:198:LEU:HD12	6:T:243:ILE:HG22	2.04	0.40
8:V:19:ARG:HG2	8:V:21:THR:HG23	2.04	0.40
11:Y:4:LEU:HD13	11:Y:161:ILE:HD11	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	236/250 (94%)	228 (97%)	7 (3%)	1 (0%)	34	72
1	O	236/250 (94%)	227 (96%)	8 (3%)	1 (0%)	34	72
2	B	242/258 (94%)	235 (97%)	4 (2%)	3 (1%)	13	48
2	P	242/258 (94%)	235 (97%)	5 (2%)	2 (1%)	19	57
3	C	238/254 (94%)	236 (99%)	1 (0%)	1 (0%)	34	72
3	Q	238/254 (94%)	236 (99%)	1 (0%)	1 (0%)	34	72
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	219 (96%)	10 (4%)	0	100	100
5	S	229/234 (98%)	219 (96%)	10 (4%)	0	100	100
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	240 (100%)	1 (0%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	189 (98%)	3 (2%)	1 (0%)	29	68
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	68
11	K	210/212 (99%)	192 (91%)	16 (8%)	2 (1%)	15	53
11	Y	210/212 (99%)	192 (91%)	16 (8%)	2 (1%)	15	53
12	L	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
12	Z	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
13	M	222/246 (90%)	213 (96%)	9 (4%)	0	100	100
13	a	222/246 (90%)	213 (96%)	9 (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%)	6056 (97%)	157 (2%)	15 (0%)	47	82

All (15) 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	Y	148	LEU
11	K	148	LEU
3	C	183	PRO
3	Q	183	PRO
2	B	51	VAL
10	J	9	VAL
10	X	9	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/209 (96%)	197 (98%)	4 (2%)	55	83
1	O	201/209 (96%)	197 (98%)	4 (2%)	55	83
2	B	203/216 (94%)	193 (95%)	10 (5%)	25	61
2	P	203/216 (94%)	194 (96%)	9 (4%)	28	65
3	C	212/226 (94%)	201 (95%)	11 (5%)	23	59
3	Q	212/226 (94%)	201 (95%)	11 (5%)	23	59
4	D	194/215 (90%)	186 (96%)	8 (4%)	30	67
4	R	194/215 (90%)	186 (96%)	8 (4%)	30	67
5	E	190/193 (98%)	179 (94%)	11 (6%)	20	55
5	S	190/193 (98%)	179 (94%)	11 (6%)	20	55
6	F	201/239 (84%)	192 (96%)	9 (4%)	27	64
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	64
7	G	206/210 (98%)	197 (96%)	9 (4%)	28	65
7	U	206/210 (98%)	197 (96%)	9 (4%)	28	65
8	H	179/194 (92%)	170 (95%)	9 (5%)	24	60
8	V	179/194 (92%)	171 (96%)	8 (4%)	27	64
9	I	172/173 (99%)	166 (96%)	6 (4%)	36	71
9	W	172/173 (99%)	167 (97%)	5 (3%)	42	76
10	J	173/175 (99%)	167 (96%)	6 (4%)	36	71
10	X	173/175 (99%)	167 (96%)	6 (4%)	36	71
11	K	169/169 (100%)	160 (95%)	9 (5%)	22	58
11	Y	169/169 (100%)	160 (95%)	9 (5%)	22	58
12	L	185/185 (100%)	177 (96%)	8 (4%)	29	66
12	Z	185/185 (100%)	177 (96%)	8 (4%)	29	66
13	M	192/208 (92%)	185 (96%)	7 (4%)	35	70
13	a	192/208 (92%)	185 (96%)	7 (4%)	35	70
14	N	162/162 (100%)	158 (98%)	4 (2%)	47	79
14	b	162/162 (100%)	158 (98%)	4 (2%)	47	79
All	All	5278/5548 (95%)	5059 (96%)	219 (4%)	30	67

All (219) 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	49	THR
3	C	51	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	202	GLN
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
5	E	55	LEU
5	E	71	LEU
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	208	ASP

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Mol	Chain	Res	Type
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	235	ARG
7	G	236	LEU
8	H	14	LEU
8	H	24	MET
8	H	78	THR
8	H	98	LEU
8	H	122	LEU
8	H	131	SER
8	H	132	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
10	J	3	ILE
10	J	35	THR
10	J	78	GLN
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	9	GLN

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Mol	Chain	Res	Type
11	K	18	SER
11	K	21	THR
11	K	35	ILE
11	K	73	ARG
11	K	100	MET
11	K	108	GLU
11	K	134	THR
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
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	48	SER

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Mol	Chain	Res	Type
3	Q	49	THR
3	Q	51	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	202	GLN
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	8	ASP
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	208	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
7	U	122	ARG
7	U	125	MET

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Mol	Chain	Res	Type
7	U	154	TYR
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	131	SER
8	V	143	ARG
8	V	201	ARG
8	V	219	LEU
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	35	THR
10	X	78	GLN
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	18	SER
11	Y	21	THR
11	Y	35	ILE
11	Y	73	ARG
11	Y	100	MET
11	Y	108	GLU
11	Y	134	THR
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
13	a	70	LEU

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Mol	Chain	Res	Type
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (133) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
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	210	GLN
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	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN

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Mol	Chain	Res	Type
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
8	H	153	ASN
9	I	71	ASN
9	I	88	GLN
10	J	55	GLN
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	176	ASN
11	K	190	ASN
12	L	3	ASN
12	L	49	ASN
12	L	55	ASN
12	L	80	ASN
12	L	152	ASN
12	L	153	GLN
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	218	ASN
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN

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Mol	Chain	Res	Type
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
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	37	ASN
9	W	71	ASN
9	W	88	GLN
10	X	55	GLN
10	X	86	GLN
10	X	146	HIS
11	Y	9	GLN

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Mol	Chain	Res	Type
11	Y	85	ASN
11	Y	133	GLN
11	Y	176	ASN
11	Y	190	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	80	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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 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	$\#\|Z\| > 2$
17	GRT	V	301	8	42,43,43	1.78	8 (19%)	53,57,57	1.45	9 (16%)
18	SO4	N	202	-	4,4,4	0.47	0	6,6,6	0.18	0
17	GRT	K	301	11	42,43,43	1.62	8 (19%)	53,57,57	1.43	8 (15%)
18	SO4	b	201	-	4,4,4	0.50	0	6,6,6	0.15	0
17	GRT	Y	301	11	42,43,43	1.66	8 (19%)	53,57,57	1.44	9 (16%)
17	GRT	H	301	8	42,43,43	1.78	8 (19%)	53,57,57	1.41	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	Y	301	11	-	5/44/44/44	0/2/2/2
17	GRT	K	301	11	-	5/44/44/44	0/2/2/2
17	GRT	V	301	8	-	3/44/44/44	0/2/2/2
17	GRT	H	301	8	-	4/44/44/44	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	301	GRT	C37-C38	-5.18	1.38	1.51
17	K	301	GRT	C37-C38	-5.13	1.39	1.51
17	H	301	GRT	C7-C3	-4.61	1.40	1.51
17	H	301	GRT	C37-C38	-4.59	1.40	1.51
17	V	301	GRT	C7-C3	-4.58	1.40	1.51
17	V	301	GRT	C37-C38	-4.58	1.40	1.51
17	V	301	GRT	N10-N9	4.55	1.35	1.23
17	K	301	GRT	C7-C3	-4.45	1.40	1.51
17	H	301	GRT	N10-N9	4.44	1.35	1.23
17	Y	301	GRT	C7-C3	-4.35	1.40	1.51
17	K	301	GRT	N10-N9	4.25	1.34	1.23
17	Y	301	GRT	N10-N9	4.16	1.34	1.23
17	V	301	GRT	C47-S48	3.92	1.83	1.78
17	H	301	GRT	O49-S48	3.79	1.52	1.44
17	V	301	GRT	O49-S48	3.64	1.52	1.44
17	Y	301	GRT	O50-S48	3.45	1.52	1.44
17	H	301	GRT	C47-S48	3.41	1.83	1.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	GRT	C44-C41	-3.35	1.39	1.51
17	V	301	GRT	O50-S48	3.22	1.51	1.44
17	H	301	GRT	C46-C47	3.17	1.55	1.52
17	K	301	GRT	O50-S48	3.14	1.51	1.44
17	V	301	GRT	C44-C41	-3.13	1.40	1.51
17	H	301	GRT	O50-S48	3.10	1.51	1.44
17	V	301	GRT	C46-C47	2.96	1.55	1.52
17	K	301	GRT	C44-C41	-2.94	1.41	1.51
17	Y	301	GRT	C44-C41	-2.94	1.41	1.51
17	Y	301	GRT	O49-S48	2.89	1.50	1.44
17	K	301	GRT	O49-S48	2.68	1.50	1.44
17	Y	301	GRT	C46-C47	2.67	1.55	1.52
17	Y	301	GRT	C47-S48	2.45	1.81	1.78
17	K	301	GRT	C47-S48	2.42	1.81	1.78
17	K	301	GRT	C46-C47	2.18	1.54	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	H	301	GRT	O50-S48-O49	-4.97	106.46	117.09
17	K	301	GRT	O50-S48-O49	-4.95	106.52	117.09
17	V	301	GRT	O50-S48-O49	-4.91	106.60	117.09
17	Y	301	GRT	O50-S48-O49	-4.45	107.59	117.09
17	Y	301	GRT	O50-S48-C51	3.69	112.61	108.91
17	Y	301	GRT	C33-C28-N27	-3.65	102.91	113.17
17	K	301	GRT	C33-C28-N27	-3.52	103.29	113.17
17	K	301	GRT	O50-S48-C51	3.46	112.39	108.91
17	V	301	GRT	C25-C15-N14	-3.19	102.49	111.16
17	V	301	GRT	C46-C36-C37	3.15	116.26	111.14
17	H	301	GRT	C25-C15-N14	-3.14	102.62	111.16
17	H	301	GRT	C46-C36-C37	3.02	116.05	111.14
17	H	301	GRT	C33-C28-N27	-2.72	105.53	113.17
17	K	301	GRT	O49-S48-C47	2.69	110.23	108.34
17	H	301	GRT	C7-C8-C12	-2.68	103.84	109.55
17	Y	301	GRT	C12-C8-N9	-2.67	102.50	108.85
17	V	301	GRT	C37-C38-C39	2.65	126.17	120.91
17	V	301	GRT	C33-C28-N27	-2.64	105.75	113.17
17	Y	301	GRT	C8-N9-N10	2.64	118.02	115.24
17	K	301	GRT	C37-C38-C39	2.62	126.10	120.91
17	V	301	GRT	C7-C8-C12	-2.61	104.01	109.55
17	Y	301	GRT	C37-C38-C39	2.56	125.99	120.91
17	K	301	GRT	C12-C8-N9	-2.49	102.94	108.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Y	301	GRT	O49-S48-C47	2.46	110.07	108.34
17	K	301	GRT	C8-N9-N10	2.44	117.81	115.24
17	H	301	GRT	C37-C38-C39	2.43	125.74	120.91
17	K	301	GRT	C37-C38-C43	-2.37	116.20	120.91
17	V	301	GRT	C46-C36-N35	-2.35	107.24	110.54
17	V	301	GRT	C51-S48-C47	2.24	113.86	105.21
17	Y	301	GRT	C37-C38-C43	-2.17	116.61	120.91
17	H	301	GRT	C46-C36-N35	-2.16	107.50	110.54
17	V	301	GRT	C37-C38-C43	-2.15	116.64	120.91
17	H	301	GRT	C51-S48-C47	2.15	113.48	105.21
17	Y	301	GRT	C37-C36-N35	-2.09	106.37	110.39

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	GRT	N11-N10-N9-C8
17	K	301	GRT	N11-N10-N9-C8
17	H	301	GRT	C36-C37-C38-C39
17	V	301	GRT	C36-C37-C38-C39
17	H	301	GRT	C36-C37-C38-C43
17	V	301	GRT	C36-C37-C38-C43
17	K	301	GRT	C36-C37-C38-C39
17	Y	301	GRT	C36-C37-C38-C39
17	Y	301	GRT	C36-C37-C38-C43
17	K	301	GRT	C36-C37-C38-C43
17	Y	301	GRT	N11-N10-N9-C8
17	H	301	GRT	C12-C8-N9-N10
17	V	301	GRT	C12-C8-N9-N10
17	Y	301	GRT	C36-C46-C47-S48
17	Y	301	GRT	C33-C28-N27-C25
17	K	301	GRT	C36-C46-C47-S48
17	K	301	GRT	C33-C28-N27-C25

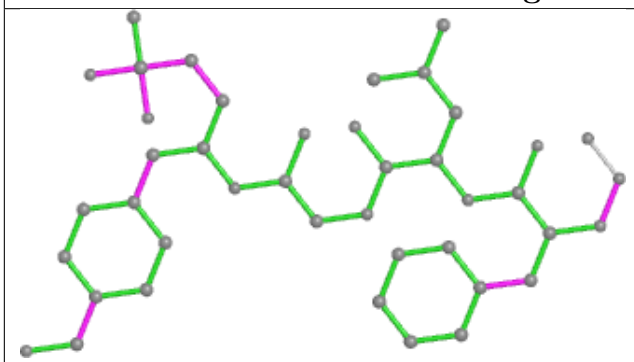
There are no ring outliers.

3 monomers are involved in 6 short contacts:

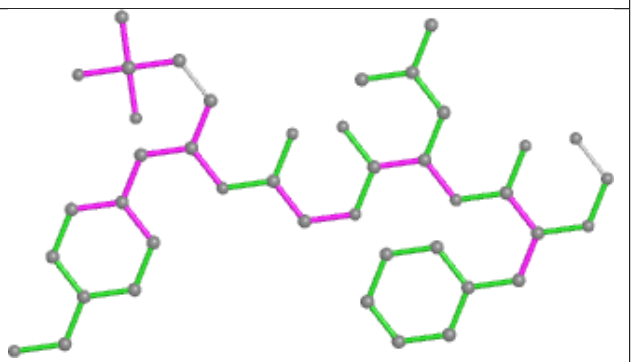
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	V	301	GRT	3	0
17	K	301	GRT	1	0
17	H	301	GRT	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

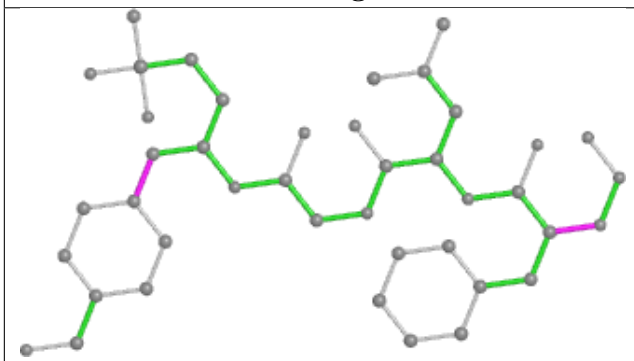
Ligand GRT V 301



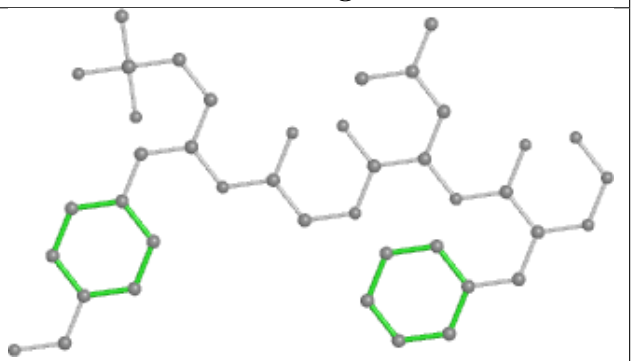
Bond lengths



Bond angles

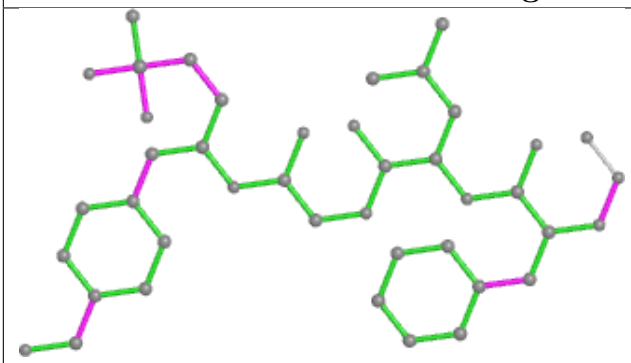


Torsions

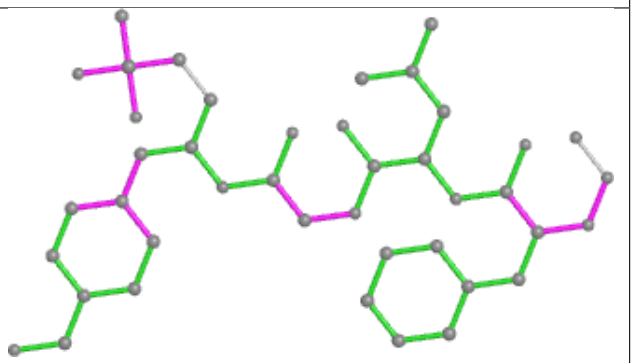


Rings

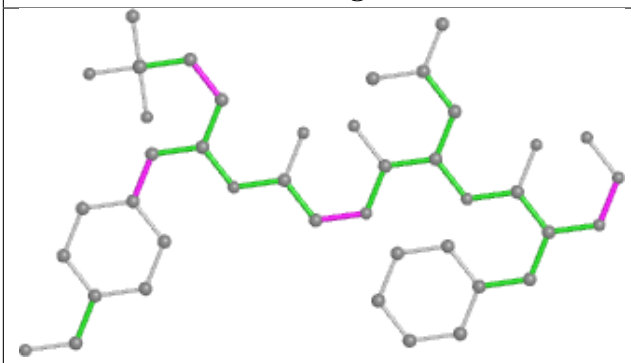
Ligand GRT K 301



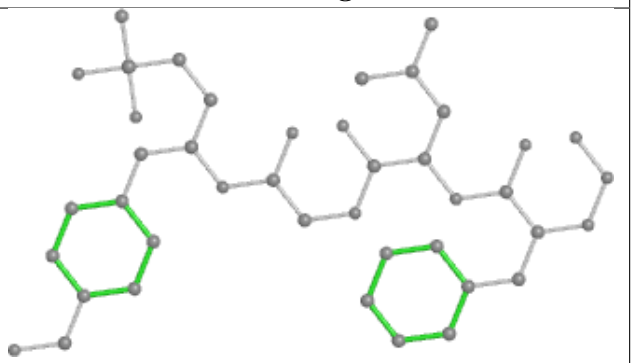
Bond lengths



Bond angles

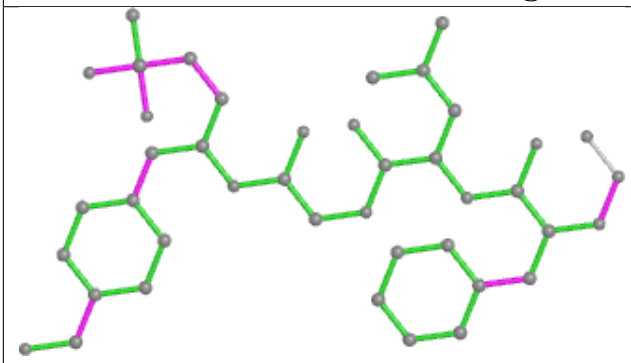


Torsions

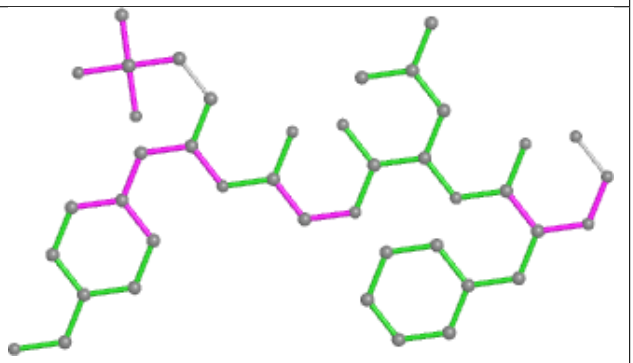


Rings

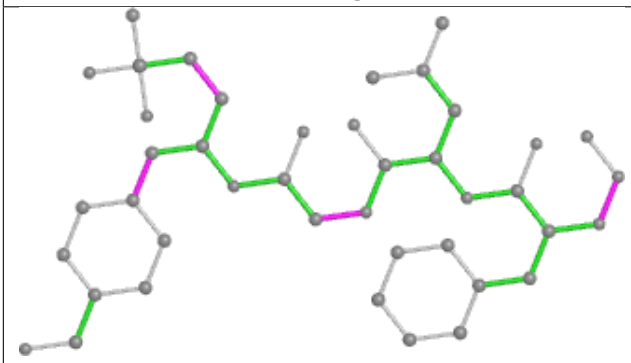
Ligand GRT Y 301



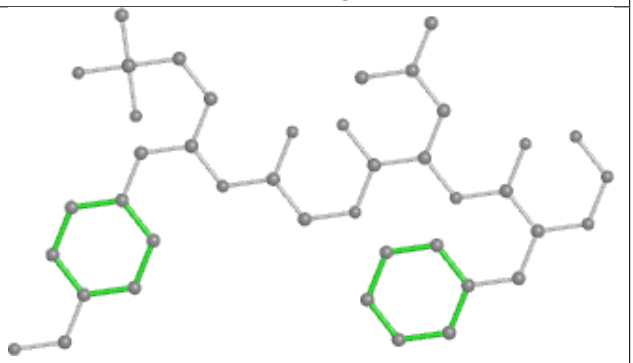
Bond lengths



Bond angles

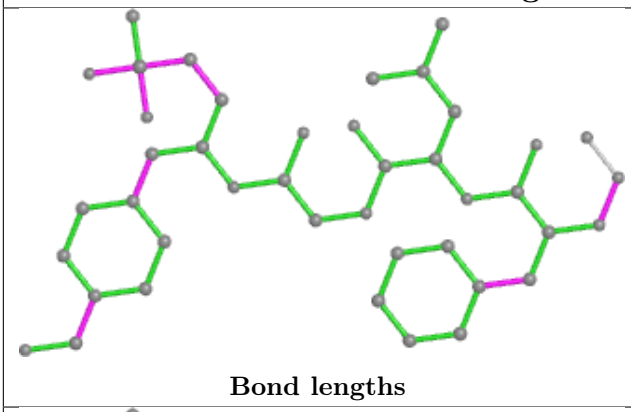


Torsions

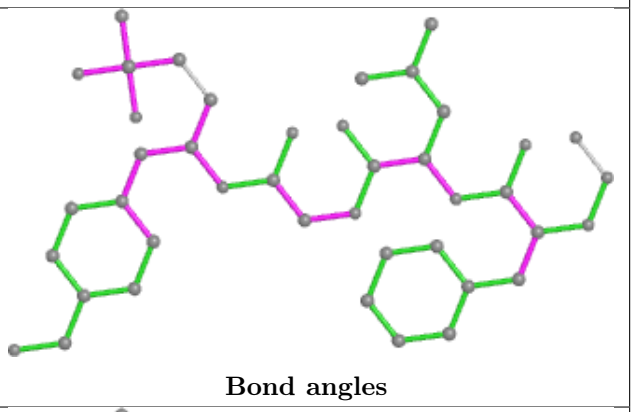


Rings

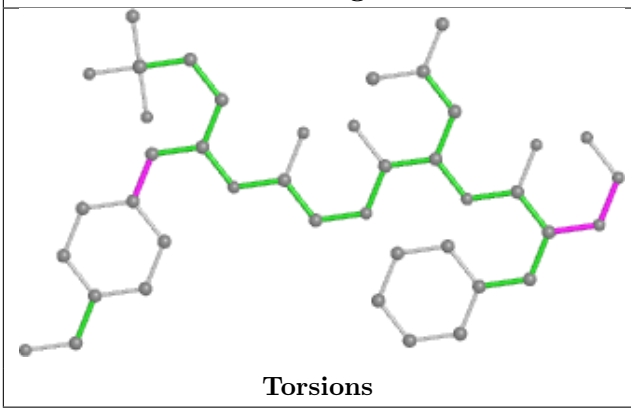
Ligand GRT H 301



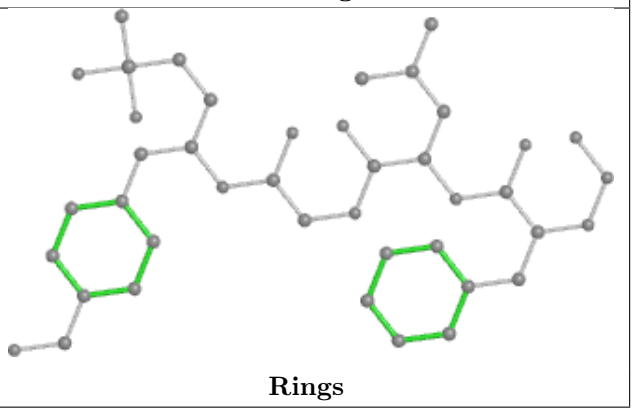
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	240/250 (96%)	-0.62	2 (0%)	86	65	47, 66, 107, 142	0
1	O	240/250 (96%)	-0.52	4 (1%)	70	41	54, 77, 122, 156	0
2	B	244/258 (94%)	-0.54	5 (2%)	65	36	47, 70, 118, 173	0
2	P	244/258 (94%)	-0.53	8 (3%)	46	20	52, 72, 119, 168	0
3	C	240/254 (94%)	-0.53	5 (2%)	63	34	48, 71, 133, 162	0
3	Q	240/254 (94%)	-0.37	8 (3%)	46	20	60, 89, 167, 184	0
4	D	235/260 (90%)	-0.67	2 (0%)	84	63	49, 70, 102, 143	0
4	R	235/260 (90%)	-0.57	2 (0%)	84	63	57, 79, 120, 150	0
5	E	231/234 (98%)	-0.61	1 (0%)	92	79	52, 72, 110, 149	0
5	S	231/234 (98%)	-0.47	5 (2%)	62	33	54, 85, 131, 169	0
6	F	243/288 (84%)	-0.69	1 (0%)	92	79	47, 67, 115, 146	0
6	T	243/288 (84%)	-0.64	1 (0%)	92	79	49, 79, 131, 163	0
7	G	241/252 (95%)	-0.73	0	100	100	47, 64, 101, 150	0
7	U	241/252 (95%)	-0.63	1 (0%)	92	79	54, 69, 103, 146	0
8	H	219/234 (93%)	-0.65	1 (0%)	91	75	42, 60, 114, 131	0
8	V	219/234 (93%)	-0.60	4 (1%)	68	40	46, 64, 119, 148	0
9	I	204/205 (99%)	-0.88	0	100	100	40, 56, 82, 111	0
9	W	204/205 (99%)	-0.85	2 (0%)	82	59	42, 57, 84, 107	0
10	J	195/198 (98%)	-0.73	1 (0%)	91	75	43, 61, 86, 133	0
10	X	195/198 (98%)	-0.70	2 (1%)	82	59	45, 64, 88, 151	0
11	K	212/212 (100%)	-0.77	0	100	100	50, 67, 96, 121	0
11	Y	212/212 (100%)	-0.65	2 (0%)	84	63	52, 70, 101, 128	0
12	L	222/222 (100%)	-0.76	0	100	100	41, 59, 100, 130	0
12	Z	222/222 (100%)	-0.74	0	100	100	41, 60, 100, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	224/246 (91%)	-0.67	2 (0%) 84 63	42, 63, 92, 132	0
13	a	224/246 (91%)	-0.66	5 (2%) 62 33	40, 61, 90, 135	0
14	N	196/196 (100%)	-0.80	1 (0%) 91 75	42, 56, 89, 112	0
14	b	196/196 (100%)	-0.79	0 100 100	43, 59, 89, 118	0
All	All	6292/6618 (95%)	-0.65	65 (1%) 82 59	40, 67, 116, 184	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	221	ASP	5.6
2	B	221	ASP	5.5
2	P	219	ALA	4.6
13	a	224	ASP	4.5
13	a	216	ASN	4.4
2	B	220	ASN	4.4
1	O	230	ASP	4.2
5	S	202	ASP	3.9
3	Q	49	THR	3.8
3	Q	239	GLN	3.8
2	B	51	VAL	3.7
2	P	59	ASP	3.6
5	E	202	ASP	3.6
2	P	220	ASN	3.5
1	A	230	ASP	3.4
13	M	1	THR	3.4
3	C	202	GLN	3.3
13	a	1	THR	3.3
8	V	196	GLY	3.2
13	M	216	ASN	3.1
8	H	196	GLY	3.1
10	X	1	MET	3.0
1	O	1	MET	3.0
3	Q	240	GLU	3.0
3	Q	50	LEU	2.9
8	V	219	LEU	2.9
11	Y	147	ASP	2.9
1	O	231	LYS	2.8
3	Q	48	SER	2.8
10	X	194	ASP	2.8
1	A	1	MET	2.8
13	a	215	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
5	S	54	GLU	2.7
6	T	181	GLU	2.7
5	S	204	SER	2.6
2	B	218	GLY	2.6
13	a	220	ASP	2.6
2	B	222	GLY	2.5
3	C	206	LYS	2.5
1	O	249	ALA	2.5
3	C	50	LEU	2.5
3	C	239	GLN	2.5
8	V	218	PRO	2.5
3	Q	236	GLN	2.4
2	P	223	GLU	2.4
3	Q	206	LYS	2.4
2	P	218	GLY	2.4
4	D	242	GLU	2.3
2	P	203	SER	2.3
2	P	51	VAL	2.3
5	S	180	LYS	2.2
9	W	1	SER	2.2
4	R	1	ASP	2.2
3	Q	202	GLN	2.2
10	J	1	MET	2.2
7	U	242	GLN	2.2
4	R	125	LEU	2.2
8	V	194	LYS	2.2
4	D	241	ALA	2.1
14	N	195	GLN	2.1
5	S	225	ASP	2.1
6	F	205	GLU	2.0
3	C	238	LYS	2.0
11	Y	106	ARG	2.0
9	W	133	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

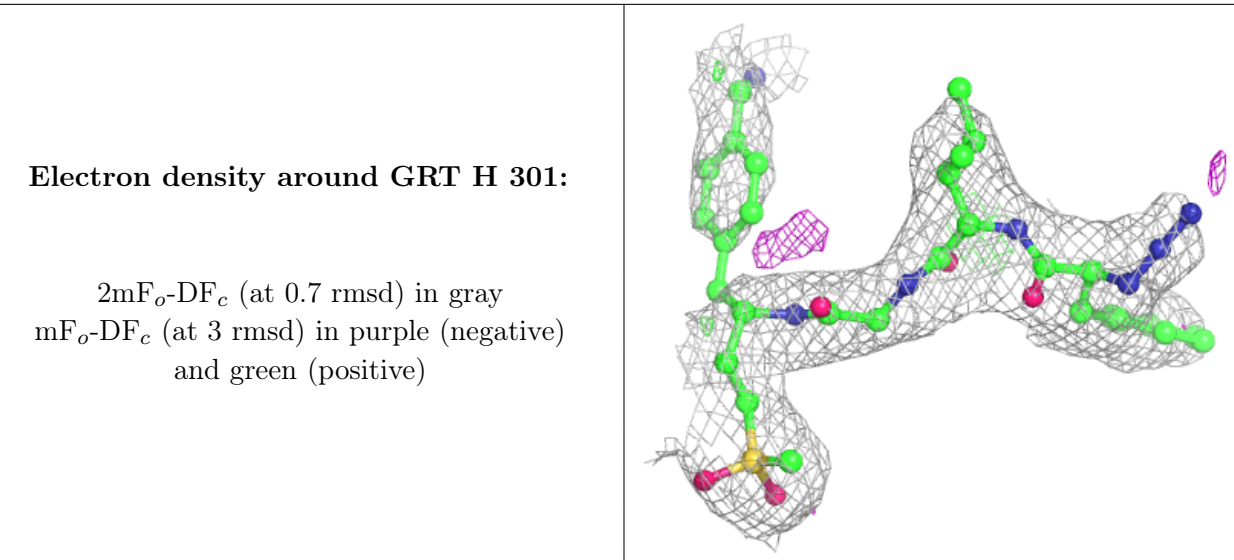
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

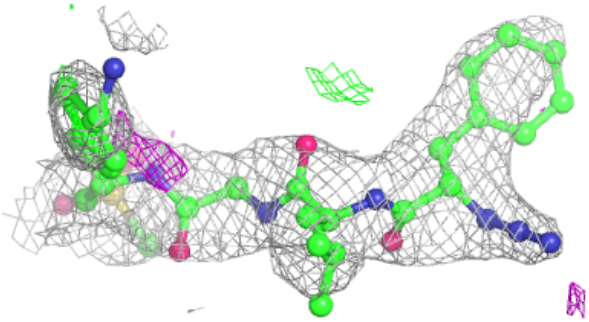
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	W	301	1/1	0.91	0.38	80,80,80,80	0
15	MG	Z	301	1/1	0.91	0.35	68,68,68,68	0
17	GRT	H	301	42/42	0.91	0.24	82,88,102,108	0
17	GRT	V	301	42/42	0.91	0.25	79,89,97,104	0
17	GRT	Y	301	42/42	0.91	0.22	62,86,103,108	0
15	MG	I	301	1/1	0.92	0.36	78,78,78,78	0
15	MG	K	302	1/1	0.93	0.15	84,84,84,84	0
15	MG	Y	302	1/1	0.93	0.19	96,96,96,96	0
16	CL	U	301	1/1	0.94	0.51	93,93,93,93	0
17	GRT	K	301	42/42	0.94	0.18	61,83,101,104	0
18	SO4	b	201	5/5	0.94	0.29	75,84,89,91	0
18	SO4	N	202	5/5	0.95	0.31	76,81,83,91	0
15	MG	N	201	1/1	0.95	0.22	70,70,70,70	0
16	CL	G	302	1/1	0.96	0.41	80,80,80,80	0
15	MG	V	302	1/1	0.96	0.20	83,83,83,83	0
15	MG	G	301	1/1	0.98	0.04	68,68,68,68	0

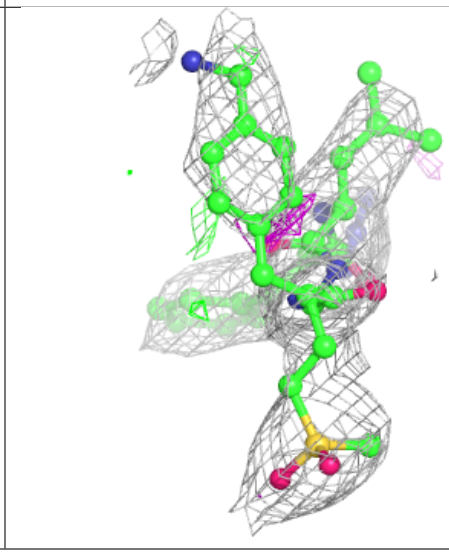
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

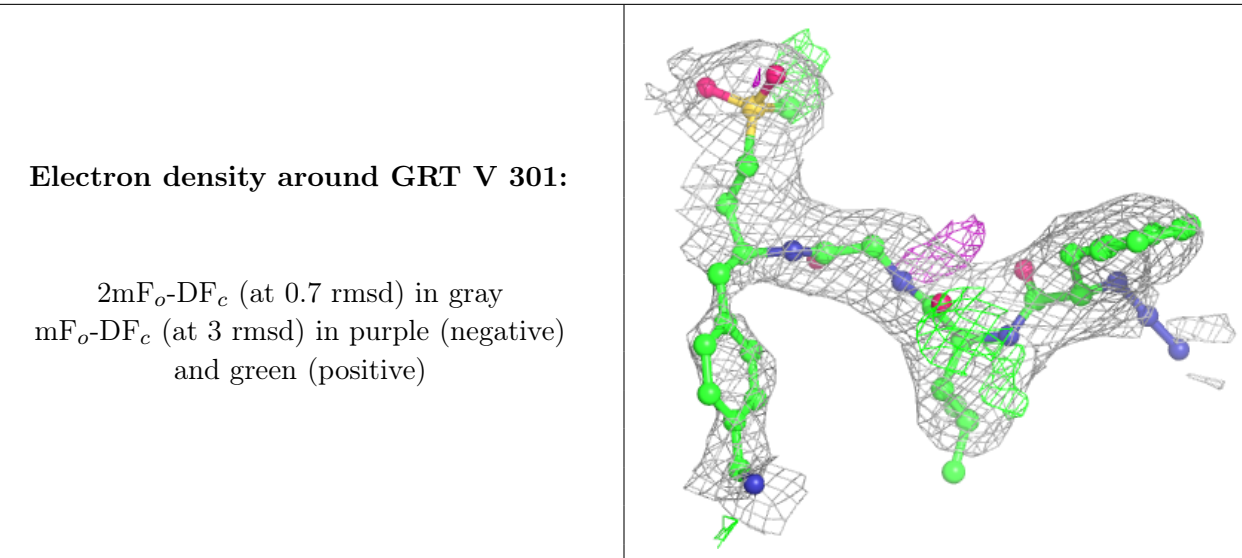


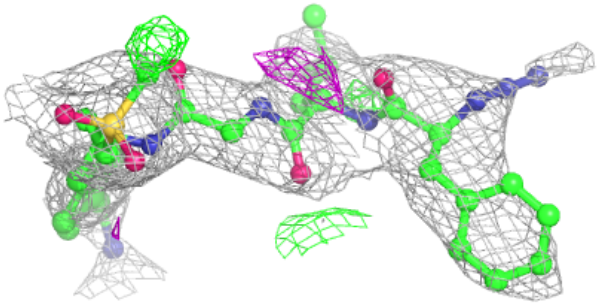


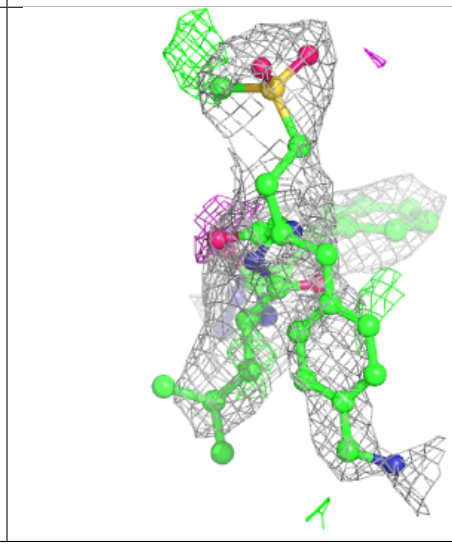


Electron density around GRT V 301:

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

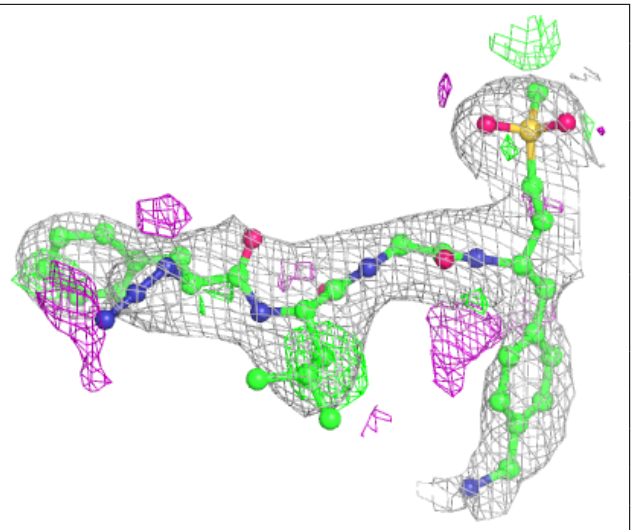


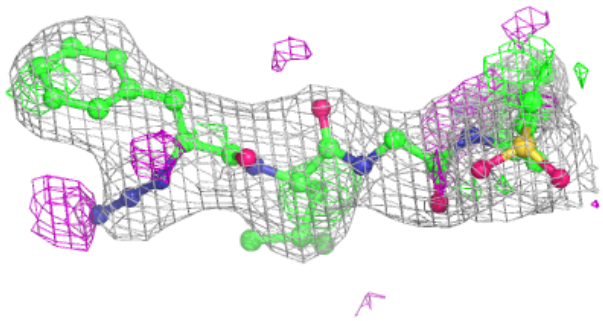




Electron density around GRT Y 301:

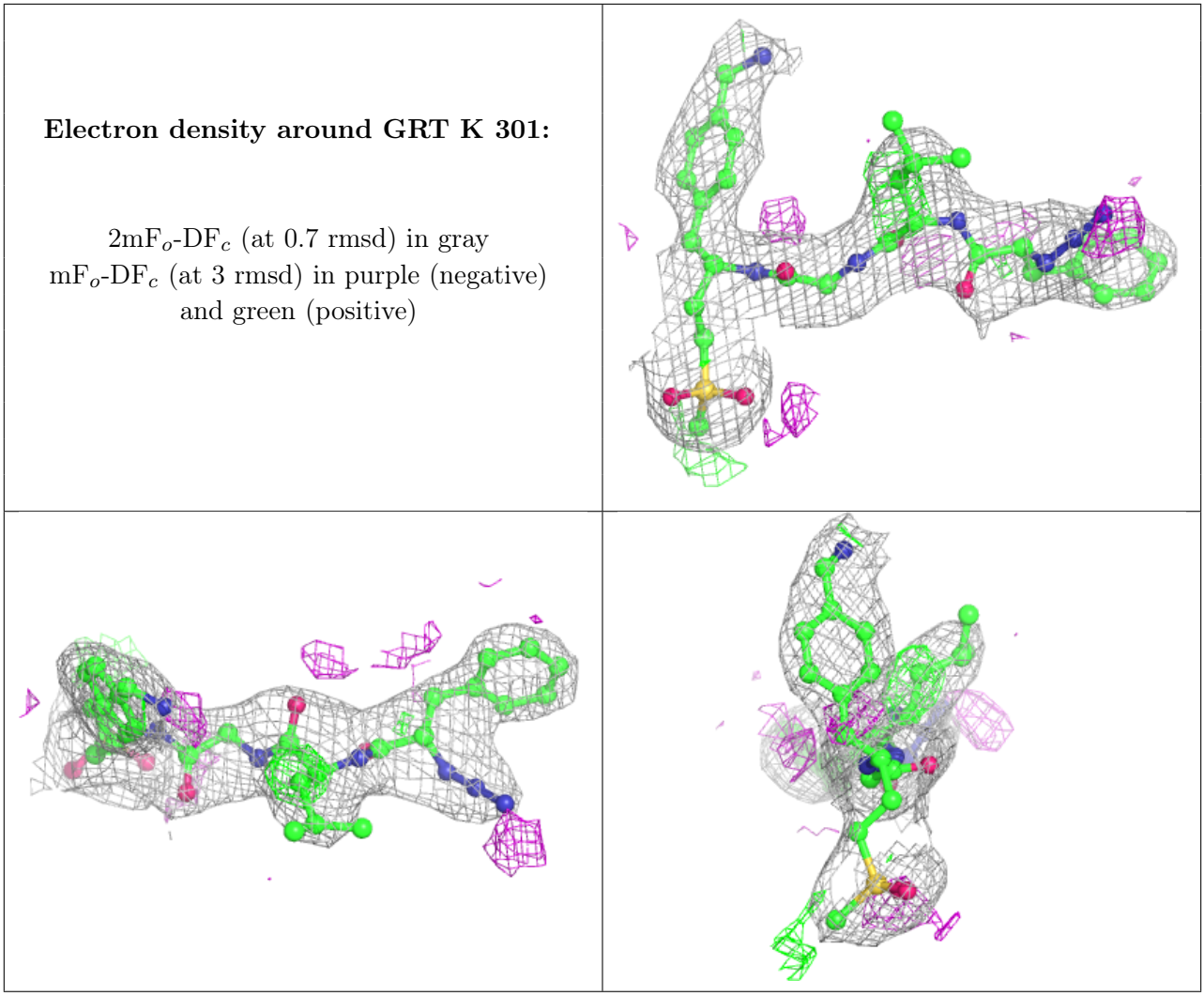
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





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)



6.5 Other polymers

There are no such residues in this entry.