Full wwPDB X-ray Structure Validation Report (i)

Jan 16, 2024 – 01:25 am GMT

PDB ID	:	6HV4
Title	:	Yeast 20S proteasome with human beta2i (1-53) in complex with ONX 0914
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2018-10-10
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:

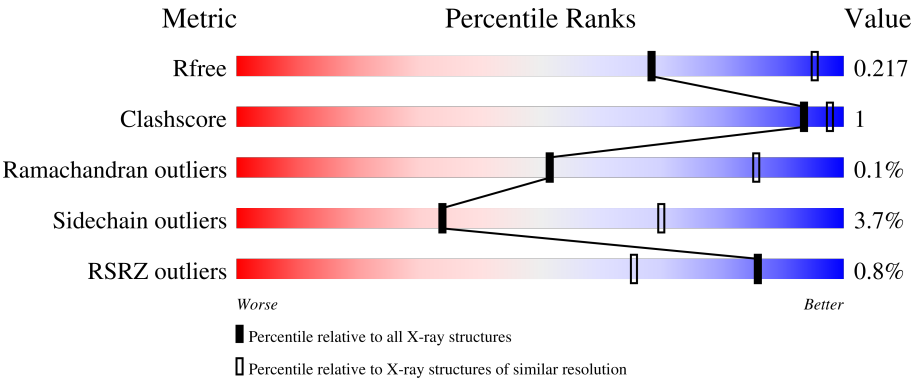
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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	97% ·
1	O	250	98% ·
2	B	258	88% 5% · 5%
2	P	258	89% 6% 5%
3	C	254	87% 6% · 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	4% 87% 7% 6%
4	D	260	85% 5% 10%
4	R	260	85% 5% 10%
5	E	234	93% 6%
5	S	234	91% 7%
6	F	288	81% 16%
6	T	288	80% 16%
7	G	252	90% 6%
7	U	252	90% 5%
8	H	226	93% 5%
8	V	226	92% 5%
9	I	205	95%
9	W	205	96%
10	J	198	92% 6%
10	X	198	91% 7%
11	K	212	92% 7%
11	Y	212	92% 7%
12	L	222	92% 8%
12	Z	222	92% 8%
13	M	246	87% 10%
13	a	246	88% 10%
14	N	196	97%
14	b	196	98%

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 49728 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 8 is a protein called Proteasome subunit beta type-10,Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1716	1081	291	336	8			
8	V	223	Total	C	N	O	S	0	0	0
			1688	1066	287	327	8			

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	222	Total	C	N	O	S	0	0	0
			1736	1098	297	334	7			
13	a	222	Total	C	N	O	S	0	0	0
			1736	1098	297	334	7			

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

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

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

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

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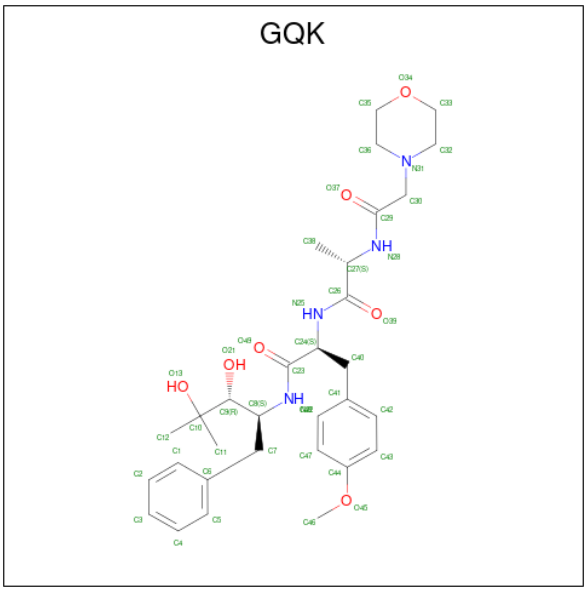
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	W	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

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

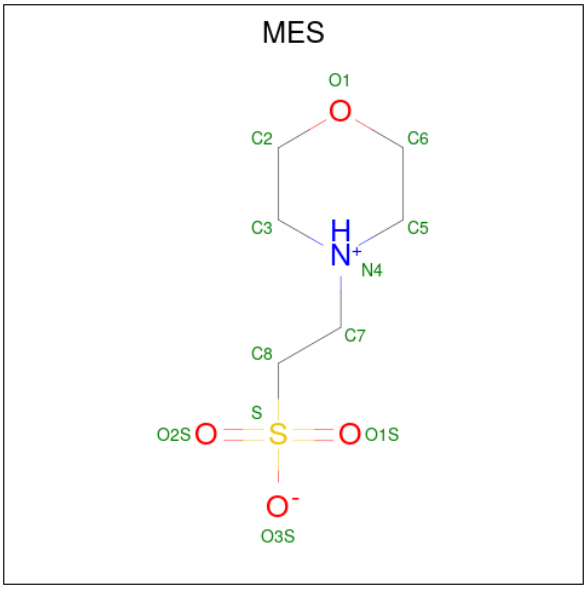
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is (2 {S})-3-(4-methoxyphenyl)- {N}-[(2 {S},3 {R})-4-methyl-3,4-bis(oxidanyl) -1-phenyl-pentan-2-yl]-2-[[(2 {S})-2-(2-morpholin-4-ylethanoylamino)propanoyl]amino]prop anamide (three-letter code: GQK) (formula: $C_{31}H_{44}N_4O_7$).



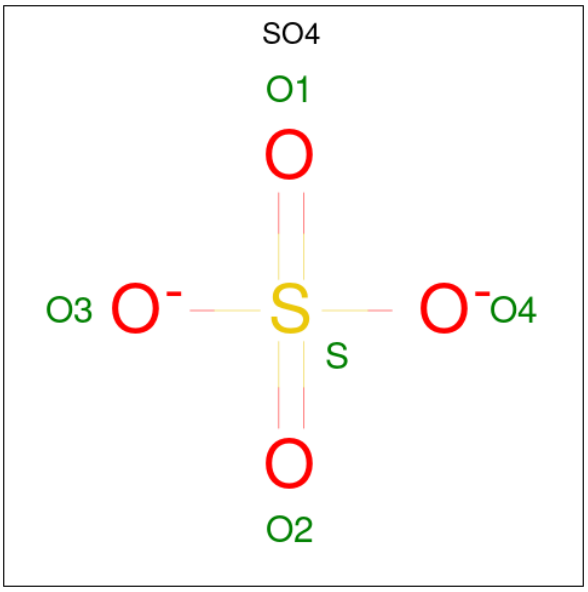
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	1	Total C N O 42 31 4 7	0	0
17	K	1	Total C N O 42 31 4 7	0	0
17	N	1	Total C N O 42 31 4 7	0	0
17	V	1	Total C N O 42 31 4 7	0	0
17	Y	1	Total C N O 42 31 4 7	0	0
17	b	1	Total C N O 42 31 4 7	0	0

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 19 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 20 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	6	Total O 6 6	0	0
20	B	12	Total O 12 12	0	0
20	C	7	Total O 7 7	0	0
20	D	11	Total O 11 11	0	0
20	E	7	Total O 7 7	0	0
20	F	6	Total O 6 6	0	0
20	G	11	Total O 11 11	0	0
20	H	12	Total O 12 12	0	0
20	I	6	Total O 6 6	0	0
20	J	14	Total O 14 14	0	0

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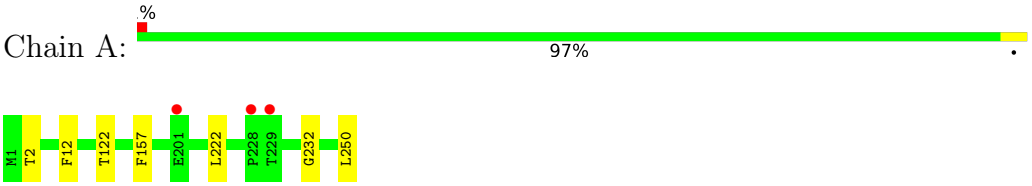
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	K	16	Total O 16 16	0	0
20	L	13	Total O 13 13	0	0
20	M	15	Total O 15 15	0	0
20	N	4	Total O 4 4	0	0
20	O	3	Total O 3 3	0	0
20	P	6	Total O 6 6	0	0
20	Q	2	Total O 2 2	0	0
20	R	3	Total O 3 3	0	0
20	S	8	Total O 8 8	0	0
20	T	9	Total O 9 9	0	0
20	U	9	Total O 9 9	0	0
20	V	9	Total O 9 9	0	0
20	W	5	Total O 5 5	0	0
20	X	10	Total O 10 10	0	0
20	Y	19	Total O 19 19	0	0
20	Z	11	Total O 11 11	0	0
20	a	13	Total O 13 13	0	0
20	b	5	Total O 5 5	0	0

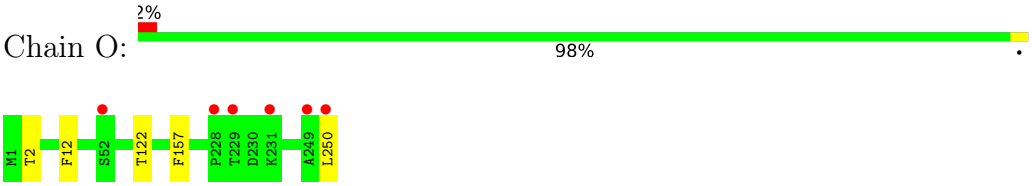
3 Residue-property plots (i)

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.

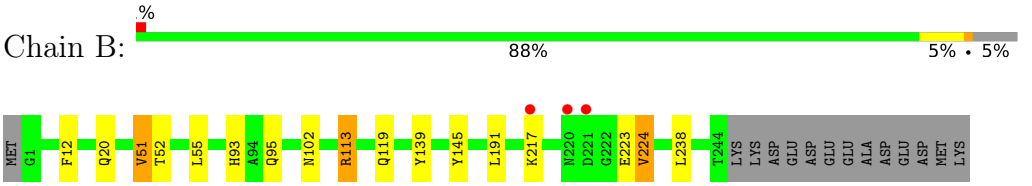
• Molecule 1: Proteasome subunit alpha type-2



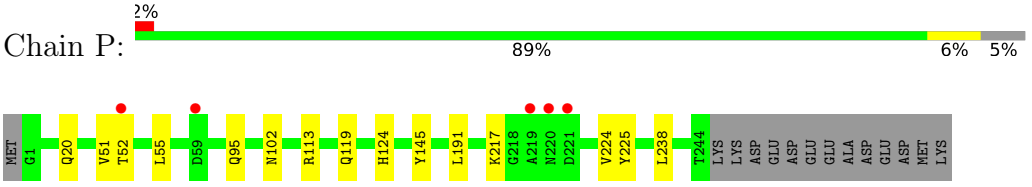
• Molecule 1: Proteasome subunit alpha type-2



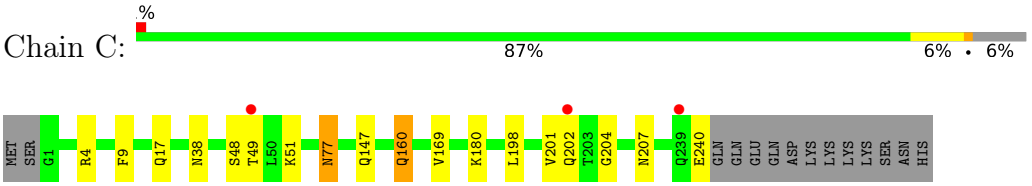
• Molecule 2: Proteasome subunit alpha type-3



• Molecule 2: Proteasome subunit alpha type-3

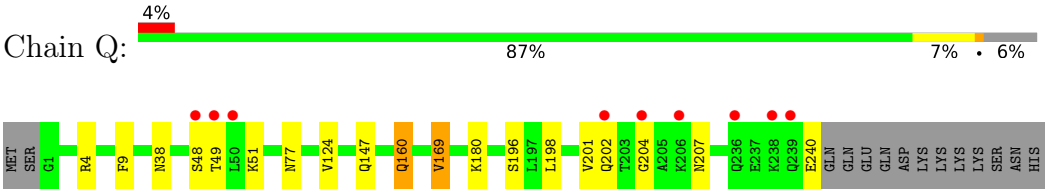


• Molecule 3: Proteasome subunit alpha type-4



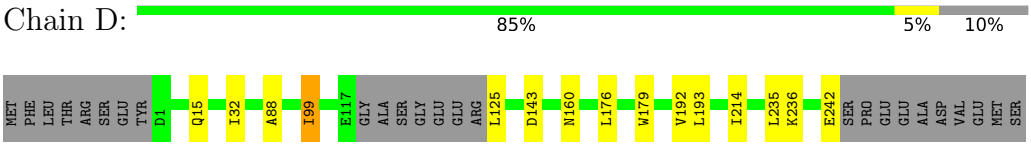
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



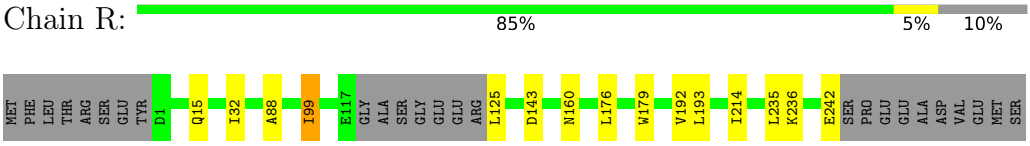
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



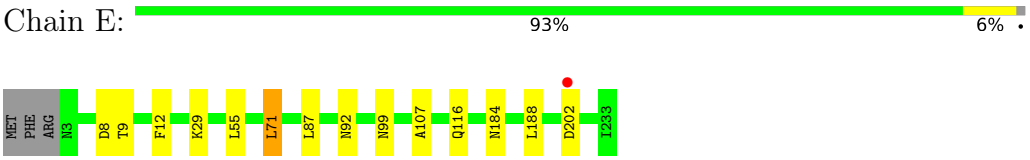
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



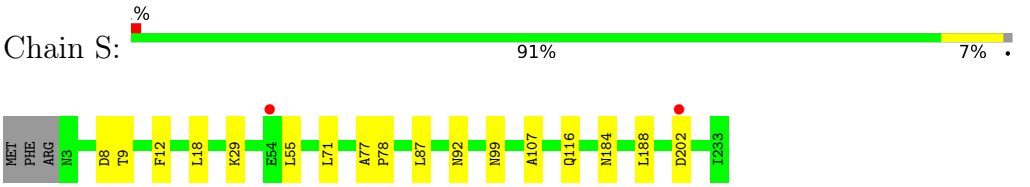
• Molecule 5: Proteasome subunit alpha type-6

Chain E:



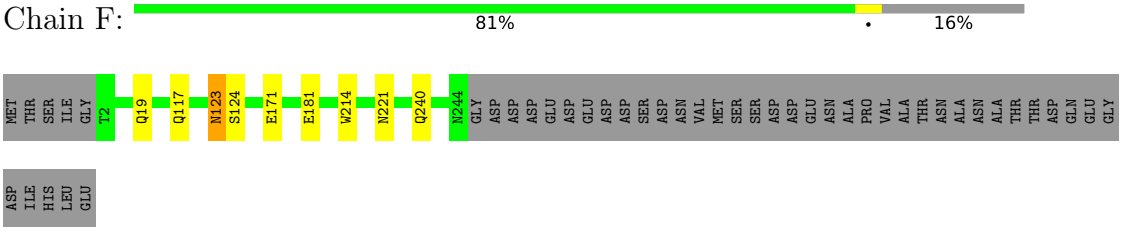
• Molecule 5: Proteasome subunit alpha type-6

Chain S:



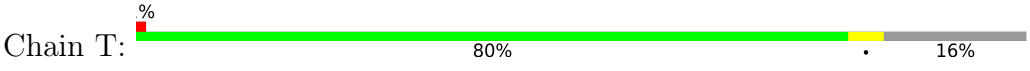
• Molecule 6: Probable proteasome subunit alpha type-7

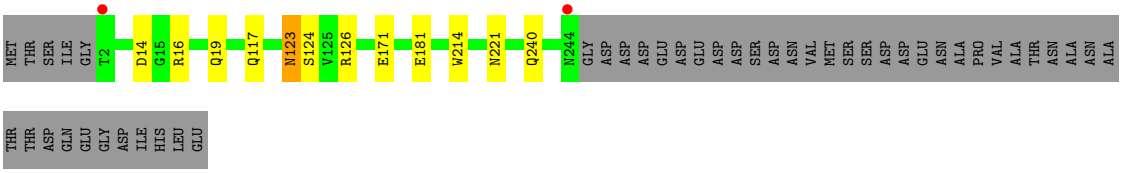
Chain F:



• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:





• Molecule 7: Proteasome subunit alpha type-1

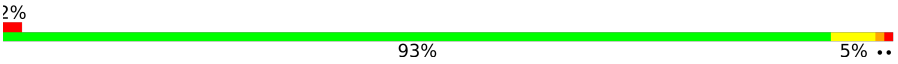
Chain G:

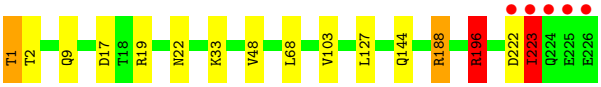
• Molecule 7: Proteasome subunit alpha type-1

Chain U:

• Molecule 8: Proteasome subunit beta type-10,Proteasome subunit beta type-2

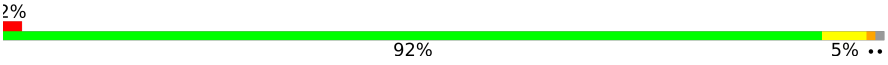
Chain H:





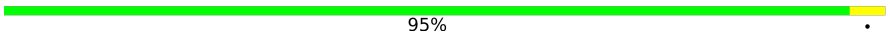
• Molecule 8: Proteasome subunit beta type-10,Proteasome subunit beta type-2

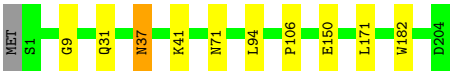
Chain V:



• Molecule 9: Proteasome subunit beta type-3

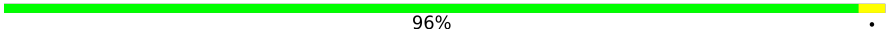
Chain I:

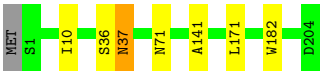




• Molecule 9: Proteasome subunit beta type-3

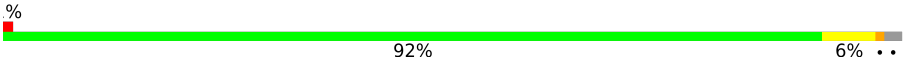
Chain W:

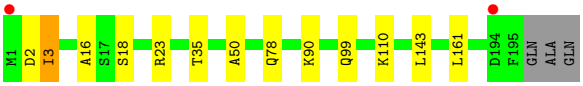




• Molecule 10: Proteasome subunit beta type-4

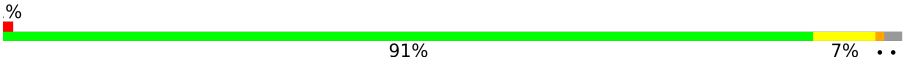
Chain J:

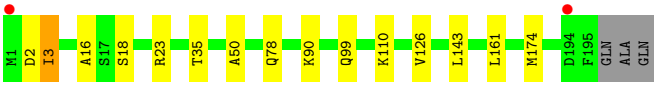




• Molecule 10: Proteasome subunit beta type-4

Chain X:





• Molecule 11: Proteasome subunit beta type-5

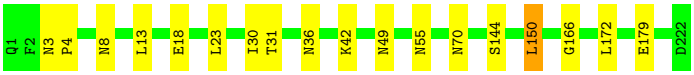
Chain K:

• Molecule 11: Proteasome subunit beta type-5

Chain Y:

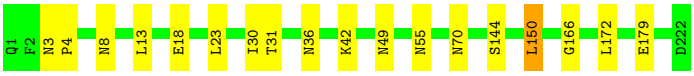
• Molecule 12: Proteasome subunit beta type-6

Chain L:



• Molecule 12: Proteasome subunit beta type-6

Chain Z:

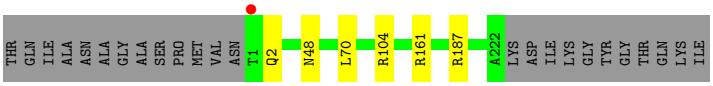


• Molecule 13: Proteasome subunit beta type-7

Chain M:

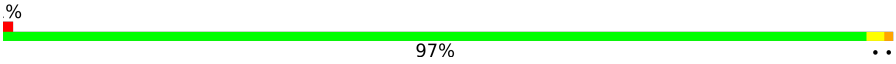
• Molecule 13: Proteasome subunit beta type-7

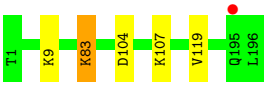
Chain a:



• Molecule 14: Proteasome subunit beta type-1

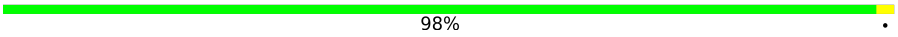
Chain N:





• Molecule 14: Proteasome subunit beta type-1

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	134.99Å 298.78Å 143.44Å 90.00° 112.52° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (15.00-3.00) 97.4 (15.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.184 , 0.214 0.191 , 0.217	Depositor DCC
R_{free} test set	10084 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	64.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	49728	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, SO4, MG, GQK, 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	0.37	0/1952	0.57	0/2642
1	O	0.36	0/1952	0.58	0/2642
2	B	0.38	0/1934	0.66	2/2618 (0.1%)
2	P	0.37	0/1934	0.66	2/2618 (0.1%)
3	C	0.36	0/1910	0.64	0/2586
3	Q	0.36	0/1910	0.64	0/2586
4	D	0.36	0/1837	0.59	0/2475
4	R	0.35	0/1837	0.59	0/2475
5	E	0.35	0/1800	0.59	1/2433 (0.0%)
5	S	0.35	0/1800	0.59	0/2433
6	F	0.36	0/1932	0.57	0/2609
6	T	0.35	0/1932	0.57	0/2609
7	G	0.37	0/1945	0.59	0/2634
7	U	0.37	0/1945	0.58	0/2634
8	H	0.36	0/1746	0.85	7/2365 (0.3%)
8	V	0.34	0/1718	0.84	4/2329 (0.2%)
9	I	0.36	0/1611	0.60	0/2174
9	W	0.35	0/1611	0.59	0/2174
10	J	0.36	0/1589	0.64	0/2142
10	X	0.36	0/1589	0.64	0/2142
11	K	0.37	0/1681	0.91	5/2274 (0.2%)
11	Y	0.36	0/1681	0.92	5/2274 (0.2%)
12	L	0.37	0/1795	0.62	0/2420
12	Z	0.37	0/1795	0.62	0/2420
13	M	0.37	0/1766	0.64	0/2398
13	a	0.37	0/1766	0.65	0/2398
14	N	0.35	0/1541	0.60	0/2087
14	b	0.35	0/1541	0.60	0/2087
All	All	0.36	0/50050	0.65	26/67678 (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
8	H	0	1
8	V	0	1
11	K	0	1
11	Y	0	1
All	All	0	4

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	V	188	ARG	NE-CZ-NH2	-21.17	109.71	120.30
11	K	73	ARG	NE-CZ-NH2	-20.36	110.12	120.30
11	Y	73	ARG	NE-CZ-NH1	-19.76	110.42	120.30
8	H	188	ARG	NE-CZ-NH1	-18.50	111.05	120.30
11	Y	73	ARG	NE-CZ-NH2	16.23	128.41	120.30
8	H	188	ARG	NE-CZ-NH2	15.02	127.81	120.30
11	K	73	ARG	NE-CZ-NH1	14.35	127.47	120.30
8	V	188	ARG	NE-CZ-NH1	14.24	127.42	120.30
11	Y	4	LEU	CD1-CG-CD2	-12.25	73.75	110.50
11	K	4	LEU	CD1-CG-CD2	-12.01	74.46	110.50
11	Y	4	LEU	CB-CG-CD1	10.98	129.67	111.00
11	K	4	LEU	CB-CG-CD2	10.56	128.96	111.00
8	V	188	ARG	CD-NE-CZ	10.34	138.07	123.60
11	K	73	ARG	CD-NE-CZ	10.15	137.81	123.60
8	H	1	THR	CA-CB-OG1	9.74	129.45	109.00
11	Y	73	ARG	CD-NE-CZ	9.28	136.59	123.60
8	H	188	ARG	CD-NE-CZ	8.78	135.89	123.60
8	H	1	THR	N-CA-CB	-6.21	98.51	110.30
2	P	224	VAL	CG1-CB-CG2	5.75	120.10	110.90
8	H	1	THR	CA-CB-CG2	-5.67	104.46	112.40
2	B	51	VAL	CG1-CB-CG2	5.43	119.59	110.90
2	B	224	VAL	CG1-CB-CG2	5.43	119.59	110.90
8	V	196	ARG	NE-CZ-NH1	5.27	122.94	120.30
5	E	71	LEU	CA-CB-CG	5.24	127.34	115.30
2	P	51	VAL	CG1-CB-CG2	5.22	119.25	110.90
8	H	196	ARG	NE-CZ-NH1	5.19	122.89	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	188	ARG	Sidechain
11	K	73	ARG	Sidechain
8	V	188	ARG	Sidechain
11	Y	73	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	1915	0	1929	2	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	8	0
2	P	1904	0	1904	9	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	5	0
5	S	1773	0	1775	7	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	5	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1716	0	1701	13	0
8	V	1688	0	1681	8	0
9	I	1581	0	1574	6	0
9	W	1581	0	1574	5	0
10	J	1561	0	1569	5	0
10	X	1561	0	1569	7	0
11	K	1644	0	1593	11	0
11	Y	1644	0	1593	12	0
12	L	1757	0	1711	10	0
12	Z	1757	0	1711	10	0
13	M	1736	0	1737	1	0
13	a	1736	0	1737	0	0
14	N	1512	0	1479	1	0
14	b	1512	0	1479	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	2	0
17	N	42	0	0	1	0
17	V	42	0	0	0	0
17	Y	42	0	0	1	0
17	b	42	0	0	0	0
18	H	12	0	13	1	0
18	K	12	0	13	1	0
18	V	12	0	13	0	0
18	Y	12	0	13	0	0
19	N	5	0	0	1	0
19	b	5	0	0	0	0
20	A	6	0	0	0	0
20	B	12	0	0	2	0
20	C	7	0	0	0	0
20	D	11	0	0	0	0
20	E	7	0	0	0	0
20	F	6	0	0	0	0
20	G	11	0	0	0	0
20	H	12	0	0	0	0
20	I	6	0	0	1	0
20	J	14	0	0	0	0
20	K	16	0	0	0	0
20	L	13	0	0	0	0
20	M	15	0	0	0	0
20	N	4	0	0	0	0
20	O	3	0	0	0	0
20	P	6	0	0	0	0
20	Q	2	0	0	0	0
20	R	3	0	0	0	0
20	S	8	0	0	0	0
20	T	9	0	0	0	0
20	U	9	0	0	1	0
20	V	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	W	5	0	0	0	0
20	X	10	0	0	1	0
20	Y	19	0	0	0	0
20	Z	11	0	0	0	0
20	a	13	0	0	0	0
20	b	5	0	0	0	0
All	All	49728	0	48928	131	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 (131) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:1:THR:HG23	8:H:33:LYS:NZ	1.86	0.90
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.48	0.78
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.48	0.78
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.32	0.76
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.34	0.75
11:K:142:SER:OG	10:X:143:LEU:HD21	1.87	0.74
8:H:1:THR:HG23	8:H:33:LYS:HZ2	1.53	0.73
8:H:1:THR:HG23	8:H:33:LYS:HZ3	1.54	0.72
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.58	0.69
2:P:145:TYR:OH	2:P:217:LYS:N	2.26	0.67
2:B:145:TYR:OH	2:B:217:LYS:N	2.28	0.67
17:N:201:GQK:O21	19:N:203:SO4:O2	2.12	0.67
10:J:143:LEU:HD21	11:Y:142:SER:OG	1.96	0.66
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.61	0.65
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.61	0.65
2:B:93:HIS:HB3	20:B:301:HOH:O	1.97	0.64
6:T:123:ASN:HD22	6:T:124:SER:N	1.95	0.64
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.62	0.64
6:F:123:ASN:HD22	6:F:124:SER:N	1.97	0.63
1:O:12:PHE:H	2:P:20:GLN:HE22	1.47	0.63
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	1.99	0.61
7:G:23:PHE:O	7:G:26:THR:HB	2.01	0.60
5:E:92:ASN:HD21	12:L:70:ASN:ND2	1.99	0.59
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	1.99	0.59
7:U:23:PHE:O	7:U:26:THR:HB	2.02	0.59
5:E:92:ASN:ND2	12:L:70:ASN:HD21	1.99	0.59
10:J:50:ALA:O	11:K:91:LYS:NZ	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:1:THR:CG2	8:H:33:LYS:HZ3	2.16	0.58
10:X:174:MET:HB2	20:X:204:HOH:O	2.04	0.57
8:V:1:THR:HG23	8:V:33:LYS:NZ	2.19	0.57
5:S:12:PHE:H	6:T:19:GLN:HE22	1.52	0.56
11:K:176:ASN:ND2	11:K:190:ASN:HD22	2.04	0.56
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.88	0.55
11:Y:176:ASN:ND2	11:Y:190:ASN:HD22	2.05	0.55
8:H:1:THR:HG22	8:H:2:THR:N	2.21	0.55
8:H:1:THR:HG21	8:H:33:LYS:HD3	1.88	0.55
2:P:225:TYR:CD1	8:V:223:ILE:HG13	2.42	0.54
8:H:1:THR:HG23	8:H:17:ASP:OD1	2.07	0.54
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.90	0.54
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.89	0.54
7:U:122:ARG:HD2	20:U:405:HOH:O	2.06	0.53
8:H:1:THR:CG2	8:H:33:LYS:NZ	2.65	0.53
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.92	0.52
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.90	0.52
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.40	0.51
17:H:301:GQK:O21	18:H:302:MES:O2S	2.29	0.51
3:C:198:LEU:HA	3:C:201:VAL:HG12	1.92	0.51
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.92	0.51
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.41	0.51
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.92	0.50
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.22	0.50
2:P:145:TYR:HH	2:P:217:LYS:N	2.09	0.50
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.60	0.50
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.44	0.49
1:A:12:PHE:H	2:B:20:GLN:HE22	1.60	0.49
3:C:9:PHE:H	4:D:15:GLN:HE22	1.58	0.49
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.22	0.49
6:T:123:ASN:HD22	6:T:123:ASN:C	2.16	0.48
5:E:12:PHE:H	6:F:19:GLN:HE22	1.60	0.48
11:K:209:ASN:O	9:W:37:ASN:ND2	2.45	0.48
8:H:19:ARG:O	8:H:33:LYS:NZ	2.44	0.48
2:B:12:PHE:H	3:C:17:GLN:HE22	1.62	0.48
11:Y:18:SER:OG	11:Y:29:GLN:O	2.31	0.48
11:Y:176:ASN:HD21	11:Y:190:ASN:HD22	1.63	0.47
11:Y:208:ASN:HD22	11:Y:208:ASN:N	2.12	0.47
17:K:301:GQK:O21	18:K:303:MES:O2S	2.33	0.47
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.63	0.47
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.80	0.47
8:H:196:ARG:NH2	9:I:150:GLU:O	2.48	0.47
2:P:225:TYR:CD1	8:V:223:ILE:HG21	2.50	0.46
8:V:1:THR:HG23	8:V:33:LYS:HZ3	1.79	0.46
11:K:176:ASN:HD21	11:K:190:ASN:HD22	1.62	0.46
11:K:208:ASN:HD22	11:K:208:ASN:N	2.13	0.46
8:V:223:ILE:H	8:V:223:ILE:HD13	1.81	0.45
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.48	0.45
11:K:18:SER:OG	11:K:29:GLN:O	2.32	0.45
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.17	0.45
3:C:202:GLN:O	3:C:202:GLN:CG	2.65	0.45
8:H:223:ILE:H	8:H:223:ILE:HD13	1.82	0.45
8:V:19:ARG:O	8:V:33:LYS:NZ	2.45	0.45
8:V:223:ILE:HD13	8:V:223:ILE:N	2.32	0.45
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.15	0.45
6:F:123:ASN:HD22	6:F:123:ASN:C	2.19	0.44
3:Q:202:GLN:CG	3:Q:202:GLN:O	2.65	0.44
2:B:113:ARG:NE	20:B:301:HOH:O	2.41	0.44
7:G:73:VAL:HG12	7:G:133:THR:HB	1.99	0.44
8:H:223:ILE:HD13	8:H:223:ILE:N	2.32	0.44
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.83	0.44
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.98	0.44
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.98	0.44
10:J:23:ARG:NH2	11:K:118:ASP:OD2	2.40	0.44
2:B:145:TYR:HH	2:B:217:LYS:N	2.16	0.43
3:C:48:SER:HB2	3:C:207:ASN:HD21	1.83	0.43
7:U:73:VAL:HG12	7:U:133:THR:HB	2.00	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.53	0.43
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.00	0.43
11:K:209:ASN:N	11:K:209:ASN:HD22	2.17	0.43
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.43
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.83	0.43
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.49	0.43
9:I:31:GLN:HG2	20:I:402:HOH:O	2.18	0.43
11:K:31:VAL:HG11	17:K:301:GQK:C4	2.49	0.43
3:Q:48:SER:HB2	3:Q:207:ASN:HD21	1.84	0.42
11:Y:31:VAL:HG11	17:Y:301:GQK:C4	2.49	0.42
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.00	0.42
10:X:23:ARG:NH2	11:Y:118:ASP:OD2	2.42	0.42
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.00	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.02	0.42
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.85	0.41
11:Y:209:ASN:HD22	11:Y:209:ASN:N	2.18	0.41
11:Y:44:THR:HG21	11:Y:100:MET:HE3	2.02	0.41
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.02	0.41
5:S:18:LEU:HD21	6:T:126:ARG:HD2	2.02	0.41
8:H:48:VAL:HG22	17:H:301:GQK:C46	2.51	0.41
4:R:32:ILE:HD12	4:R:192:VAL:HG23	2.02	0.41
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.02	0.41
1:A:222:LEU:HD13	1:A:232:GLY:HA2	2.03	0.41
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.03	0.41
2:P:145:TYR:OH	2:P:217:LYS:HB2	2.21	0.41
6:T:14:ASP:CB	6:T:16:ARG:HD3	2.51	0.41
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.02	0.41
4:D:32:ILE:HD12	4:D:192:VAL:HG23	2.03	0.41
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.02	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.56	0.40
9:I:94:LEU:HD11	9:I:106:PRO:HG2	2.03	0.40
3:C:77:ASN:HD22	3:C:77:ASN:N	2.19	0.40
13:M:179:ASN:HD22	13:M:182:ARG:NH1	2.20	0.40
8:V:1:THR:HG22	8:V:2:THR:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
1	O	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	233 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	242/258 (94%)	232 (96%)	10 (4%)	0	100	100
3	C	238/254 (94%)	235 (99%)	2 (1%)	1 (0%)	34	72
3	Q	238/254 (94%)	235 (99%)	2 (1%)	1 (0%)	34	72
4	D	231/260 (89%)	224 (97%)	7 (3%)	0	100	100
4	R	231/260 (89%)	224 (97%)	7 (3%)	0	100	100
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	224/226 (99%)	218 (97%)	5 (2%)	1 (0%)	34	72
8	V	221/226 (98%)	216 (98%)	5 (2%)	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%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
12	L	220/222 (99%)	213 (97%)	6 (3%)	1 (0%)	29	68
12	Z	220/222 (99%)	213 (97%)	6 (3%)	1 (0%)	29	68
13	M	220/246 (89%)	210 (96%)	10 (4%)	0	100	100
13	a	220/246 (89%)	212 (96%)	8 (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	6259/6602 (95%)	6099 (97%)	155 (2%)	5 (0%)	51	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	223	ILE
3	C	204	GLY
3	Q	204	GLY

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Mol	Chain	Res	Type
12	L	166	GLY
12	Z	166	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	205 (98%)	4 (2%)	57	84
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	84
2	B	203/216 (94%)	194 (96%)	9 (4%)	28	65
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	72
3	C	212/226 (94%)	202 (95%)	10 (5%)	26	63
3	Q	212/226 (94%)	202 (95%)	10 (5%)	26	63
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	64
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	64
5	E	190/193 (98%)	180 (95%)	10 (5%)	22	58
5	S	190/193 (98%)	180 (95%)	10 (5%)	22	58
6	F	201/239 (84%)	194 (96%)	7 (4%)	36	71
6	T	201/239 (84%)	194 (96%)	7 (4%)	36	71
7	G	206/210 (98%)	198 (96%)	8 (4%)	32	69
7	U	206/210 (98%)	198 (96%)	8 (4%)	32	69
8	H	184/184 (100%)	175 (95%)	9 (5%)	25	61
8	V	181/184 (98%)	172 (95%)	9 (5%)	24	60
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	85
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	85
10	J	173/175 (99%)	166 (96%)	7 (4%)	31	68
10	X	173/175 (99%)	166 (96%)	7 (4%)	31	68
11	K	169/169 (100%)	163 (96%)	6 (4%)	35	70
11	Y	169/169 (100%)	163 (96%)	6 (4%)	35	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	L	185/185 (100%)	178 (96%)	7 (4%)	33 69
12	Z	185/185 (100%)	178 (96%)	7 (4%)	33 69
13	M	190/208 (91%)	184 (97%)	6 (3%)	39 74
13	a	190/208 (91%)	184 (97%)	6 (3%)	39 74
14	N	162/162 (100%)	158 (98%)	4 (2%)	47 79
14	b	162/162 (100%)	158 (98%)	4 (2%)	47 79
All	All	5297/5528 (96%)	5101 (96%)	196 (4%)	34 70

All (196) 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	51	VAL
2	B	52	THR
2	B	55	LEU
2	B	102	ASN
2	B	113	ARG
2	B	119	GLN
2	B	191	LEU
2	B	223	GLU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	49	THR
3	C	51	LYS
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE

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Mol	Chain	Res	Type
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	8	ASP
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	99	ASN
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	117	GLN
6	F	123	ASN
6	F	171	GLU
6	F	181	GLU
6	F	214	TRP
6	F	221	ASN
6	F	240	GLN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	9	GLN
8	H	22	ASN
8	H	68	LEU
8	H	103	VAL
8	H	127	LEU
8	H	144	GLN
8	H	196	ARG
8	H	222	ASP
8	H	223	ILE
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	2	ASP
10	J	3	ILE

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Mol	Chain	Res	Type
10	J	35	THR
10	J	78	GLN
10	J	90	LYS
10	J	99	GLN
10	J	110	LYS
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	100	MET
11	K	107	LYS
11	K	209	ASN
12	L	18	GLU
12	L	23	LEU
12	L	49	ASN
12	L	144	SER
12	L	150	LEU
12	L	172	LEU
12	L	179	GLU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	2	THR
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	52	THR
2	P	55	LEU
2	P	102	ASN
2	P	113	ARG
2	P	119	GLN
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	49	THR

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Mol	Chain	Res	Type
3	Q	51	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	8	ASP
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	99	ASN
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	117	GLN
6	T	123	ASN
6	T	171	GLU
6	T	181	GLU
6	T	214	TRP
6	T	221	ASN
6	T	240	GLN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	9	GLN

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Mol	Chain	Res	Type
8	V	22	ASN
8	V	68	LEU
8	V	103	VAL
8	V	127	LEU
8	V	144	GLN
8	V	196	ARG
8	V	222	ASP
8	V	223	ILE
9	W	37	ASN
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
10	X	110	LYS
11	Y	9	GLN
11	Y	35	ILE
11	Y	73	ARG
11	Y	100	MET
11	Y	107	LYS
11	Y	209	ASN
12	Z	18	GLU
12	Z	23	LEU
12	Z	49	ASN
12	Z	144	SER
12	Z	150	LEU
12	Z	172	LEU
12	Z	179	GLU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126)

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
4	D	15	GLN
4	D	91	HIS
4	D	146	GLN
4	D	160	ASN
4	D	225	ASN
5	E	59	GLN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
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
8	H	172	ASN
9	I	71	ASN
10	J	55	GLN
10	J	118	GLN
11	K	9	GLN

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Mol	Chain	Res	Type
11	K	85	ASN
11	K	176	ASN
11	K	209	ASN
12	L	3	ASN
12	L	29	ASN
12	L	36	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	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
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	167	ASN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	146	GLN
4	R	160	ASN
4	R	225	ASN
5	S	59	GLN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN

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Mol	Chain	Res	Type
5	S	120	GLN
5	S	184	ASN
6	T	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	165	ASN
8	V	172	ASN
9	W	71	ASN
10	X	55	GLN
10	X	78	GLN
10	X	86	GLN
10	X	118	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	209	ASN
12	Z	3	ASN
12	Z	29	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	79	HIS
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	69	GLN
14	b	161	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 10 are monoatomic - leaving 12 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	GQK	V	301	8	44,44,44	1.37	4 (9%)	59,60,60	1.34	8 (13%)
17	GQK	K	301	11	44,44,44	1.27	4 (9%)	59,60,60	1.63	7 (11%)
17	GQK	H	301	8	44,44,44	1.71	6 (13%)	59,60,60	2.48	13 (22%)
18	MES	V	303	-	12,12,12	2.28	1 (8%)	14,16,16	1.73	2 (14%)
18	MES	H	302	-	12,12,12	2.25	1 (8%)	14,16,16	1.43	2 (14%)
17	GQK	Y	301	11	44,44,44	1.30	5 (11%)	59,60,60	1.64	8 (13%)
17	GQK	N	201	14	44,44,44	1.38	4 (9%)	59,60,60	1.27	9 (15%)
18	MES	K	303	-	12,12,12	2.18	1 (8%)	14,16,16	1.73	3 (21%)
17	GQK	b	201	14	44,44,44	1.40	5 (11%)	59,60,60	1.25	8 (13%)
19	SO4	b	202	-	4,4,4	0.48	0	6,6,6	0.18	0
19	SO4	N	203	-	4,4,4	0.46	0	6,6,6	0.28	0
18	MES	Y	303	-	12,12,12	2.22	1 (8%)	14,16,16	1.62	2 (14%)

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	GQK	V	301	8	-	4/44/52/52	0/3/3/3
17	GQK	K	301	11	-	10/44/52/52	0/3/3/3
17	GQK	H	301	8	-	9/44/52/52	0/3/3/3
18	MES	V	303	-	-	5/6/14/14	0/1/1/1
18	MES	H	302	-	-	1/6/14/14	0/1/1/1
17	GQK	Y	301	11	-	9/44/52/52	0/3/3/3
17	GQK	N	201	14	-	7/44/52/52	0/3/3/3
18	MES	K	303	-	-	0/6/14/14	0/1/1/1
17	GQK	b	201	14	-	7/44/52/52	0/3/3/3
18	MES	Y	303	-	-	3/6/14/14	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	303	MES	C8-S	-7.74	1.66	1.77
18	H	302	MES	C8-S	-7.63	1.66	1.77
18	Y	303	MES	C8-S	-7.29	1.67	1.77
18	K	303	MES	C8-S	-7.23	1.67	1.77
17	H	301	GQK	C40-C41	-5.49	1.38	1.51
17	H	301	GQK	C7-C6	-5.45	1.38	1.51
17	b	201	GQK	C40-C41	-4.98	1.39	1.51
17	N	201	GQK	C40-C41	-4.89	1.39	1.51
17	V	301	GQK	C40-C41	-4.82	1.39	1.51
17	K	301	GQK	C40-C41	-4.46	1.40	1.51
17	V	301	GQK	C11-C10	4.37	1.59	1.52
17	Y	301	GQK	C40-C41	-4.28	1.41	1.51
17	b	201	GQK	C11-C10	4.03	1.59	1.52
17	N	201	GQK	C11-C10	3.90	1.59	1.52
17	H	301	GQK	O21-C9	-3.69	1.35	1.42
17	H	301	GQK	C10-C9	-3.55	1.47	1.54
17	N	201	GQK	C9-C8	3.47	1.57	1.53
17	b	201	GQK	C9-C8	3.43	1.57	1.53
17	K	301	GQK	C11-C10	3.22	1.57	1.52
17	Y	301	GQK	C11-C10	3.17	1.57	1.52
17	b	201	GQK	C7-C6	-2.99	1.44	1.51
17	V	301	GQK	C7-C6	-2.95	1.44	1.51
17	Y	301	GQK	C7-C6	-2.94	1.44	1.51
17	V	301	GQK	C9-C8	2.91	1.57	1.53
17	H	301	GQK	O13-C10	-2.88	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	201	GQK	C7-C6	-2.86	1.44	1.51
17	H	301	GQK	C11-C10	-2.84	1.47	1.52
17	K	301	GQK	C7-C6	-2.76	1.44	1.51
17	Y	301	GQK	C9-C8	2.41	1.56	1.53
17	K	301	GQK	C9-C8	2.31	1.56	1.53
17	b	201	GQK	C30-C29	2.17	1.55	1.52
17	Y	301	GQK	C10-C9	2.02	1.58	1.54

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	H	301	GQK	O13-C10-C9	10.24	131.73	107.64
17	H	301	GQK	O13-C10-C12	-8.54	89.56	107.90
17	K	301	GQK	C12-C10-C11	-7.50	99.84	110.56
17	Y	301	GQK	C12-C10-C11	-7.37	100.02	110.56
17	H	301	GQK	C12-C10-C11	-7.36	100.04	110.56
18	Y	303	MES	O3S-S-C8	4.63	113.26	105.77
17	H	301	GQK	C8-N22-C23	4.58	131.17	123.07
18	V	303	MES	O3S-S-C8	4.06	112.34	105.77
18	K	303	MES	O1S-S-C8	3.76	111.44	106.92
17	Y	301	GQK	C30-N31-C36	-3.67	105.41	111.09
17	K	301	GQK	C30-N31-C36	-3.58	105.55	111.09
17	V	301	GQK	C30-N31-C36	-3.57	105.55	111.09
17	Y	301	GQK	C46-O45-C44	3.47	125.03	117.51
18	H	302	MES	O3S-S-C8	3.44	111.33	105.77
17	K	301	GQK	C46-O45-C44	3.34	124.77	117.51
18	K	303	MES	O2S-S-C8	3.29	110.88	106.92
17	V	301	GQK	C12-C10-C11	-3.25	105.90	110.56
17	H	301	GQK	C40-C41-C42	-3.23	114.50	120.91
17	b	201	GQK	C7-C6-C5	3.22	127.30	120.91
17	H	301	GQK	C40-C41-C48	3.21	127.27	120.91
17	K	301	GQK	C7-C6-C5	3.18	127.22	120.91
17	N	201	GQK	O34-C35-C36	-3.15	104.85	111.80
17	N	201	GQK	C46-O45-C44	3.12	124.29	117.51
18	V	303	MES	O1S-S-C8	3.07	110.61	106.92
17	b	201	GQK	O34-C35-C36	-3.06	105.05	111.80
17	N	201	GQK	C7-C6-C5	3.01	126.88	120.91
17	Y	301	GQK	C7-C6-C5	3.00	126.86	120.91
17	V	301	GQK	C11-C10-C9	2.96	116.82	111.28
17	b	201	GQK	C46-O45-C44	2.92	123.84	117.51
17	V	301	GQK	C7-C6-C5	2.89	126.64	120.91
17	K	301	GQK	C11-C10-C9	2.88	116.66	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	b	201	GQK	C11-C10-C9	2.87	116.65	111.28
17	N	201	GQK	C11-C10-C9	2.85	116.62	111.28
17	H	301	GQK	C11-C10-C9	2.75	116.43	111.28
17	H	301	GQK	O13-C10-C11	-2.70	102.09	107.90
17	V	301	GQK	C46-O45-C44	2.69	123.34	117.51
17	N	201	GQK	C29-C30-N31	-2.59	107.35	113.36
17	Y	301	GQK	C11-C10-C9	2.57	116.09	111.28
17	V	301	GQK	O34-C35-C36	-2.56	106.15	111.80
17	K	301	GQK	O34-C35-C36	-2.54	106.20	111.80
17	Y	301	GQK	O34-C35-C36	-2.54	106.20	111.80
18	Y	303	MES	O1S-S-C8	2.47	109.89	106.92
17	b	201	GQK	C29-C30-N31	-2.45	107.67	113.36
17	N	201	GQK	C12-C10-C11	-2.44	107.07	110.56
17	b	201	GQK	C12-C10-C11	-2.32	107.24	110.56
17	H	301	GQK	C30-N31-C32	-2.32	107.50	111.09
17	K	301	GQK	C7-C6-C1	-2.30	116.34	120.91
17	V	301	GQK	C29-C30-N31	-2.30	108.03	113.36
17	Y	301	GQK	C7-C6-C1	-2.29	116.36	120.91
17	H	301	GQK	C6-C7-C8	2.27	117.28	113.33
17	H	301	GQK	C38-C27-C26	-2.21	105.94	110.14
17	V	301	GQK	C33-C32-N31	-2.18	106.80	110.10
18	K	303	MES	O3S-S-C8	2.12	109.20	105.77
17	N	201	GQK	O13-C10-C11	-2.11	103.36	107.90
18	H	302	MES	O2S-S-C8	2.11	109.46	106.92
17	b	201	GQK	C7-C6-C1	-2.11	116.72	120.91
17	Y	301	GQK	C12-C10-C9	2.11	115.22	111.28
17	H	301	GQK	O34-C35-C36	-2.10	107.17	111.80
17	H	301	GQK	C38-C27-N28	-2.08	106.47	110.38
17	N	201	GQK	C30-N31-C36	-2.08	107.87	111.09
17	N	201	GQK	C7-C6-C1	-2.06	116.83	120.91
17	b	201	GQK	C30-N31-C36	-2.00	107.99	111.09

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	301	GQK	C11-C10-C9-C8
17	K	301	GQK	C11-C10-C9-O21
17	K	301	GQK	C12-C10-C9-C8
17	K	301	GQK	C12-C10-C9-O21
17	K	301	GQK	O13-C10-C9-C8
17	K	301	GQK	O13-C10-C9-O21

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Mol	Chain	Res	Type	Atoms
17	Y	301	GQK	C11-C10-C9-C8
17	Y	301	GQK	C11-C10-C9-O21
17	Y	301	GQK	C12-C10-C9-C8
17	Y	301	GQK	C12-C10-C9-O21
17	Y	301	GQK	O13-C10-C9-C8
17	Y	301	GQK	O13-C10-C9-O21
18	V	303	MES	C7-C8-S-O1S
18	V	303	MES	C7-C8-S-O3S
18	Y	303	MES	C7-C8-S-O1S
18	Y	303	MES	C7-C8-S-O3S
17	H	301	GQK	C47-C44-O45-C46
17	H	301	GQK	C43-C44-O45-C46
17	V	301	GQK	C5-C6-C7-C8
17	V	301	GQK	C1-C6-C7-C8
17	b	201	GQK	N25-C24-C40-C41
17	N	201	GQK	N25-C24-C40-C41
17	Y	301	GQK	C5-C6-C7-C8
17	K	301	GQK	C5-C6-C7-C8
17	Y	301	GQK	C1-C6-C7-C8
17	H	301	GQK	C1-C6-C7-C8
17	K	301	GQK	C1-C6-C7-C8
17	b	201	GQK	C5-C6-C7-C8
17	N	201	GQK	N28-C29-C30-N31
17	b	201	GQK	N28-C29-C30-N31
17	H	301	GQK	C5-C6-C7-C8
17	N	201	GQK	C5-C6-C7-C8
17	N	201	GQK	O37-C29-C30-N31
17	b	201	GQK	C1-C6-C7-C8
17	N	201	GQK	C1-C6-C7-C8
17	b	201	GQK	O37-C29-C30-N31
17	b	201	GQK	C23-C24-C40-C41
17	N	201	GQK	C23-C24-C40-C41
18	V	303	MES	C8-C7-N4-C3
17	H	301	GQK	C29-C30-N31-C32
18	V	303	MES	C7-C8-S-O2S
18	Y	303	MES	C7-C8-S-O2S
17	V	301	GQK	N28-C29-C30-N31
18	H	302	MES	N4-C7-C8-S
18	V	303	MES	C8-C7-N4-C5
17	H	301	GQK	N28-C29-C30-N31
17	V	301	GQK	O37-C29-C30-N31
17	H	301	GQK	O49-C23-C24-N25

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Mol	Chain	Res	Type	Atoms
17	K	301	GQK	O49-C23-C24-N25
17	Y	301	GQK	O49-C23-C24-N25
17	H	301	GQK	O37-C29-C30-N31
17	N	201	GQK	C6-C7-C8-C9
17	b	201	GQK	C6-C7-C8-C9
17	H	301	GQK	N22-C23-C24-N25
17	K	301	GQK	N22-C23-C24-N25

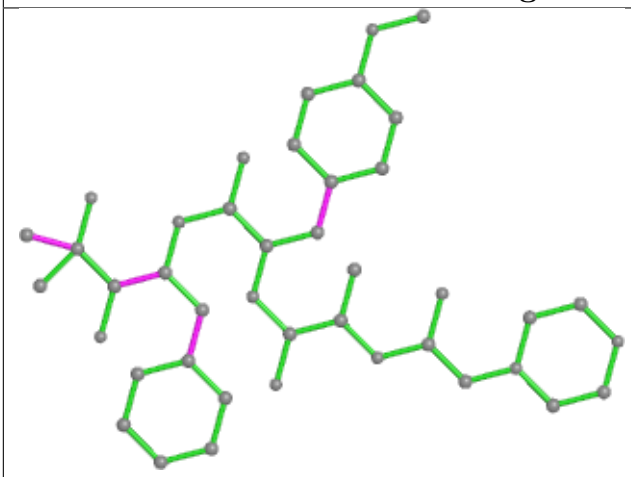
There are no ring outliers.

7 monomers are involved in 6 short contacts:

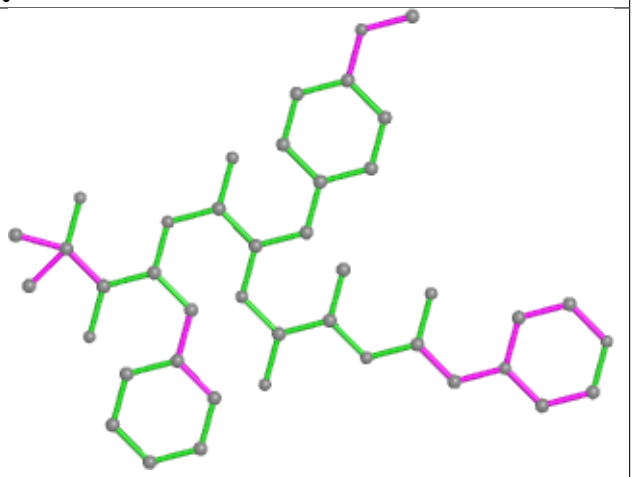
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	301	GQK	2	0
17	H	301	GQK	2	0
18	H	302	MES	1	0
17	Y	301	GQK	1	0
17	N	201	GQK	1	0
18	K	303	MES	1	0
19	N	203	SO4	1	0

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

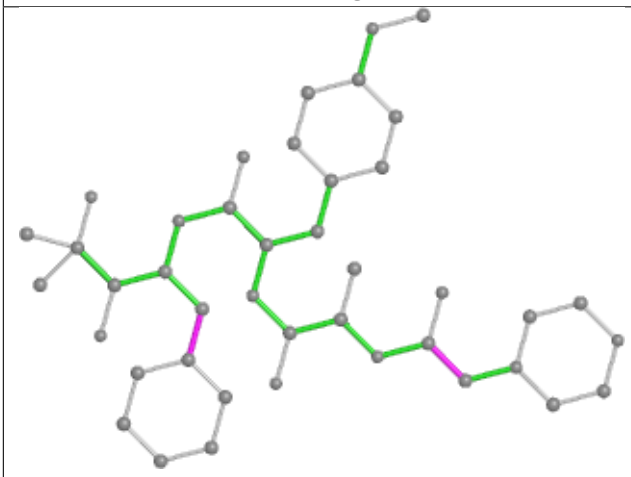
Ligand GQK V 301



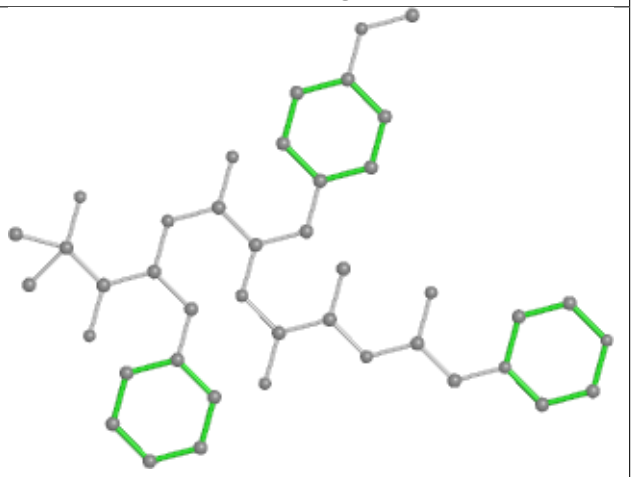
Bond lengths



Bond angles

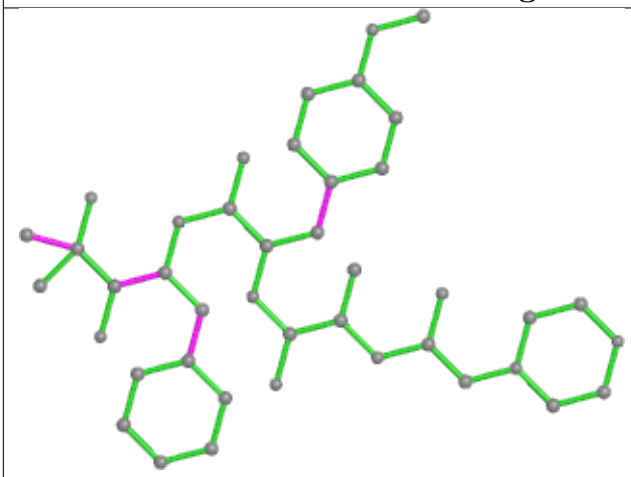


Torsions

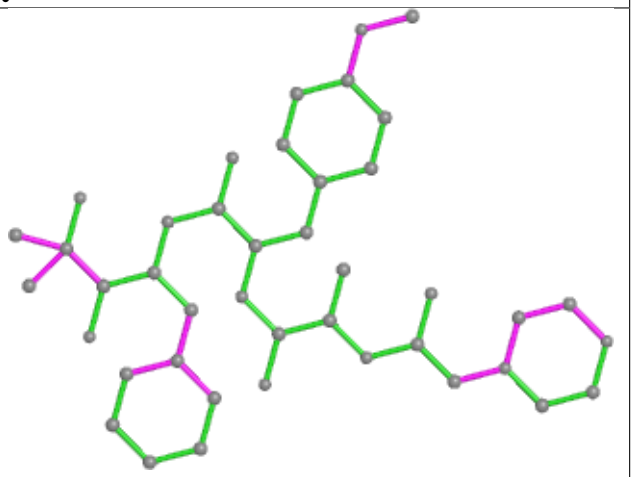


Rings

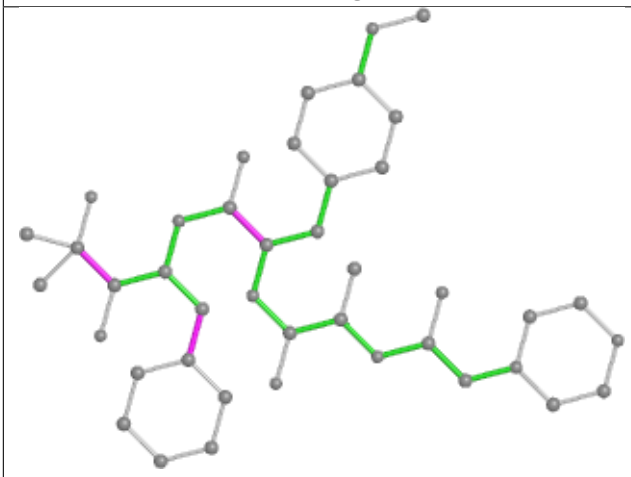
Ligand GQK K 301



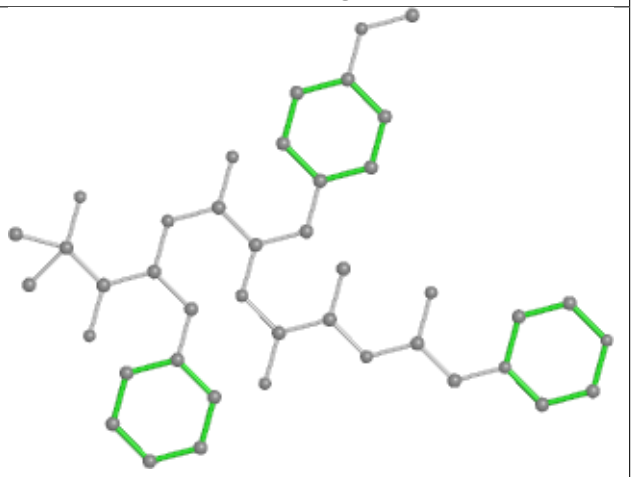
Bond lengths



Bond angles

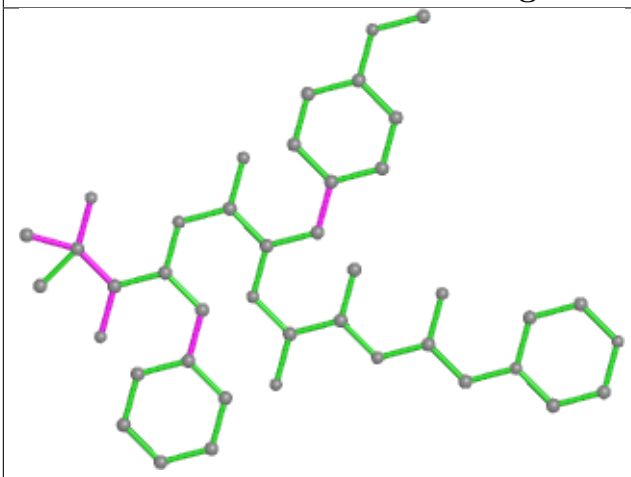


Torsions

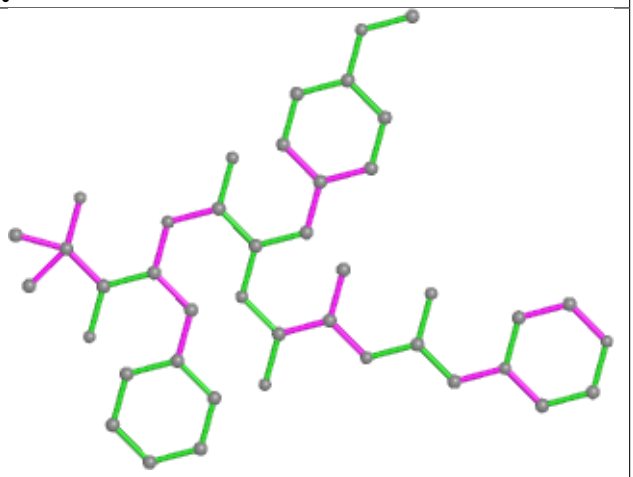


Rings

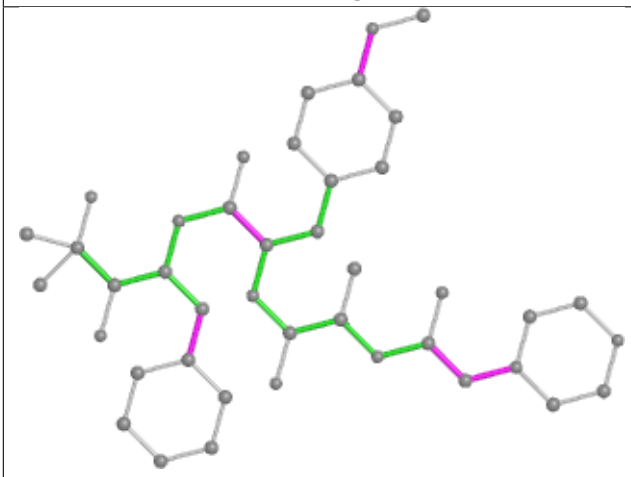
Ligand GQK H 301



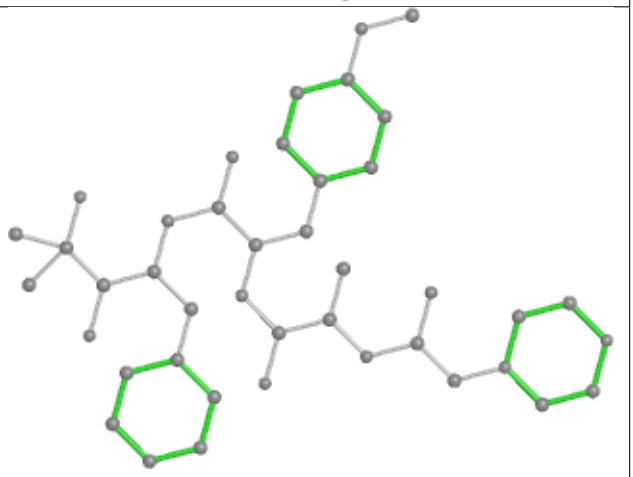
Bond lengths



Bond angles

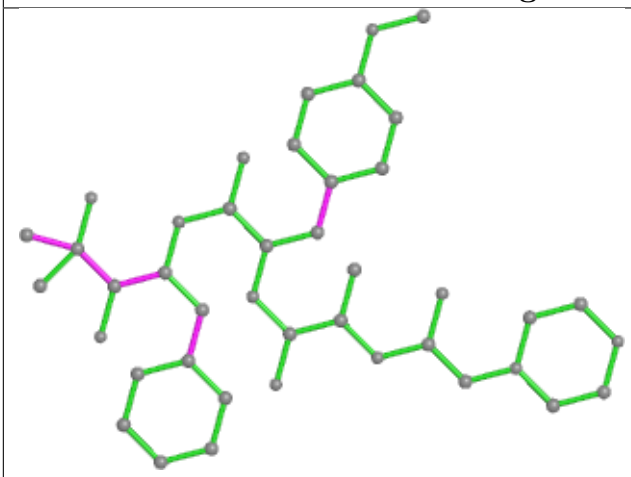


Torsions

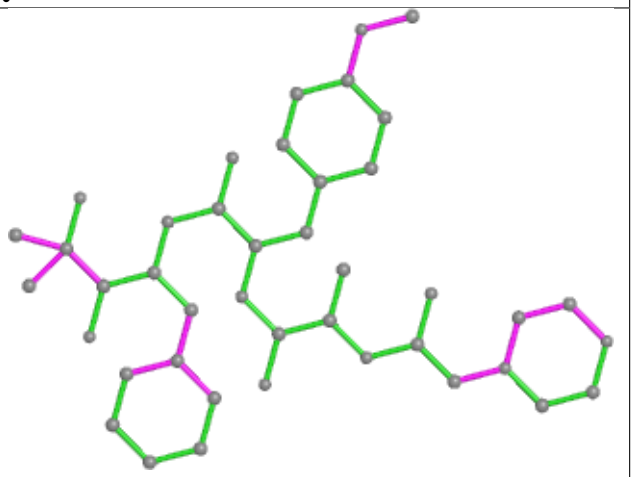


Rings

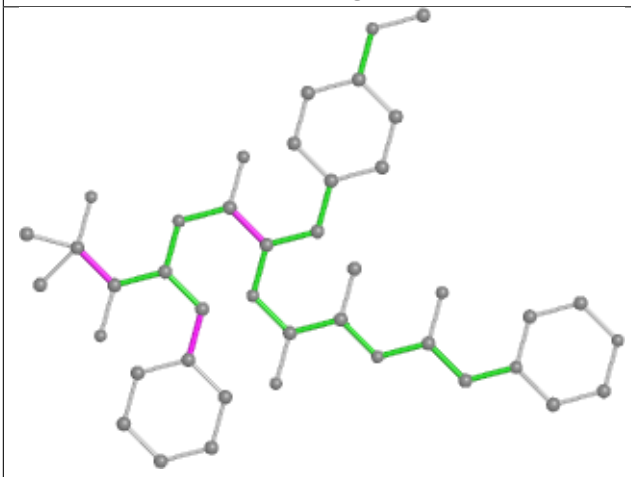
Ligand GQK Y 301



Bond lengths



Bond angles



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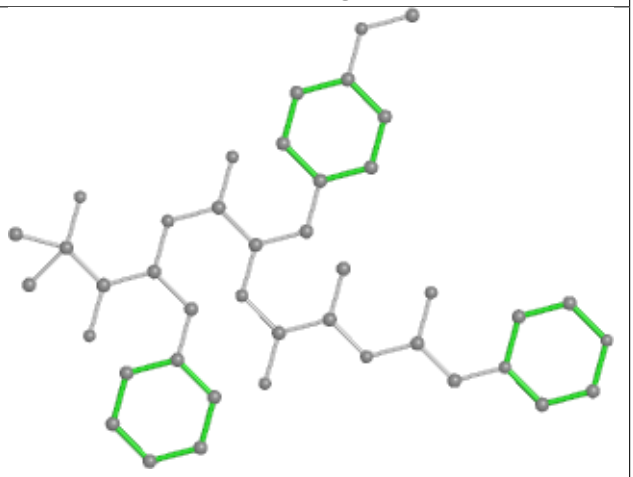
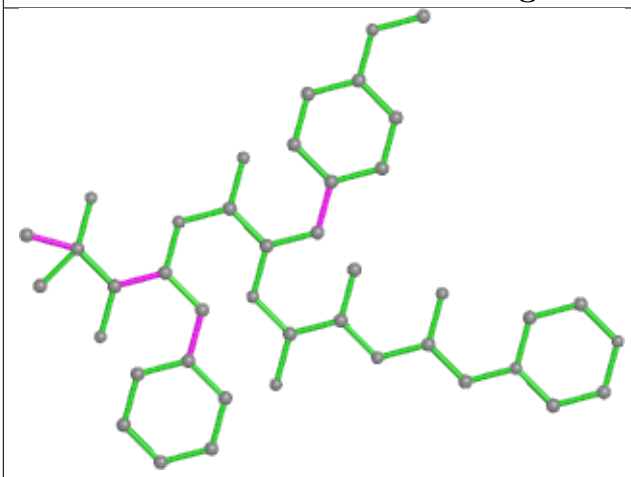
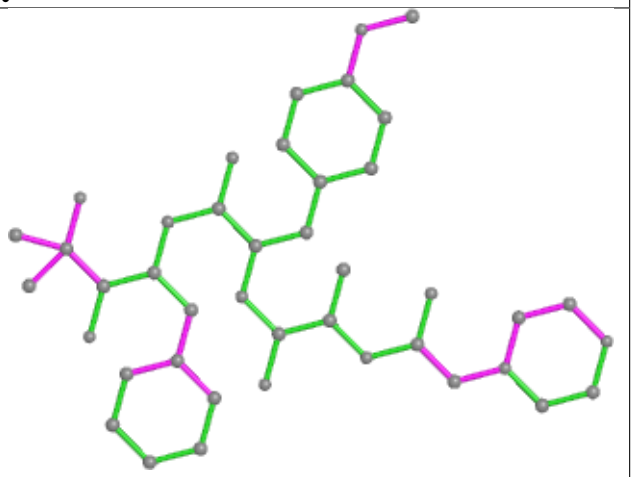


Rings

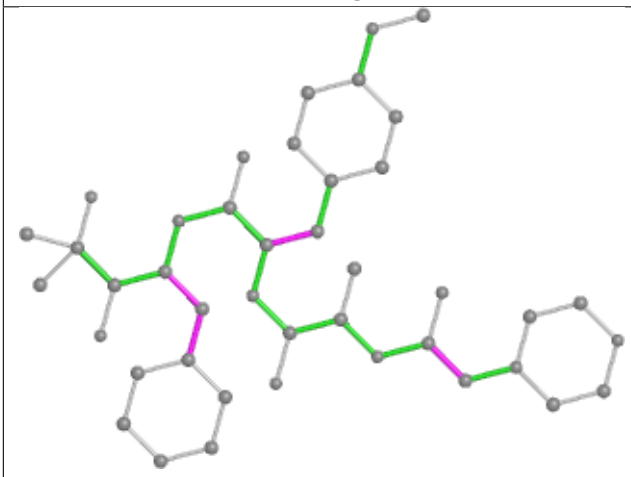
Ligand GQK N 201



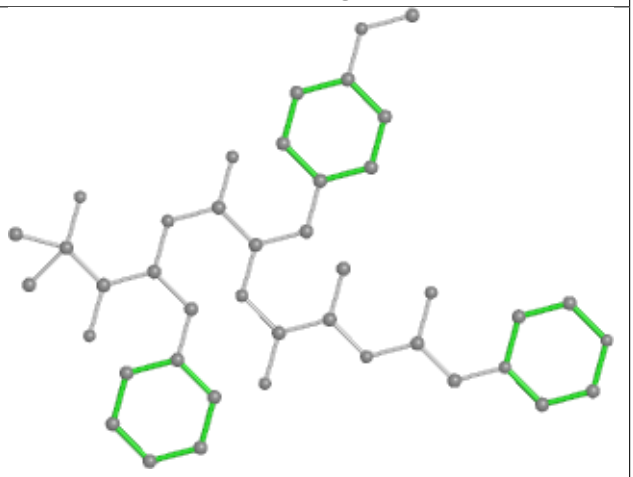
Bond lengths



Bond angles

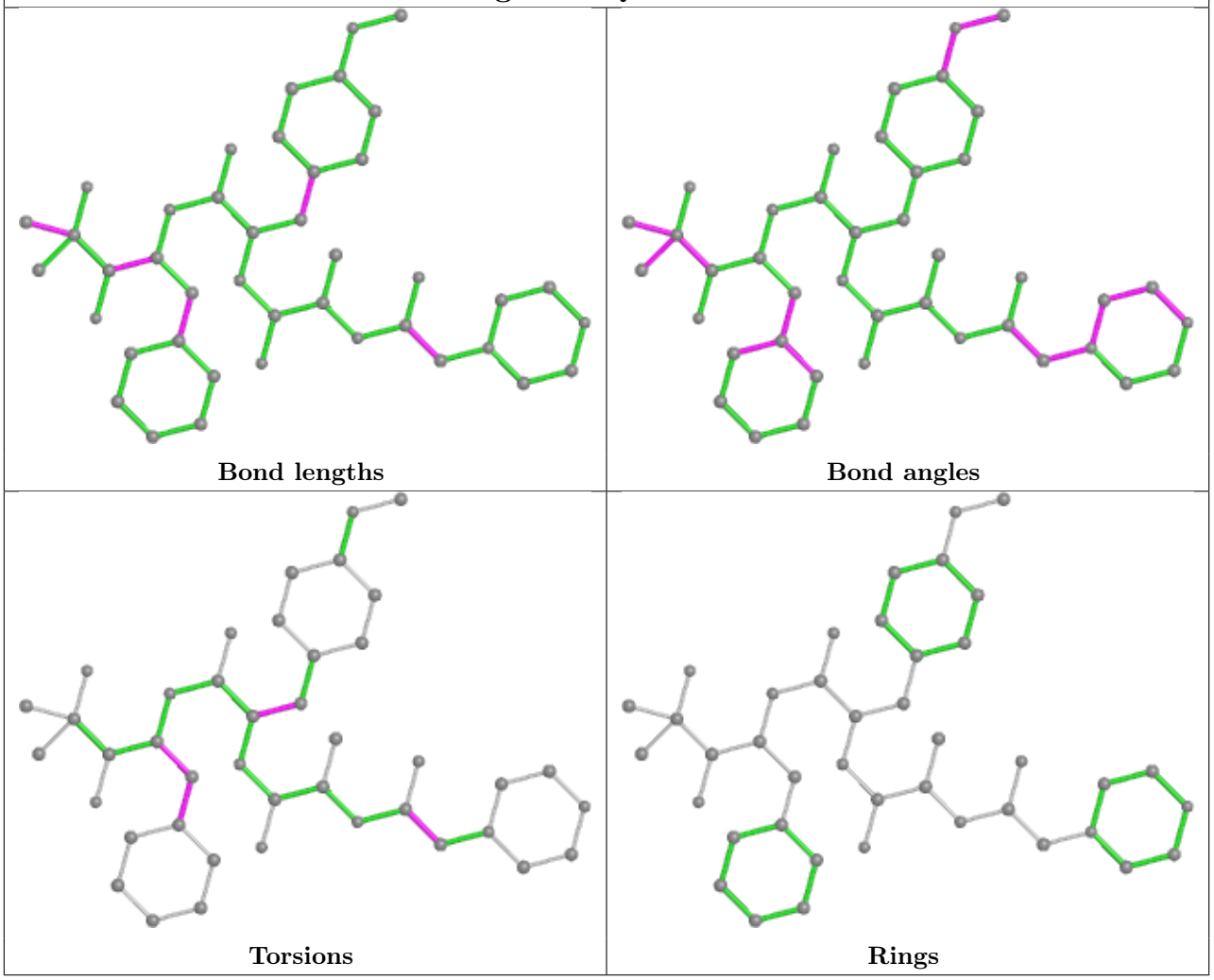


Torsions



Rings

Ligand GQK b 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.56	3 (1%) 79 54	52, 69, 109, 133	0
1	O	250/250 (100%)	-0.51	6 (2%) 59 30	56, 77, 119, 145	0
2	B	244/258 (94%)	-0.56	3 (1%) 79 54	52, 72, 112, 132	0
2	P	244/258 (94%)	-0.51	5 (2%) 65 36	56, 76, 114, 141	0
3	C	240/254 (94%)	-0.48	3 (1%) 77 51	49, 77, 129, 167	0
3	Q	240/254 (94%)	-0.29	9 (3%) 40 16	59, 93, 163, 209	0
4	D	235/260 (90%)	-0.59	0 100 100	55, 75, 105, 146	0
4	R	235/260 (90%)	-0.47	0 100 100	67, 86, 119, 155	0
5	E	231/234 (98%)	-0.52	1 (0%) 92 79	59, 79, 118, 138	0
5	S	231/234 (98%)	-0.46	2 (0%) 84 63	64, 89, 131, 153	0
6	F	243/288 (84%)	-0.63	0 100 100	51, 74, 116, 135	0
6	T	243/288 (84%)	-0.55	2 (0%) 86 65	51, 82, 126, 152	0
7	G	241/252 (95%)	-0.65	1 (0%) 92 79	52, 70, 104, 148	0
7	U	241/252 (95%)	-0.62	1 (0%) 92 79	56, 71, 102, 138	0
8	H	226/226 (100%)	-0.62	5 (2%) 62 33	51, 65, 96, 153	0
8	V	223/226 (98%)	-0.61	4 (1%) 68 40	50, 67, 94, 131	0
9	I	204/205 (99%)	-0.82	0 100 100	44, 60, 86, 104	0
9	W	204/205 (99%)	-0.81	0 100 100	46, 63, 86, 104	0
10	J	195/198 (98%)	-0.68	2 (1%) 82 59	47, 64, 89, 109	0
10	X	195/198 (98%)	-0.66	2 (1%) 82 59	51, 67, 92, 119	0
11	K	212/212 (100%)	-0.74	0 100 100	38, 63, 87, 100	0
11	Y	212/212 (100%)	-0.77	0 100 100	39, 65, 90, 104	0
12	L	222/222 (100%)	-0.74	0 100 100	50, 64, 93, 111	0
12	Z	222/222 (100%)	-0.73	0 100 100	51, 65, 95, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	222/246 (90%)	-0.73	2 (0%) 84 63	44, 63, 87, 109	0
13	a	222/246 (90%)	-0.71	1 (0%) 91 75	46, 63, 85, 101	0
14	N	196/196 (100%)	-0.71	1 (0%) 91 75	46, 62, 90, 104	0
14	b	196/196 (100%)	-0.73	0 100 100	45, 64, 93, 105	0
All	All	6319/6602 (95%)	-0.62	53 (0%) 86 65	38, 70, 115, 209	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	224	GLN	6.6
2	P	220	ASN	5.2
3	Q	49	THR	4.6
8	H	225	GLU	4.5
8	H	226	GLU	4.3
8	V	222	ASP	4.1
2	B	220	ASN	4.1
8	H	222	ASP	3.9
2	B	221	ASP	3.9
3	Q	239	GLN	3.8
5	E	202	ASP	3.6
3	Q	238	LYS	3.5
1	A	229	THR	3.5
5	S	54	GLU	3.4
1	A	228	PRO	3.3
1	O	228	PRO	3.3
10	X	1	MET	3.3
13	a	1	THR	3.3
8	V	223	ILE	3.2
10	J	1	MET	3.2
3	C	49	THR	3.2
3	Q	48	SER	3.1
3	C	202	GLN	3.0
3	Q	204	GLY	3.0
1	O	249	ALA	3.0
2	P	221	ASP	3.0
5	S	202	ASP	2.9
3	Q	50	LEU	2.9
2	P	219	ALA	2.9
3	Q	236	GLN	2.8
13	M	220	ASP	2.7
7	U	222	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
8	H	223	ILE	2.6
1	O	229	THR	2.6
2	P	52	THR	2.5
3	Q	206	LYS	2.4
2	P	59	ASP	2.3
13	M	1	THR	2.3
10	X	194	ASP	2.3
3	Q	202	GLN	2.2
1	O	52	SER	2.2
6	T	2	THR	2.2
2	B	217	LYS	2.2
10	J	194	ASP	2.2
8	V	221	CYS	2.1
1	O	250	LEU	2.1
3	C	239	GLN	2.1
7	G	222	ASP	2.1
8	V	9	GLN	2.1
14	N	195	GLN	2.1
1	O	231	LYS	2.0
6	T	244	ASN	2.0
1	A	201	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	K	302	1/1	0.92	0.13	67,67,67,67	0
17	GQK	N	201	42/42	0.92	0.21	48,66,85,91	0

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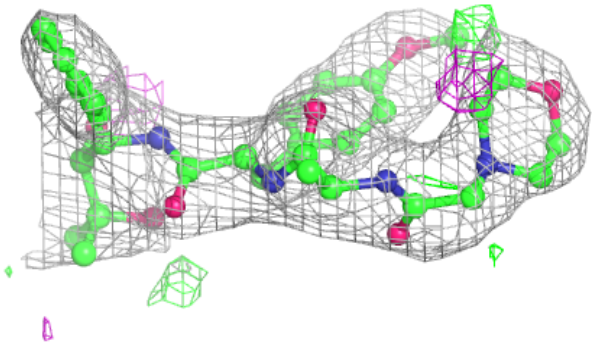
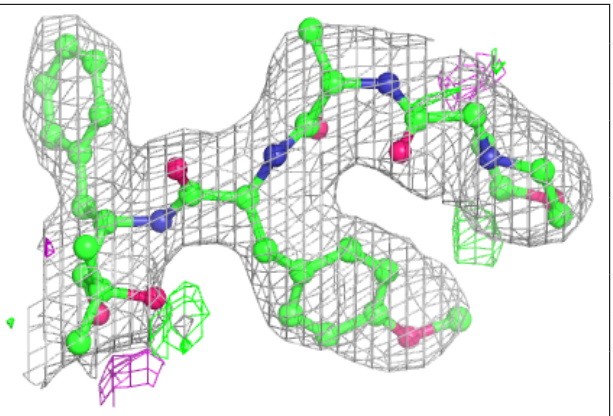
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	GQK	H	301	42/42	0.93	0.19	51,61,87,90	0
17	GQK	b	201	42/42	0.93	0.17	47,64,89,93	0
17	GQK	V	301	42/42	0.94	0.16	47,56,89,92	0
17	GQK	K	301	42/42	0.95	0.16	36,52,69,71	0
16	CL	U	301	1/1	0.95	0.19	57,57,57,57	0
18	MES	V	303	12/12	0.95	0.17	47,73,78,78	12
15	MG	Z	301	1/1	0.96	0.15	76,76,76,76	0
18	MES	H	302	12/12	0.96	0.18	45,68,76,77	12
17	GQK	Y	301	42/42	0.96	0.16	37,53,72,73	0
19	SO4	b	202	5/5	0.96	0.27	42,47,50,50	5
19	SO4	N	203	5/5	0.97	0.27	44,47,52,55	5
15	MG	I	301	1/1	0.97	0.36	78,78,78,78	0
15	MG	V	302	1/1	0.98	0.13	88,88,88,88	0
15	MG	W	301	1/1	0.98	0.38	83,83,83,83	0
18	MES	K	303	12/12	0.98	0.17	29,29,37,40	12
15	MG	Y	302	1/1	0.98	0.14	69,69,69,69	0
18	MES	Y	303	12/12	0.98	0.14	28,29,32,35	12
15	MG	G	301	1/1	0.98	0.04	59,59,59,59	0
15	MG	N	202	1/1	0.98	0.12	53,53,53,53	0
16	CL	G	302	1/1	0.99	0.22	48,48,48,48	0

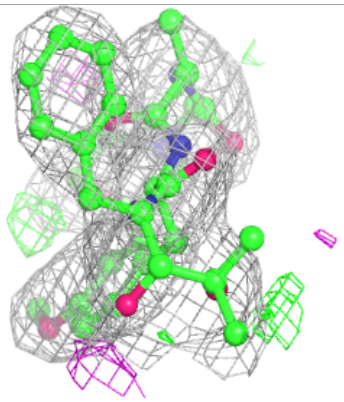
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GQK N 201:

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

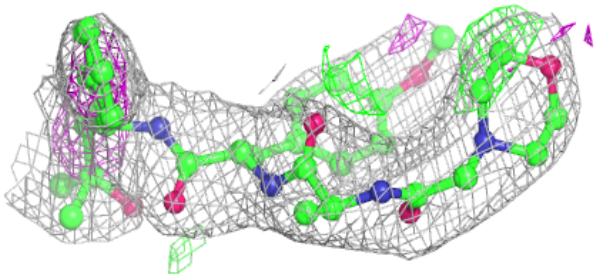


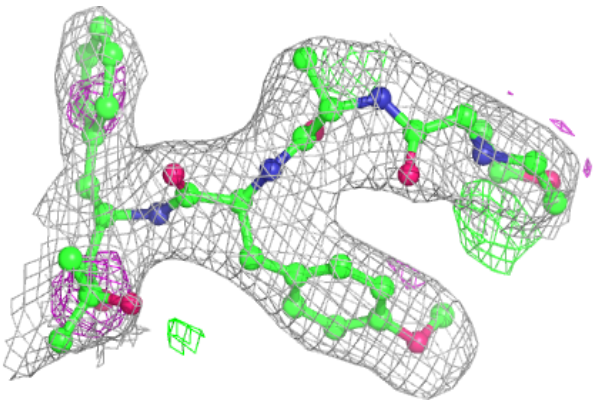


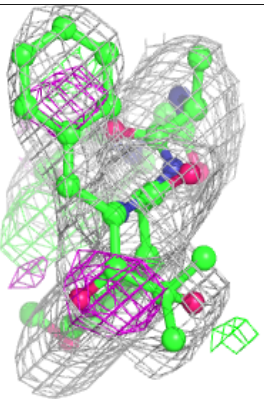


Electron density around GQK H 301:

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

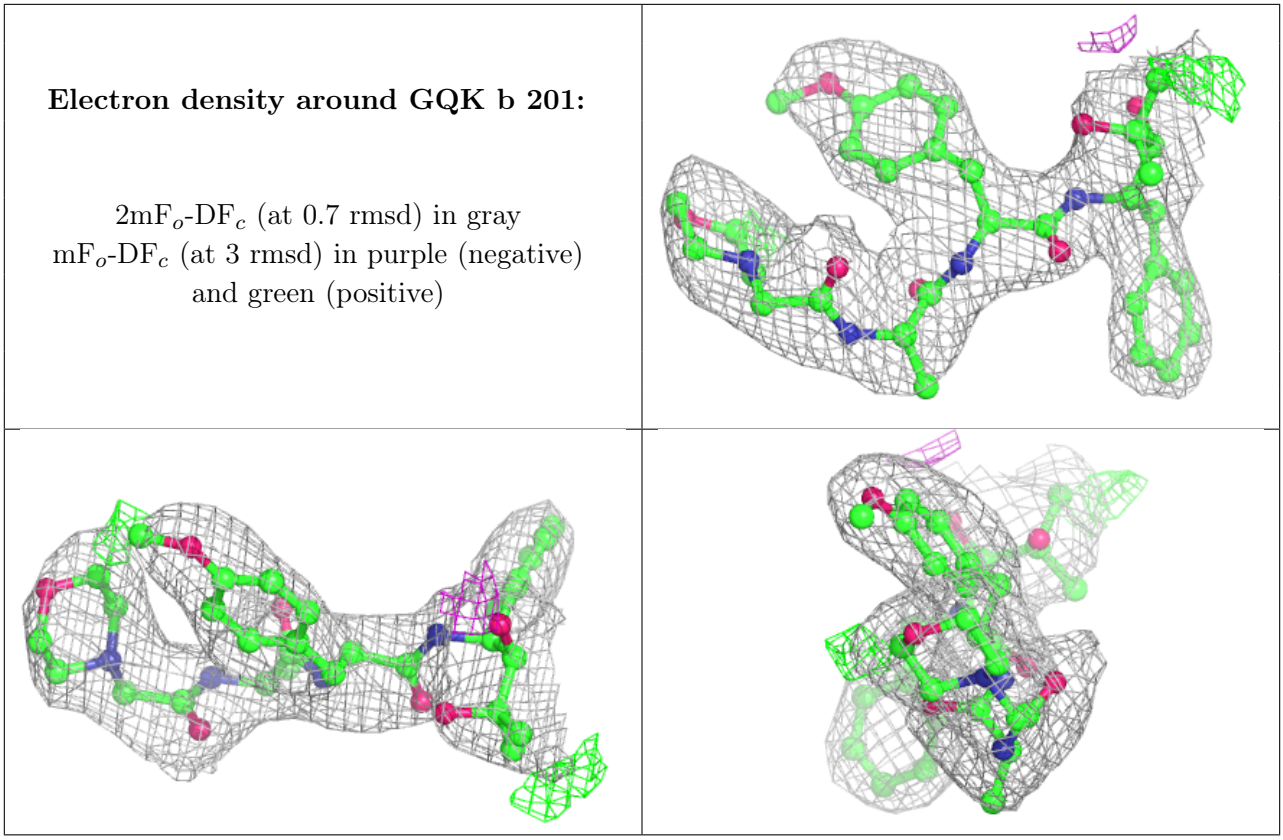






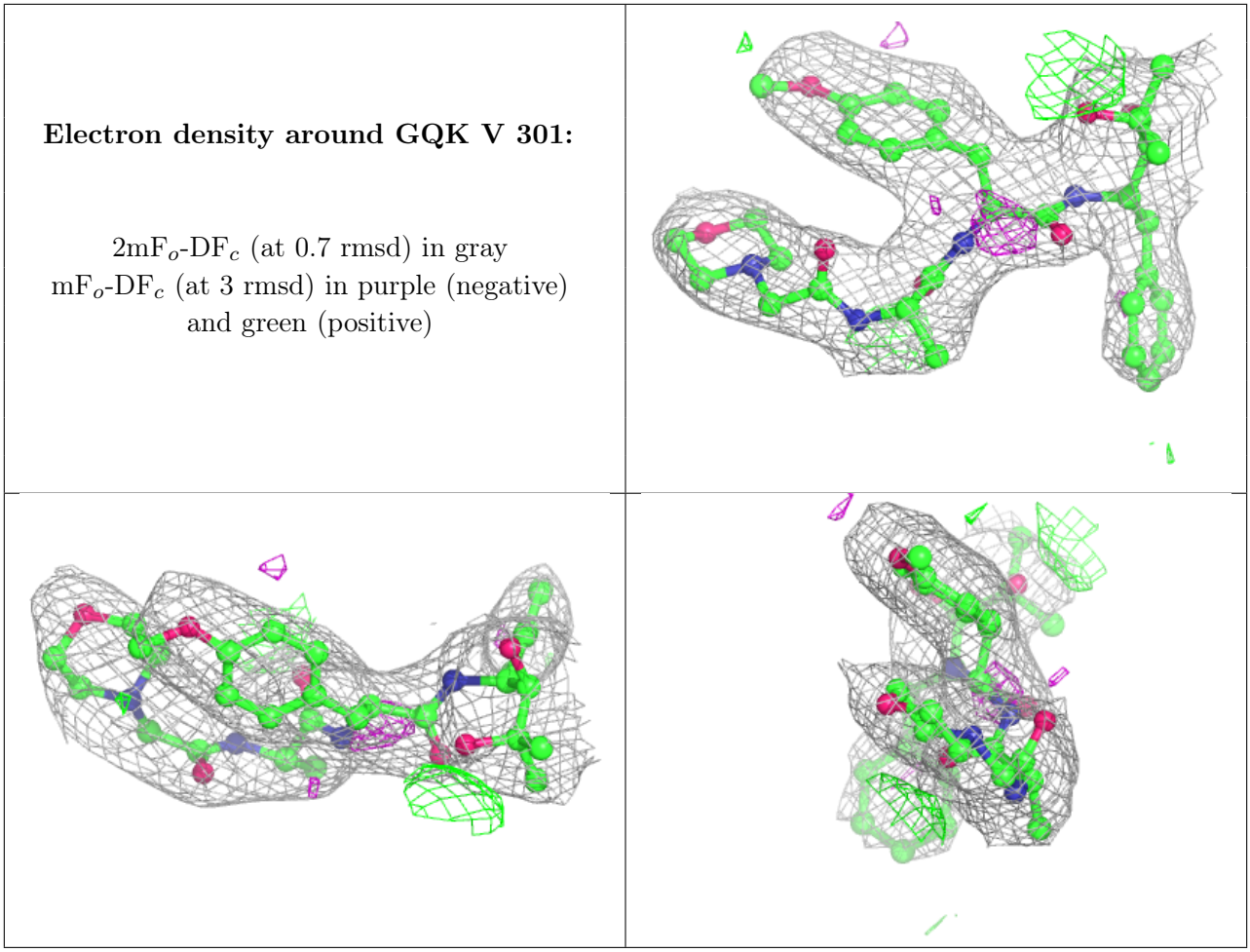
Electron density around GQK b 201:

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



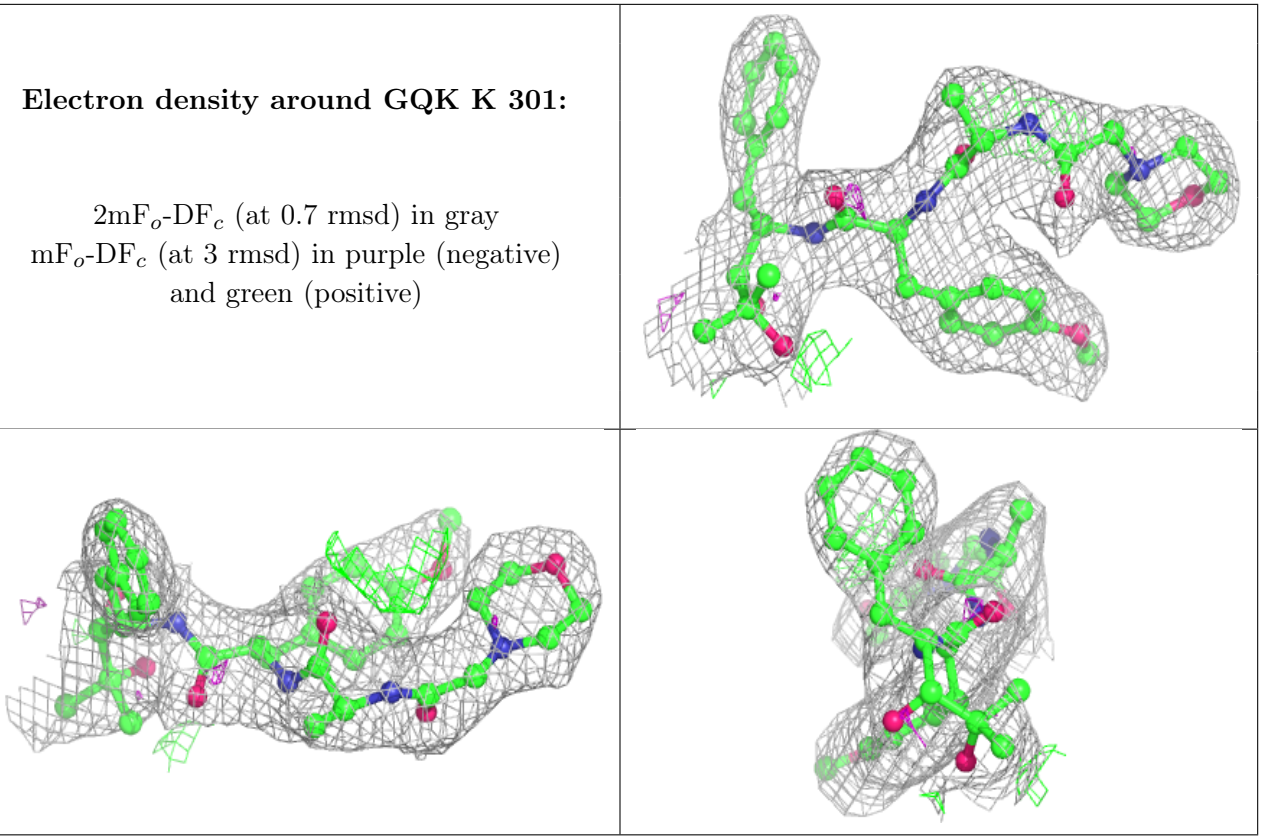
Electron density around GQK V 301:

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



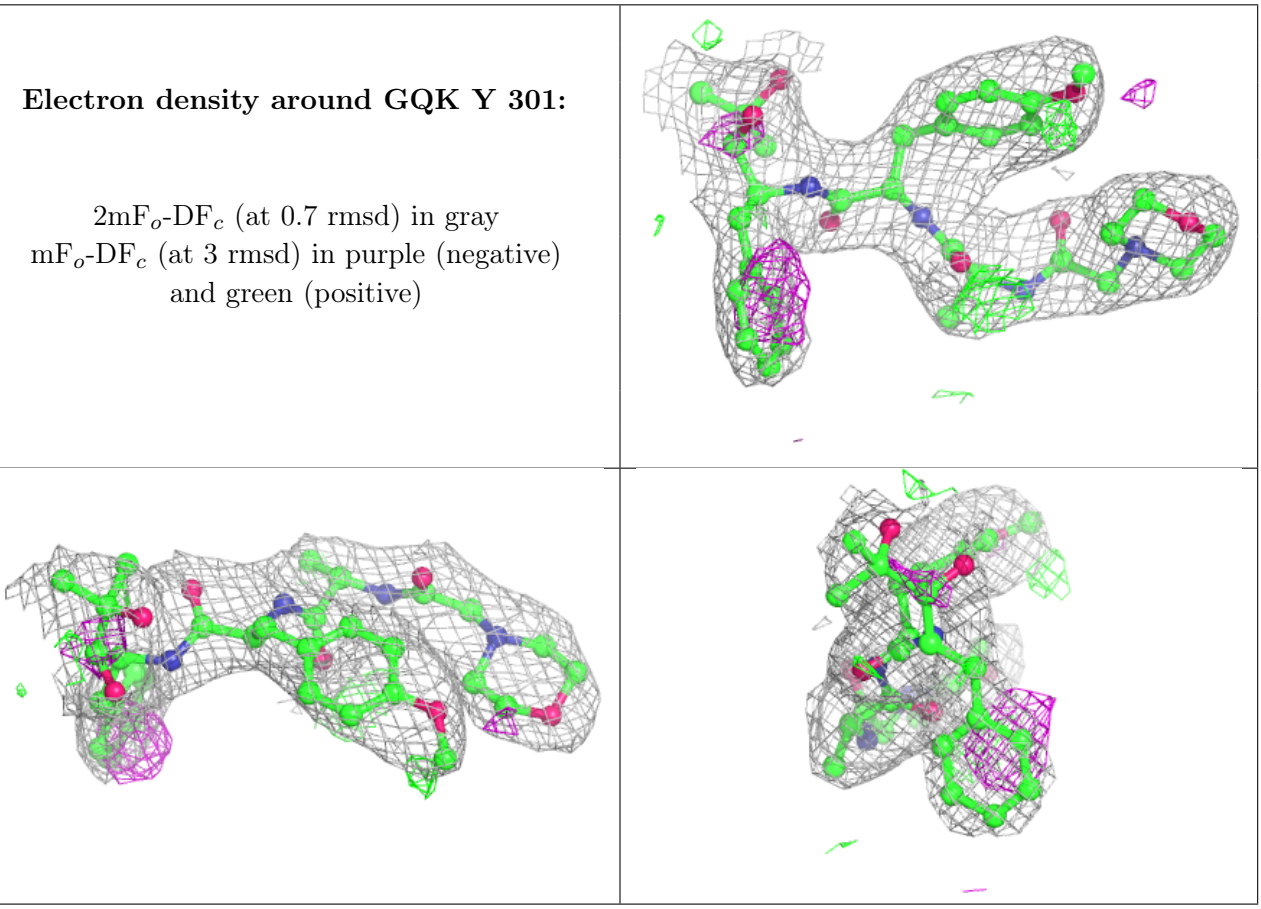
Electron density around GQK K 301:

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



Electron density around GQK 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.