



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 1, 2020 – 08:06 PM EST

PDB ID : 6W9T  
Title : Crystal structure of Neisseria meningitidis ClpP protease complex with small molecule activator ACP1-06  
Authors : Mabanglo, M.F.; Houry, W.A.  
Deposited on : 2020-03-23  
Resolution : 1.64 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
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) : 2.14.6

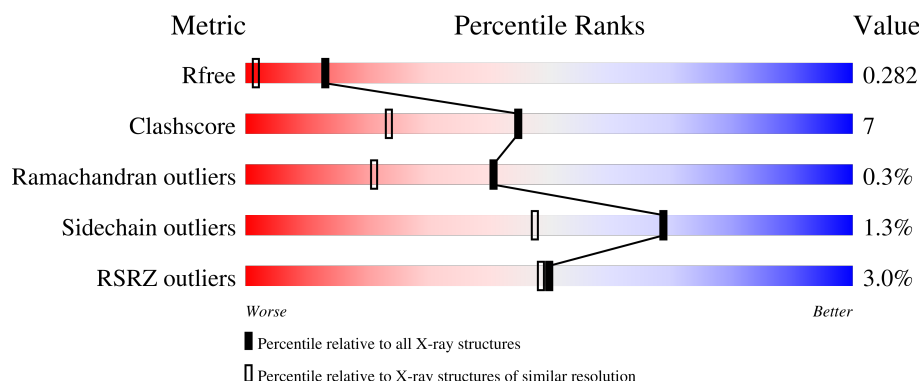
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.64 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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

Mol	Chain	Length	Quality of chain
1	A	199	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>10%</div> </div> </div>
1	B	199	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>10%</div> </div> </div>
1	C	199	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>10%</div> </div> </div>
1	D	199	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>9%</div> </div> </div>
1	E	199	<div> <div>0%</div> <div> <div></div> <div>70%</div> <div>18%</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	199	
1	G	199	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	KHS	F	301[A]	-	-	-	X
3	KHS	F	301[B]	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20410 atoms, of which 9866 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	180	Total	C	H	N	O	S	0	0	0
			2820	887	1415	239	271	8			
1	B	180	Total	C	H	N	O	S	0	0	0
			2829	893	1419	239	270	8			
1	C	180	Total	C	H	N	O	S	0	0	0
			2820	887	1415	239	271	8			
1	D	182	Total	C	H	N	O	S	0	0	0
			2864	902	1437	244	273	8			
1	E	174	Total	C	H	N	O	S	0	0	0
			2731	859	1368	233	263	8			
1	F	179	Total	C	H	N	O	S	0	0	0
			2810	887	1408	238	269	8			
1	G	174	Total	C	H	N	O	S	0	0	0
			2731	859	1368	233	263	8			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	ASP	GLY	conflict	UNP A0A0Y5K536
B	165	ASP	GLY	conflict	UNP A0A0Y5K536
C	165	ASP	GLY	conflict	UNP A0A0Y5K536
D	165	ASP	GLY	conflict	UNP A0A0Y5K536
E	165	ASP	GLY	conflict	UNP A0A0Y5K536
F	165	ASP	GLY	conflict	UNP A0A0Y5K536
G	165	ASP	GLY	conflict	UNP A0A0Y5K536

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by author).

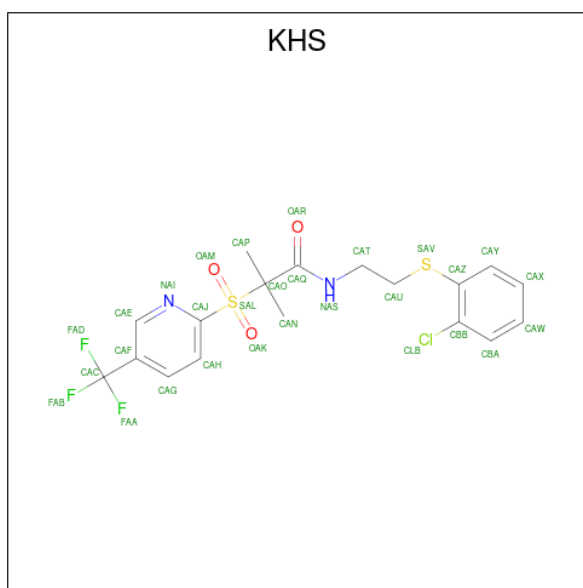
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total 1 K 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total K 1 1	0	0
2	E	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0
2	F	1	Total K 1 1	0	0

- Molecule 3 is N-{2-[(2-chlorophenyl)sulfanyl]ethyl}-2-methyl-2-{[5-(trifluoromethyl)pyridin-2-yl]sulfonyl}propanamide (three-letter code: KHS) (formula:  $C_{18}H_{18}ClF_3N_2O_3S_2$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
3	F	1	Total	C	Cl	F	H	N	O	S	0	1
			94	36	2	6	36	4	6	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	94	Total O 94 94	0	0

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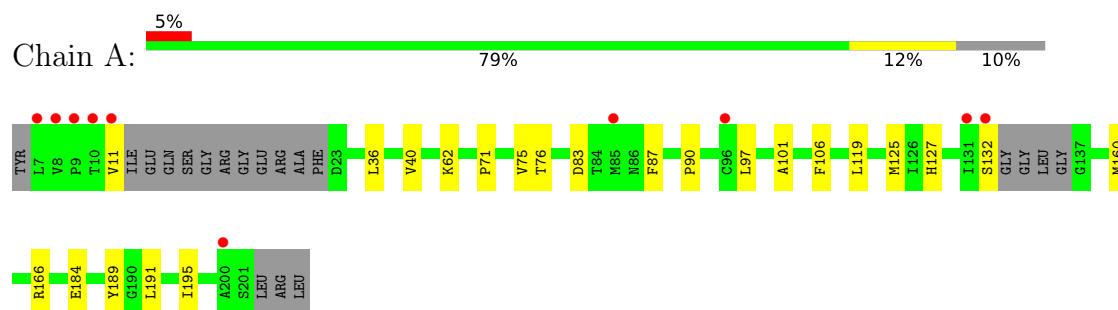
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	104	Total 104	O 104	0	0
4	C	86	Total 86	O 86	0	0
4	D	107	Total 107	O 107	0	0
4	E	93	Total 93	O 93	0	0
4	F	99	Total 99	O 99	0	0
4	G	121	Total 121	O 121	0	0

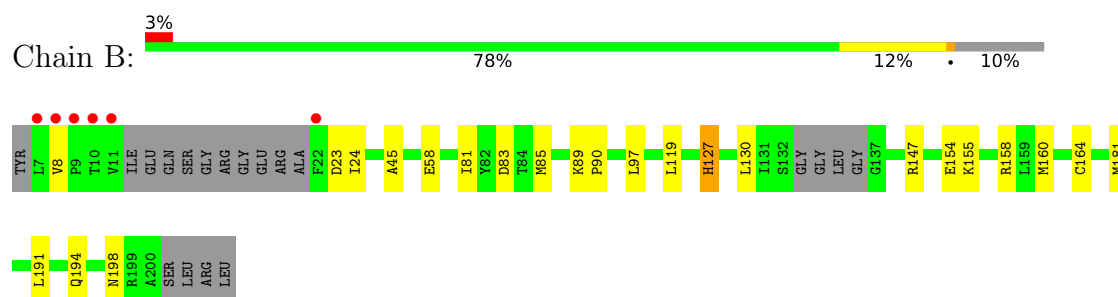
### 3 Residue-property plots [i](#)

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.

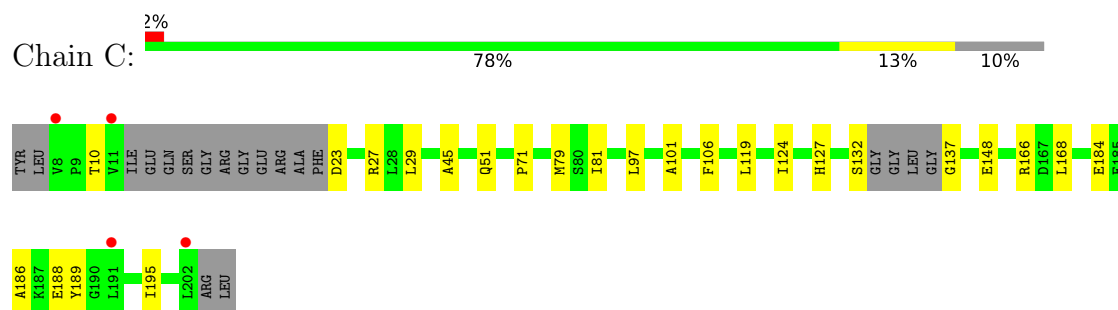
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



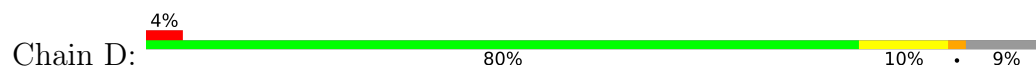
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

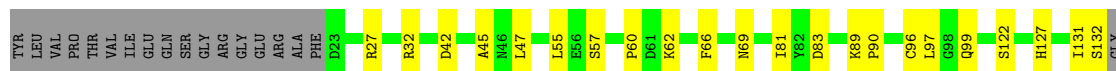


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

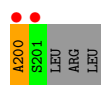
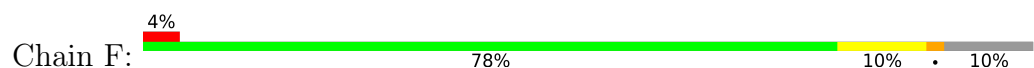




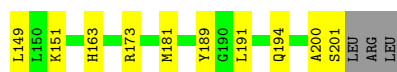
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.33Å 119.15Å 127.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	97.33 – 1.64 97.33 – 1.64	Depositor EDS
% Data completeness (in resolution range)	98.2 (97.33-1.64) 98.2 (97.33-1.64)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 1.63Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, $R_{free}$	0.237 , 0.282 0.237 , 0.282	Depositor DCC
$R_{free}$ test set	2010 reflections (1.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 57.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20410	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, KHS

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	0.56	0/1424	0.75	1/1917 (0.1%)
1	B	0.57	0/1430	0.77	1/1925 (0.1%)
1	C	0.69	1/1424 (0.1%)	0.74	2/1917 (0.1%)
1	D	0.51	0/1447	0.70	0/1947
1	E	0.54	0/1382	0.78	3/1859 (0.2%)
1	F	0.67	4/1422 (0.3%)	0.79	1/1914 (0.1%)
1	G	0.59	0/1382	0.79	2/1859 (0.1%)
All	All	0.59	5/9911 (0.1%)	0.76	10/13338 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	188	GLU	CD-OE1	-16.39	1.07	1.25
1	F	188	GLU	CD-OE1	9.81	1.36	1.25
1	F	188	GLU	CG-CD	-8.86	1.38	1.51
1	F	188	GLU	CD-OE2	6.93	1.33	1.25
1	F	85	MET	SD-CE	-5.05	1.49	1.77

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	85	MET	CG-SD-CE	15.88	125.60	100.20
1	B	85	MET	CG-SD-CE	11.57	118.70	100.20
1	E	181	MET	CG-SD-CE	9.38	115.21	100.20
1	G	173	ARG	CG-CD-NE	8.72	130.11	111.80
1	G	181	MET	CG-SD-CE	8.71	114.14	100.20
1	C	188	GLU	CG-CD-OE2	8.10	134.49	118.30
1	C	188	GLU	OE1-CD-OE2	-6.88	115.05	123.30
1	E	181	MET	CB-CG-SD	-5.86	94.84	112.40
1	A	125	MET	CG-SD-CE	-5.59	91.26	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	66	PHE	CB-CG-CD1	5.22	124.45	120.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1405	1415	1415	21	1
1	B	1410	1419	1419	23	0
1	C	1405	1415	1415	16	0
1	D	1427	1437	1437	18	0
1	E	1363	1368	1368	28	1
1	F	1402	1408	1408	18	0
1	G	1363	1368	1368	18	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
3	F	58	36	0	4	0
4	A	94	0	0	1	0
4	B	104	0	0	1	0
4	C	86	0	0	1	1
4	D	107	0	0	1	0
4	E	93	0	0	2	0
4	F	99	0	0	4	0
4	G	121	0	0	3	0
All	All	10544	9866	9830	128	2

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 7.

All (128) 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)
1:D:8:VAL:N	4:D:401:HOH:O	2.07	0.86
1:F:67:TYR:OH	3:F:301[A]:KHS:OAR	1.95	0.84
1:D:194:GLN:NE2	1:D:202:LEU:O	2.13	0.82
1:B:194:GLN:OE1	4:B:401:HOH:O	1.99	0.81
1:E:187:LYS:HD2	1:E:195:ILE:HD12	1.64	0.80
1:F:131:ILE:HG22	4:F:482:HOH:O	1.84	0.78
1:F:42:ASP:OD2	4:F:401:HOH:O	2.07	0.72
1:C:137:GLY:N	4:C:401:HOH:O	2.23	0.70
1:E:187:LYS:HD2	1:E:195:ILE:CD1	2.22	0.68
1:A:160:MET:HA	1:A:160:MET:HE2	1.77	0.66
1:G:60:PRO:HB2	1:G:89:LYS:HD3	1.78	0.65
1:E:131:ILE:HD12	1:E:149:LEU:HD22	1.79	0.65
1:B:8:VAL:CG1	1:B:24:ILE:HG22	2.27	0.64
1:F:199:ARG:NH2	4:F:402:HOH:O	2.31	0.64
1:B:45:ALA:HA	1:B:81:ILE:HD11	1.80	0.62
1:E:155:LYS:NZ	4:E:404:HOH:O	2.33	0.62
1:B:160:MET:HE1	1:B:191:LEU:CD2	2.32	0.60
1:A:11:VAL:O	4:A:401:HOH:O	2.17	0.59
1:G:151:LYS:NZ	4:G:406:HOH:O	2.37	0.58
1:B:58:GLU:OE2	1:C:27:ARG:NH2	2.36	0.58
1:G:75:VAL:O	1:G:79:MET:HG2	2.03	0.57
1:D:97:LEU:HD23	1:D:97:LEU:H	1.68	0.57
1:G:23:ASP:OD1	1:G:26:SER:OG	2.20	0.57
1:F:164:CYS:SG	1:F:191:LEU:HD12	2.46	0.56
1:B:194:GLN:OE1	1:B:194:GLN:HA	2.05	0.56
1:E:131:ILE:CD1	1:E:149:LEU:HD22	2.36	0.55
1:D:8:VAL:CG1	1:D:24:ILE:HG22	2.36	0.55
1:A:83:ASP:HB3	1:B:119:LEU:HD13	1.88	0.55
1:B:97:LEU:H	1:B:97:LEU:HD23	1.72	0.54
1:E:97:LEU:H	1:E:97:LEU:HD23	1.71	0.54
1:B:154:GLU:HA	1:B:154:GLU:OE1	2.09	0.53
1:F:187:LYS:NZ	4:F:404:HOH:O	2.34	0.53
1:D:8:VAL:HG13	1:D:24:ILE:HG22	1.91	0.53
1:F:198:ASN:C	1:F:200:ALA:H	2.11	0.52
1:B:8:VAL:HG12	1:B:24:ILE:HG22	1.91	0.52
1:D:130:LEU:HD23	1:D:130:LEU:H	1.75	0.52
1:A:97:LEU:H	1:A:97:LEU:HD23	1.75	0.51
1:C:51:GLN:HA	1:D:24:ILE:HD11	1.93	0.50
1:D:166:ARG:HD2	1:D:189:TYR:O	2.12	0.50
1:A:189:TYR:HD2	1:A:191:LEU:HD12	1.76	0.50
1:B:8:VAL:HG11	1:B:23:ASP:OD2	2.12	0.50
1:E:60:PRO:O	1:E:89:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:ILE:HD11	3:F:301[B]:KHS:CAT	2.41	0.49
1:D:201:SER:O	1:D:202:LEU:CB	2.60	0.49
1:A:119:LEU:HD13	1:G:83:ASP:HB3	1.96	0.48
1:G:124:ILE:N	1:G:124:ILE:HD12	2.28	0.48
1:G:97:LEU:HD23	1:G:97:LEU:H	1.78	0.48
1:F:8:VAL:HG13	1:F:24:ILE:HG22	1.95	0.47
1:F:33:ILE:HD11	3:F:301[B]:KHS:CAU	2.44	0.47
1:G:23:ASP:OD2	4:G:401:HOH:O	2.20	0.47
1:A:87:PHE:CD1	1:B:198:ASN:HA	2.49	0.47
1:G:189:TYR:HB3	1:G:191:LEU:HD12	1.95	0.47
1:E:45:ALA:HA	1:E:81:ILE:HD11	1.97	0.47
1:A:11:VAL:HG12	1:G:30:LYS:NZ	2.30	0.47
1:C:184:GLU:CD	1:C:184:GLU:H	2.19	0.46
1:C:71:PRO:HA	1:C:101:ALA:HB3	1.98	0.46
1:E:199:ARG:O	1:E:200:ALA:HB2	2.16	0.46
1:E:96:CYS:SG	1:E:122:SER:HB3	2.55	0.46
1:C:29:LEU:HD23	1:D:11:VAL:HG12	1.98	0.46
1:C:97:LEU:HD23	1:C:97:LEU:H	1.80	0.45
1:B:127:HIS:CE1	1:B:130:LEU:HD11	2.51	0.45
1:E:187:LYS:HB2	1:E:195:ILE:HD11	1.99	0.45
1:E:42:ASP:OD2	4:E:401:HOH:O	2.21	0.45
1:F:102:SER:HG	1:F:127:HIS:CE1	2.33	0.45
1:A:189:TYR:CD2	1:A:191:LEU:CD1	3.00	0.45
1:B:160:MET:CE	1:B:191:LEU:CD2	2.95	0.45
1:F:33:ILE:HD11	3:F:301[A]:KHS:CAT	2.47	0.45
1:A:106:PHE:HA	1:A:160:MET:HE1	1.98	0.45
1:A:189:TYR:HD2	1:A:191:LEU:CD1	2.29	0.45
1:D:10:THR:HA	1:D:22:PHE:O	2.17	0.45
1:E:62:LYS:O	1:E:90:PRO:HB3	2.17	0.45
1:D:89:LYS:N	1:D:90:PRO:HD2	2.32	0.45
1:C:148:GLU:OE2	1:D:123:ARG:HD2	2.18	0.44
1:D:130:LEU:HD23	1:D:130:LEU:N	2.31	0.44
1:A:160:MET:HE2	1:A:160:MET:CA	2.45	0.44
1:A:75:VAL:HG13	1:A:76:THR:N	2.33	0.44
1:B:181:MET:CE	1:B:191:LEU:HD12	2.48	0.44
1:G:27:ARG:O	1:G:30:LYS:HB2	2.18	0.44
1:G:45:ALA:HA	1:G:81:ILE:HD11	2.00	0.44
1:C:45:ALA:HA	1:C:81:ILE:HD11	1.99	0.43
1:E:131:ILE:CG2	1:E:132:SER:N	2.81	0.43
1:C:124:ILE:HD13	1:C:186:ALA:CB	2.48	0.43
1:C:10:THR:HA	1:C:23:ASP:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LEU:N	1:B:97:LEU:HD23	2.34	0.43
1:B:155:LYS:HE2	1:B:158:ARG:HH22	1.84	0.42
1:C:166:ARG:HD2	1:C:189:TYR:O	2.19	0.42
1:C:168:LEU:HD12	1:C:168:LEU:O	2.19	0.42
1:E:83:ASP:HB3	1:F:119:LEU:HB3	2.01	0.42
1:A:83:ASP:CB	1:B:119:LEU:HD13	2.49	0.42
1:D:96:CYS:SG	1:D:122:SER:HB3	2.60	0.42
1:A:184:GLU:OE2	1:A:195:ILE:HD12	2.19	0.42
1:B:164:CYS:SG	1:B:191:LEU:HD23	2.59	0.42
1:E:131:ILE:O	1:E:132:SER:CB	2.67	0.42
1:E:32:ARG:HG2	1:E:55:LEU:HD22	2.01	0.42
1:E:83:ASP:HB3	1:F:119:LEU:HD13	2.01	0.42
1:D:11:VAL:O	1:D:11:VAL:HG23	2.18	0.42
1:E:157:ASN:HB3	1:E:168:LEU:CD1	2.50	0.42
1:G:131:ILE:HD11	1:G:149:LEU:HD22	2.02	0.42
1:D:120:PRO:HG3	1:D:197:GLU:HG2	2.01	0.42
1:A:11:VAL:CG1	4:G:409:HOH:O	2.67	0.41
1:A:62:LYS:O	1:A:90:PRO:HB3	2.19	0.41
1:F:36:LEU:HD21	1:F:40:VAL:HG22	2.01	0.41
1:G:123:ARG:C	1:G:124:ILE:HD12	2.41	0.41
1:G:91:ASP:OD2	1:G:115:LYS:NZ	2.50	0.41
1:G:113:LYS:HE2	1:G:163:HIS:O	2.20	0.41
1:B:89:LYS:HB3	1:B:90:PRO:HD3	2.02	0.41
1:E:47:LEU:HD11	1:F:9:PRO:HD3	2.03	0.41
1:E:171:LEU:HD13	1:E:171:LEU:HA	1.86	0.41
1:E:198:ASN:OD1	1:E:200:ALA:HB3	2.21	0.41
1:E:27:ARG:HD2	1:E:27:ARG:HA	1.94	0.41
1:C:79:MET:HE2	1:C:106:PHE:CE2	2.56	0.41
1:D:111:GLY:O	1:D:116:ARG:HD3	2.20	0.41
1:E:69:ASN:HA	1:E:99:GLN:O	2.21	0.41
1:B:160:MET:HE1	1:B:191:LEU:HD21	2.03	0.41
1:E:131:ILE:HG22	1:E:132:SER:N	2.36	0.40
1:E:157:ASN:HB3	1:E:168:LEU:HD11	2.03	0.40
1:E:187:LYS:HE2	1:E:193:ASP:O	2.21	0.40
1:E:69:ASN:HB2	1:E:97:LEU:O	2.21	0.40
1:F:45:ALA:HA	1:F:81:ILE:HD11	2.02	0.40
1:A:71:PRO:HA	1:A:101:ALA:HB3	2.03	0.40
1:B:8:VAL:CG1	1:B:23:ASP:OD2	2.69	0.40
1:B:83:ASP:HB3	1:C:119:LEU:HD13	2.02	0.40
1:A:36:LEU:HD21	1:A:40:VAL:HG22	2.03	0.40
1:C:184:GLU:HA	1:C:195:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:TYR:HA	1:F:85:MET:HE2	2.03	0.40
1:G:194:GLN:NE2	1:G:201:SER:O	2.55	0.40
1:A:160:MET:HB2	1:A:160:MET:HE3	1.83	0.40
1:A:119:LEU:HB3	1:G:83:ASP:HB3	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:SER:O	4:C:485:HOH:O[2_545]	2.11	0.09
1:E:166:ARG:HH22	1:G:31:GLU:OE1[3_545]	1.52	0.08

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	174/199 (87%)	171 (98%)	3 (2%)	0	100	100
1	B	174/199 (87%)	171 (98%)	3 (2%)	0	100	100
1	C	174/199 (87%)	171 (98%)	3 (2%)	0	100	100
1	D	176/199 (88%)	170 (97%)	4 (2%)	2 (1%)	14	2
1	E	170/199 (85%)	168 (99%)	2 (1%)	0	100	100
1	F	173/199 (87%)	168 (97%)	4 (2%)	1 (1%)	25	8
1	G	170/199 (85%)	167 (98%)	2 (1%)	1 (1%)	25	8
All	All	1211/1393 (87%)	1186 (98%)	21 (2%)	4 (0%)	41	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	202	LEU

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Mol	Chain	Res	Type
1	F	200	ALA
1	D	200	ALA
1	G	200	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	155/168 (92%)	153 (99%)	2 (1%)	69	47
1	B	155/168 (92%)	153 (99%)	2 (1%)	69	47
1	C	155/168 (92%)	153 (99%)	2 (1%)	69	47
1	D	157/168 (94%)	154 (98%)	3 (2%)	57	32
1	E	149/168 (89%)	147 (99%)	2 (1%)	69	47
1	F	154/168 (92%)	153 (99%)	1 (1%)	86	75
1	G	149/168 (89%)	147 (99%)	2 (1%)	69	47
All	All	1074/1176 (91%)	1060 (99%)	14 (1%)	69	47

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	HIS
1	A	166	ARG
1	B	127	HIS
1	B	147	ARG
1	C	127	HIS
1	C	132	SER
1	D	22	PHE
1	D	127	HIS
1	D	194	GLN
1	E	57	SER
1	E	127	HIS
1	F	127	HIS
1	G	23	ASP
1	G	127	HIS



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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
3	KHS	F	301[A]	-	28,30,30	1.92	6 (21%)	35,45,45	4.08	12 (34%)
3	KHS	F	301[B]	-	28,30,30	1.87	6 (21%)	35,45,45	3.98	13 (37%)

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
3	KHS	F	301[A]	-	-	15/30/34/34	0/2/2/2
3	KHS	F	301[B]	-	-	18/30/34/34	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	301[A]	KHS	CAQ-NAS	6.16	1.46	1.34
3	F	301[B]	KHS	CAQ-NAS	5.93	1.45	1.34
3	F	301[A]	KHS	CAZ-SAV	4.35	1.83	1.77
3	F	301[A]	KHS	OAM-SAL	3.87	1.47	1.44
3	F	301[B]	KHS	OAM-SAL	3.84	1.47	1.44
3	F	301[B]	KHS	CAZ-SAV	3.72	1.82	1.77
3	F	301[A]	KHS	OAK-SAL	3.44	1.47	1.44
3	F	301[B]	KHS	OAK-SAL	3.44	1.47	1.44
3	F	301[B]	KHS	CBB-CLB	2.85	1.80	1.73
3	F	301[A]	KHS	CBB-CLB	2.37	1.79	1.73
3	F	301[B]	KHS	OAR-CAQ	-2.27	1.18	1.22
3	F	301[A]	KHS	OAR-CAQ	-2.10	1.19	1.22

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	301[B]	KHS	OAK-SAL-OAM	-17.60	99.63	118.98
3	F	301[A]	KHS	OAK-SAL-OAM	-17.59	99.64	118.98
3	F	301[A]	KHS	OAK-SAL-CAO	7.83	113.23	107.72
3	F	301[A]	KHS	OAM-SAL-CAO	7.05	112.68	107.72
3	F	301[B]	KHS	OAK-SAL-CAO	6.89	112.56	107.72
3	F	301[B]	KHS	OAM-SAL-CAO	6.54	112.32	107.72
3	F	301[A]	KHS	CAE-NAI-CAJ	5.98	122.27	115.91
3	F	301[B]	KHS	CAE-NAI-CAJ	5.81	122.09	115.91
3	F	301[B]	KHS	OAM-SAL-CAJ	4.66	113.02	108.21
3	F	301[A]	KHS	CAO-CAQ-NAS	4.05	121.68	116.82
3	F	301[A]	KHS	CAH-CAJ-NAI	-4.00	120.89	125.28
3	F	301[B]	KHS	CAF-CAE-NAI	-3.90	119.62	123.34
3	F	301[B]	KHS	CAH-CAJ-NAI	-3.81	121.10	125.28
3	F	301[A]	KHS	CAF-CAE-NAI	-3.75	119.76	123.34
3	F	301[A]	KHS	CAU-SAV-CAZ	3.65	110.68	103.04
3	F	301[A]	KHS	OAM-SAL-CAJ	3.60	111.93	108.21
3	F	301[B]	KHS	CAO-CAQ-NAS	3.48	121.00	116.82
3	F	301[A]	KHS	CAN-CAO-CAP	-3.20	108.59	111.33
3	F	301[A]	KHS	OAK-SAL-CAJ	3.12	111.43	108.21
3	F	301[B]	KHS	CAN-CAO-CAP	-2.65	109.07	111.33
3	F	301[B]	KHS	CAU-SAV-CAZ	2.49	108.24	103.04
3	F	301[B]	KHS	OAK-SAL-CAJ	2.22	110.50	108.21
3	F	301[B]	KHS	CAG-CAF-CAE	2.09	120.09	117.69
3	F	301[A]	KHS	CAH-CAG-CAF	-2.04	118.48	121.22
3	F	301[B]	KHS	CAH-CAG-CAF	-2.01	118.53	121.22

There are no chirality outliers.

All (33) torsion outliers are listed below:

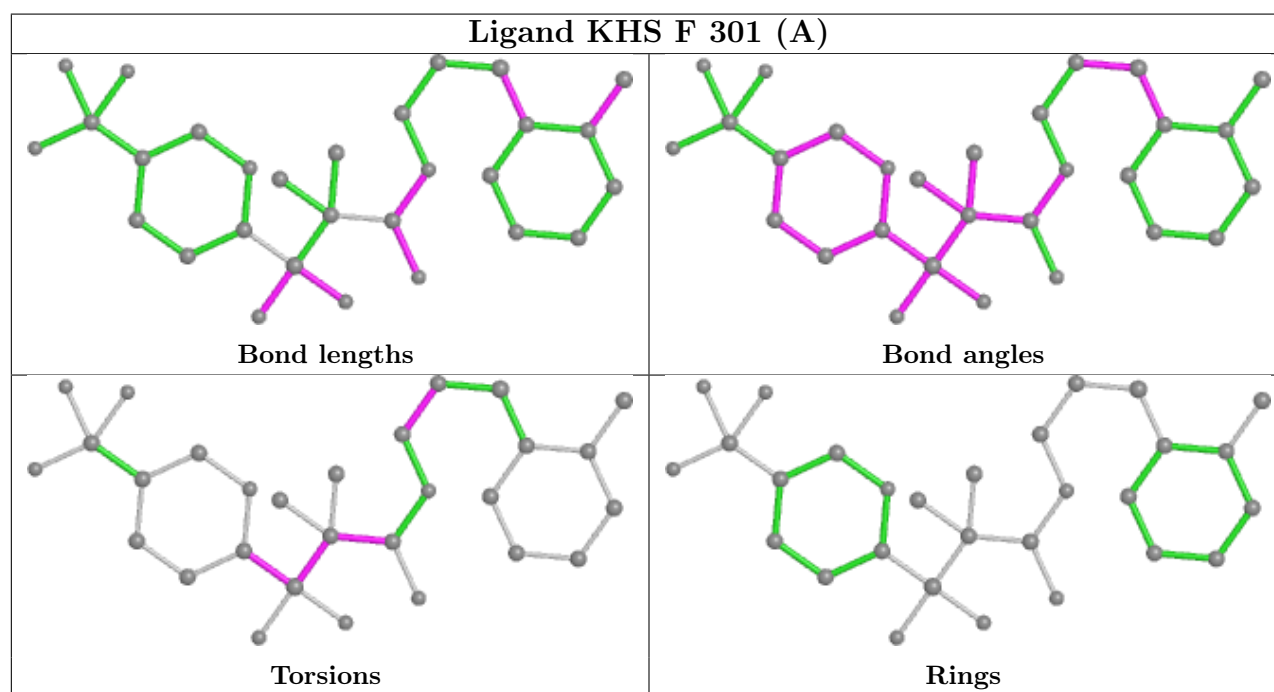
Mol	Chain	Res	Type	Atoms
3	F	301[A]	KHS	NAS-CAT-CAU-SAV
3	F	301[A]	KHS	CAQ-CAO-SAL-OAM
3	F	301[A]	KHS	CAP-CAO-SAL-OAM
3	F	301[A]	KHS	CAP-CAO-SAL-OAK
3	F	301[A]	KHS	CAP-CAO-SAL-CAJ
3	F	301[A]	KHS	CAN-CAO-SAL-OAM
3	F	301[A]	KHS	CAN-CAO-SAL-CAJ
3	F	301[A]	KHS	NAI-CAJ-SAL-OAM
3	F	301[A]	KHS	CAH-CAJ-SAL-OAM
3	F	301[A]	KHS	NAI-CAJ-SAL-OAK
3	F	301[A]	KHS	CAH-CAJ-SAL-OAK
3	F	301[B]	KHS	NAS-CAT-CAU-SAV
3	F	301[B]	KHS	CAQ-CAO-SAL-OAM
3	F	301[B]	KHS	CAQ-CAO-SAL-OAK
3	F	301[B]	KHS	CAP-CAO-SAL-OAM
3	F	301[B]	KHS	CAP-CAO-SAL-OAK
3	F	301[B]	KHS	CAP-CAO-SAL-CAJ
3	F	301[B]	KHS	CAN-CAO-SAL-OAM
3	F	301[B]	KHS	CAN-CAO-SAL-OAK
3	F	301[B]	KHS	CAN-CAO-SAL-CAJ
3	F	301[B]	KHS	NAI-CAJ-SAL-OAK
3	F	301[B]	KHS	CAH-CAJ-SAL-OAK
3	F	301[A]	KHS	CAH-CAJ-SAL-CAO
3	F	301[A]	KHS	CAN-CAO-CAQ-NAS
3	F	301[B]	KHS	CAY-CAZ-SAV-CAU
3	F	301[B]	KHS	CBB-CAZ-SAV-CAU
3	F	301[B]	KHS	NAI-CAJ-SAL-OAM
3	F	301[B]	KHS	CAH-CAJ-SAL-OAM
3	F	301[B]	KHS	CAH-CAJ-SAL-CAO
3	F	301[B]	KHS	CAT-CAU-SAV-CAZ
3	F	301[B]	KHS	CAU-CAT-NAS-CAQ
3	F	301[A]	KHS	CAQ-CAO-SAL-OAK
3	F	301[A]	KHS	CAN-CAO-CAQ-OAR

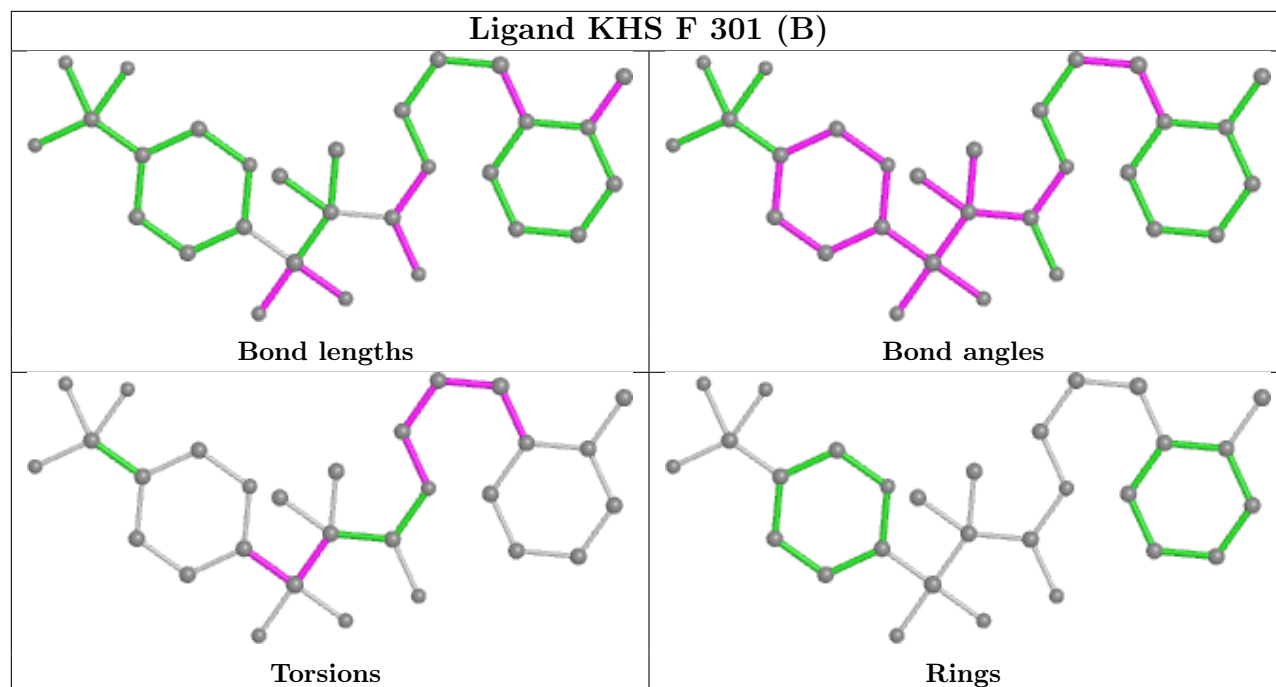
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	301[A]	KHS	2	0
3	F	301[B]	KHS	2	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	180/199 (90%)	0.27	10 (5%) 24 22	15, 22, 56, 80	0
1	B	180/199 (90%)	0.17	6 (3%) 46 44	17, 27, 50, 69	0
1	C	180/199 (90%)	0.29	4 (2%) 62 61	20, 32, 56, 73	0
1	D	182/199 (91%)	0.41	8 (4%) 34 32	17, 28, 60, 85	0
1	E	174/199 (87%)	0.12	2 (1%) 80 81	17, 27, 55, 74	0
1	F	179/199 (89%)	0.17	7 (3%) 39 37	18, 28, 63, 96	0
1	G	174/199 (87%)	-0.03	0 100 100	15, 22, 43, 57	0
All	All	1249/1393 (89%)	0.20	37 (2%) 50 48	15, 27, 56, 96	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	THR	10.7
1	D	10	THR	9.7
1	D	22	PHE	8.8
1	A	8	VAL	7.7
1	D	11	VAL	6.9
1	D	202	LEU	6.6
1	B	8	VAL	6.5
1	A	7	LEU	5.7
1	C	11	VAL	5.1
1	C	202	LEU	5.1
1	D	8	VAL	4.9
1	A	9	PRO	4.8
1	A	11	VAL	4.2
1	B	22	PHE	3.8
1	A	200	ALA	3.6
1	B	10	THR	3.6
1	D	9	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	96	CYS	3.6
1	D	201	SER	3.5
1	B	7	LEU	3.4
1	B	9	PRO	3.3
1	F	10	THR	3.1
1	F	8	VAL	3.1
1	F	200	ALA	3.0
1	F	22	PHE	2.9
1	C	8	VAL	2.9
1	E	200	ALA	2.6
1	F	11	VAL	2.5
1	B	11	VAL	2.4
1	C	191	LEU	2.4
1	D	132	SER	2.4
1	F	201	SER	2.3
1	F	9	PRO	2.2
1	A	85	MET	2.1
1	A	131	ILE	2.1
1	A	132	SER	2.0
1	E	199	ARG	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	KHS	F	301[A]	29/29	0.66	0.50	53,71,89,93	47
3	KHS	F	301[B]	29/29	0.66	0.50	24,73,88,94	47
2	K	D	301	1/1	0.98	0.08	30,30,30,30	0

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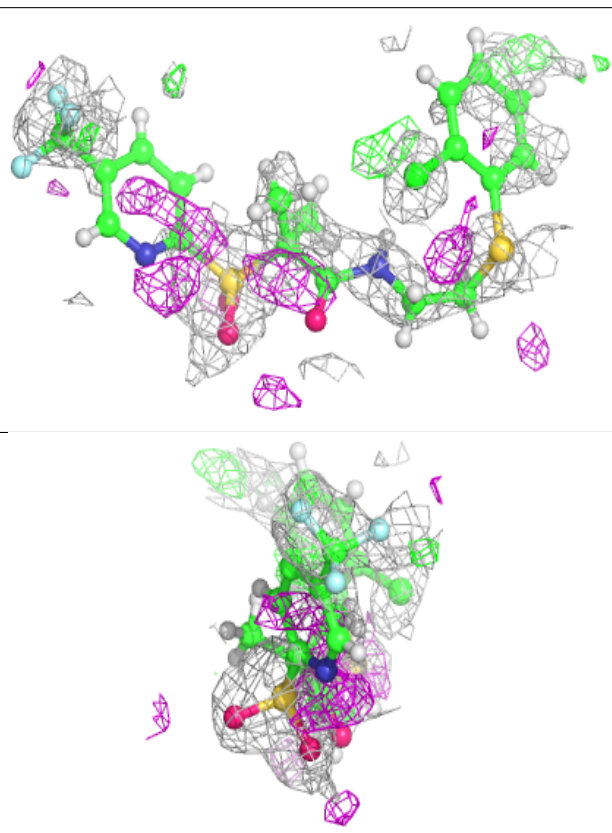
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	K	B	301	1/1	0.98	0.11	29,29,29,29	0
2	K	C	301	1/1	0.98	0.06	35,35,35,35	0
2	K	E	301	1/1	0.98	0.09	26,26,26,26	0
2	K	F	302	1/1	0.99	0.10	27,27,27,27	0
2	K	A	301	1/1	0.99	0.13	22,22,22,22	0
2	K	G	301	1/1	1.00	0.11	21,21,21,21	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 KHS F 301 (A):**

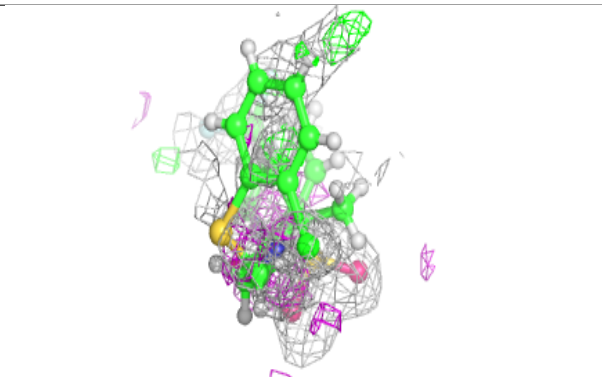
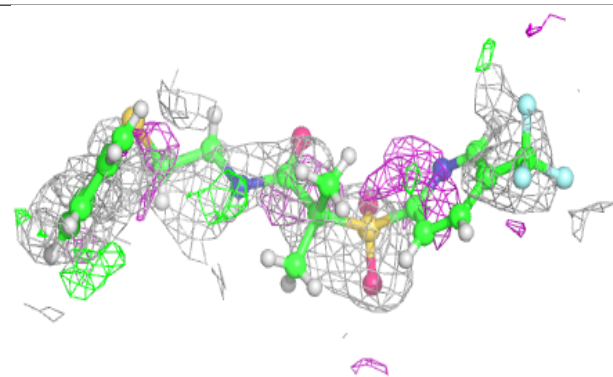
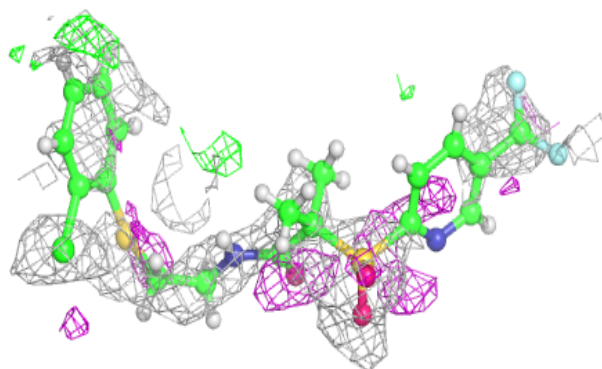
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





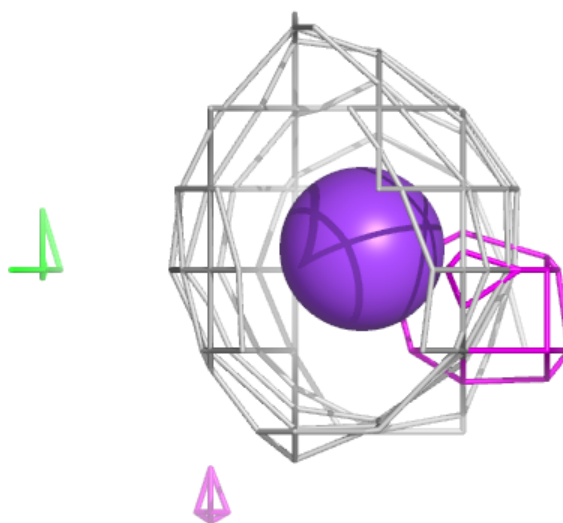
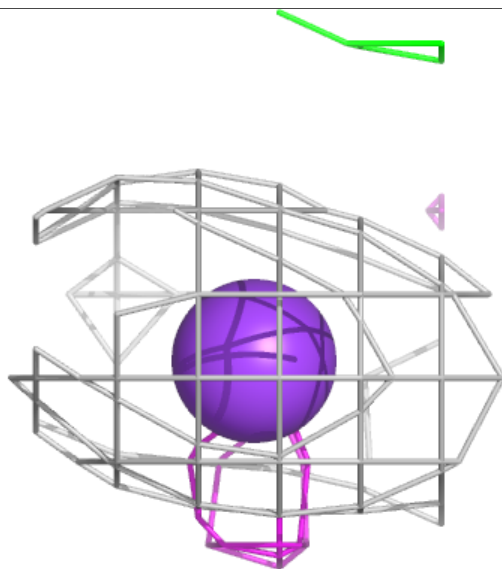
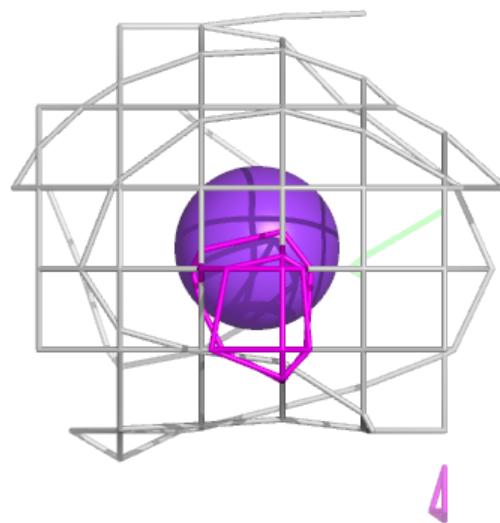
**Electron density around KHS F 301 (B):**

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



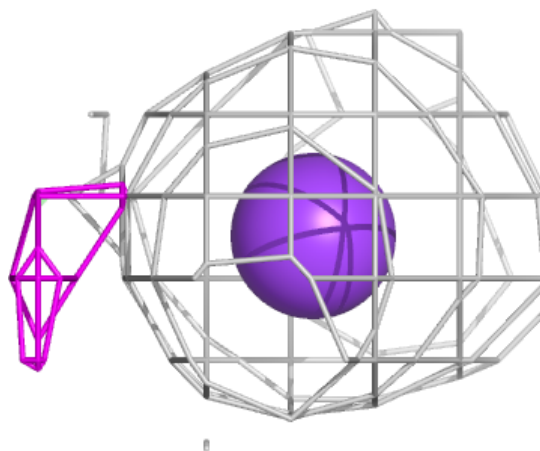
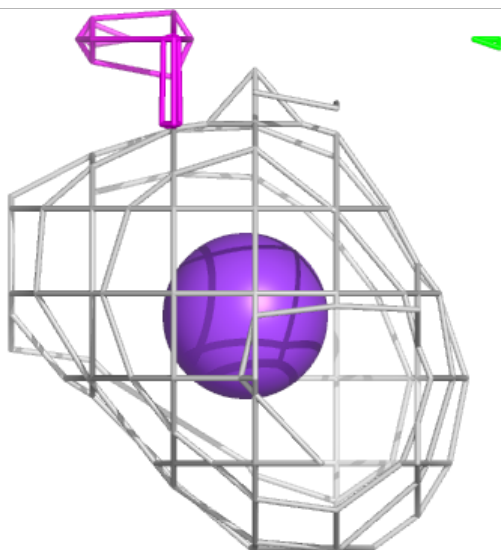
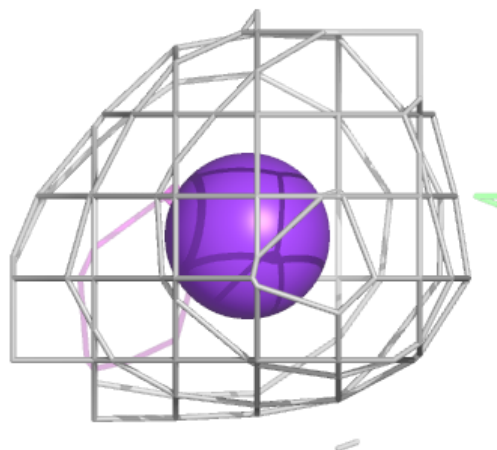
**Electron density around K D 301:**

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



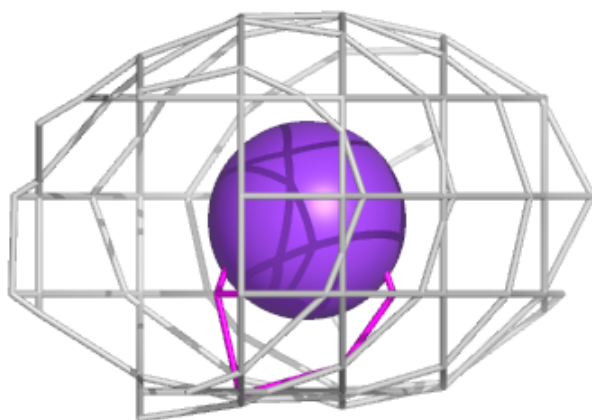
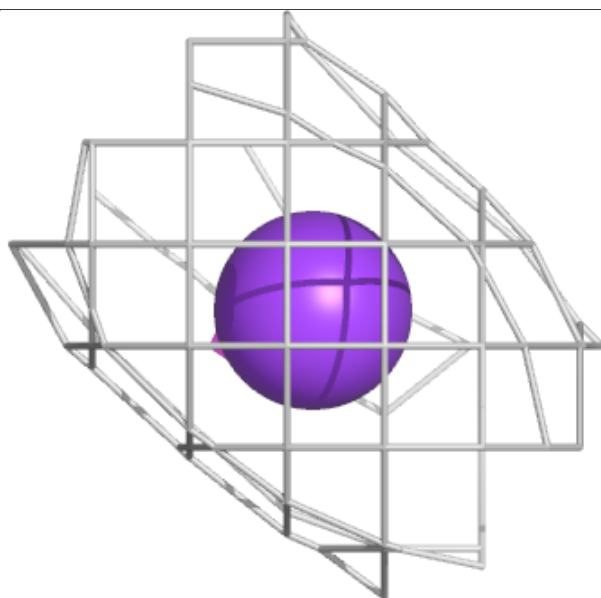
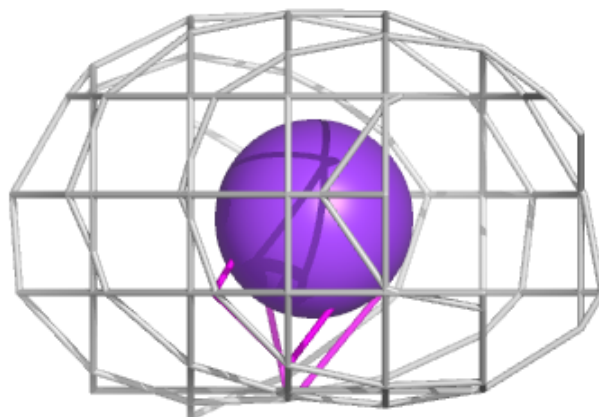
**Electron density around K B 301:**

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



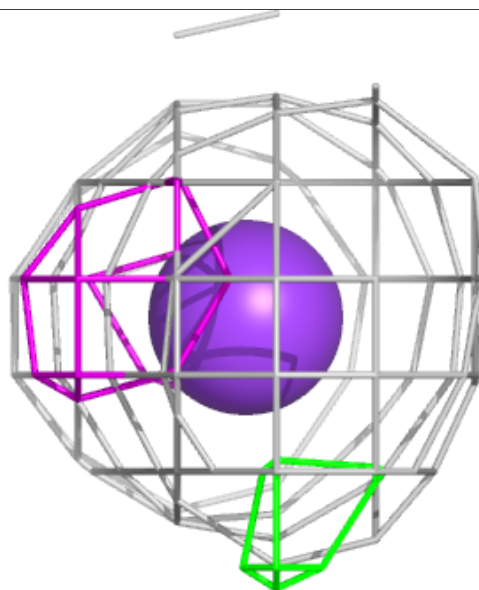
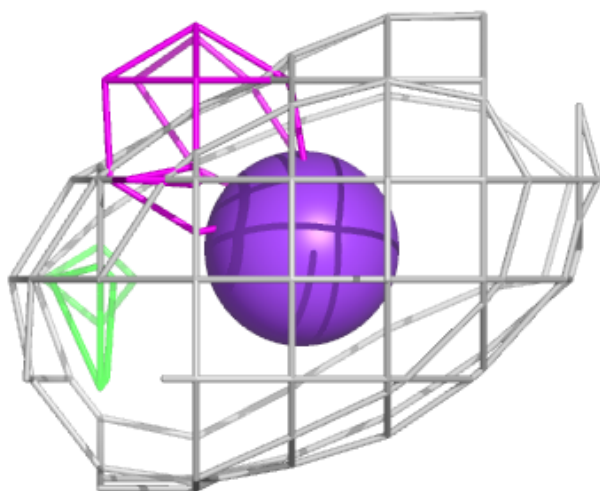
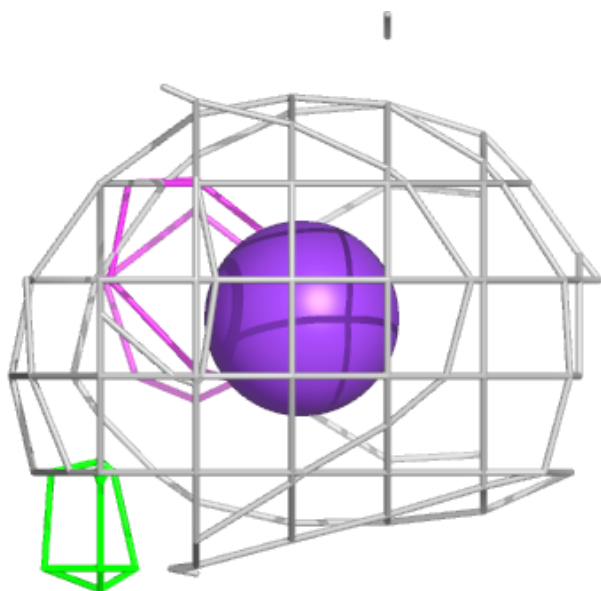
**Electron density around K C 301:**

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



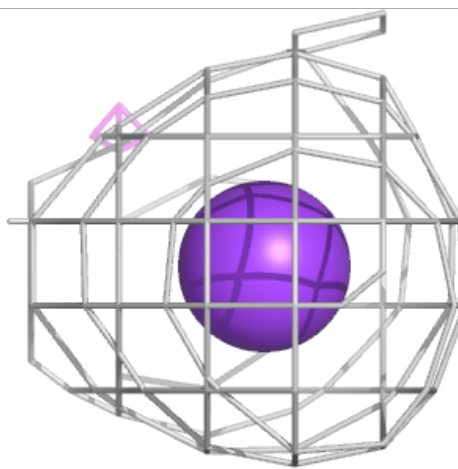
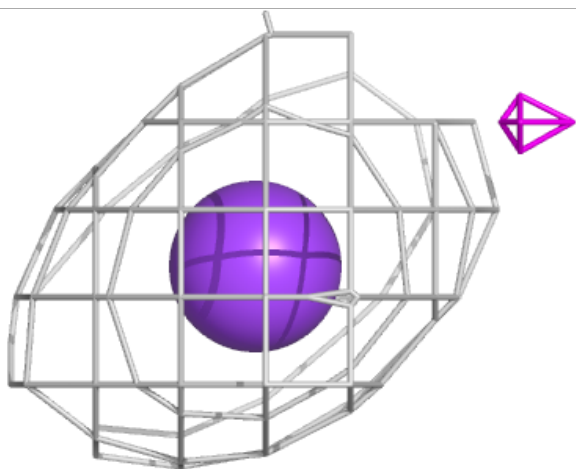
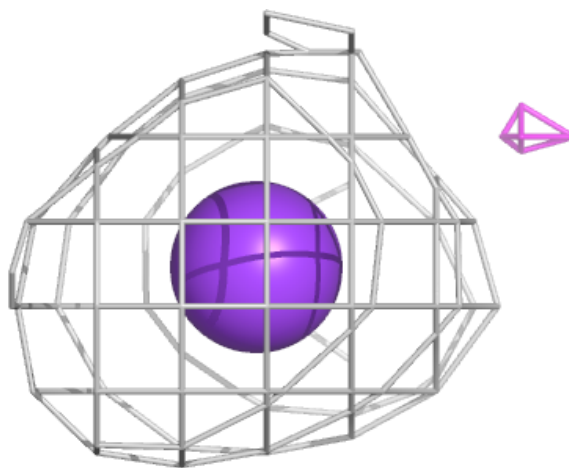
**Electron density around K E 301:**

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



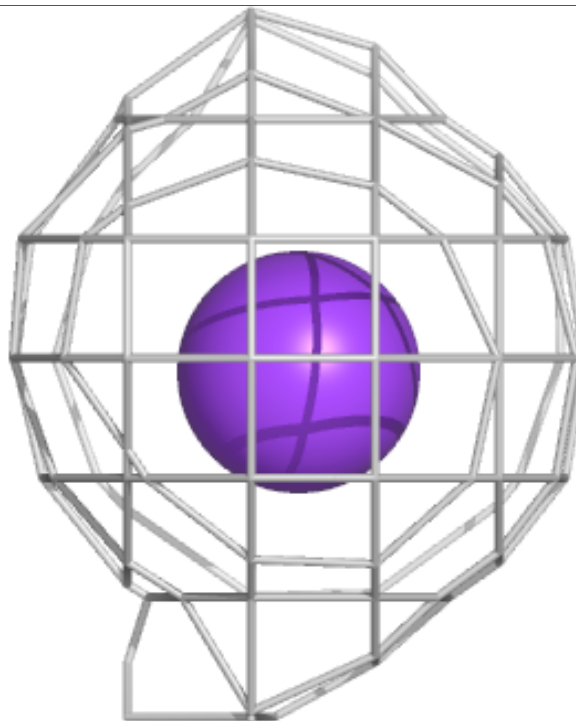
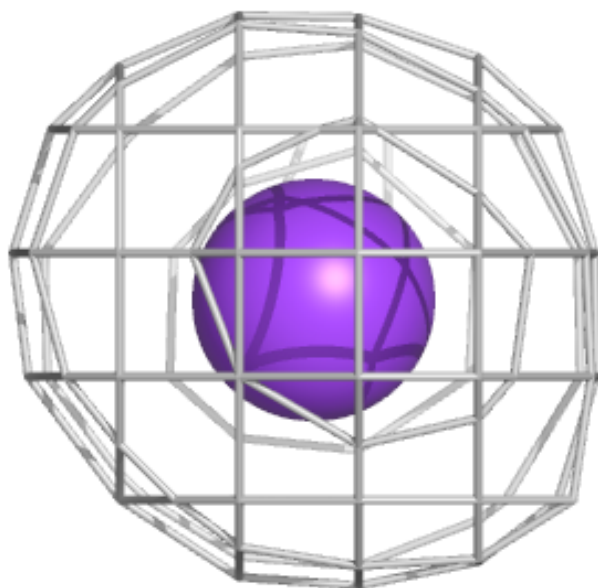
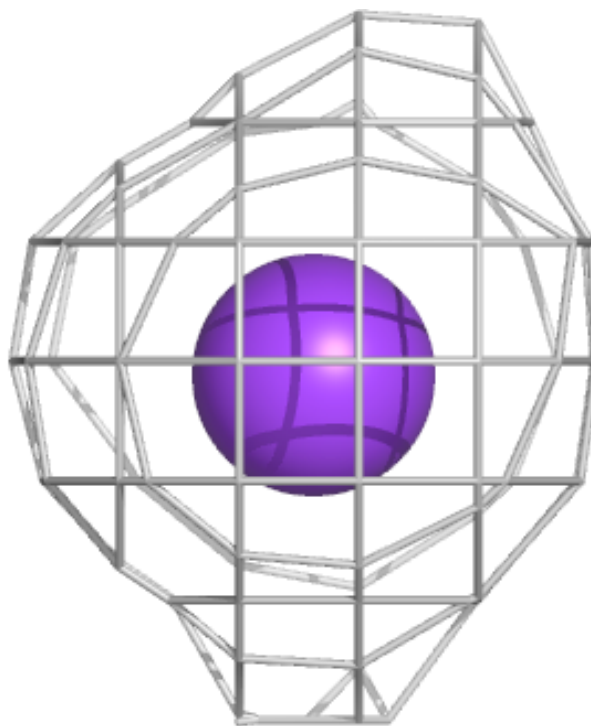
**Electron density around K F 302:**

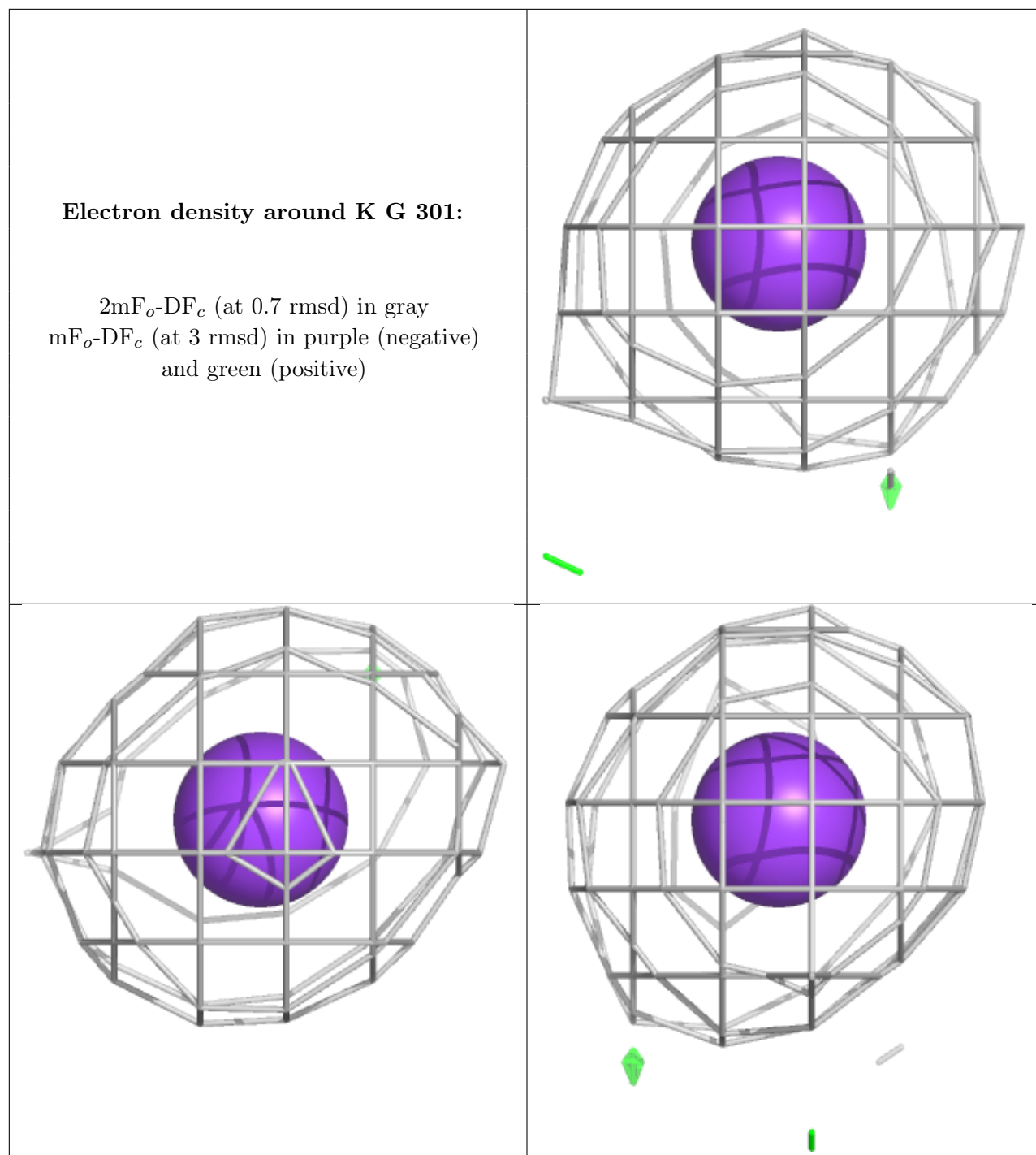
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around K A 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.