Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2023 – 04:37 AM EDT

PDB ID	:	7LJ5
Title	:	Human TRAAK K+ channel FHIEG mutant A198E in a K+ bound conductive conformation
Authors	:	Rietmeijer, R.A.; Brohawn, S.G.
Deposited on	:	2021-01-28
Resolution	:	2.26 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:

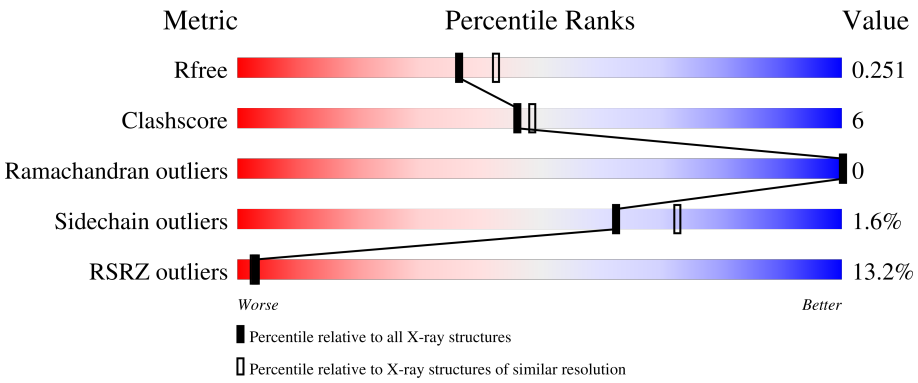
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	299	21% 70% 14% 15%
1	B	299	27% 76% 9% 15%
2	D	211	% 86% 13% •
2	F	211	4% 86% 13%
3	E	217	3% 83% 14% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	217	8% 84% 12%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10660 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 Isoform 2 of Potassium channel subfamily K member 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	253	1967	1301	318	342	6	0	0	0
1	B	255	1984	1310	321	347	6	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	GLN	ASN	engineered mutation	UNP Q9NYG8-2
A	108	GLN	ASN	engineered mutation	UNP Q9NYG8-2
A	198	GLU	ALA	engineered mutation	UNP Q9NYG8-2
A	291	SER	-	expression tag	UNP Q9NYG8-2
A	292	ASN	-	expression tag	UNP Q9NYG8-2
A	293	SER	-	expression tag	UNP Q9NYG8-2
A	294	LEU	-	expression tag	UNP Q9NYG8-2
A	295	GLU	-	expression tag	UNP Q9NYG8-2
A	296	VAL	-	expression tag	UNP Q9NYG8-2
A	297	LEU	-	expression tag	UNP Q9NYG8-2
A	298	PHE	-	expression tag	UNP Q9NYG8-2
A	299	GLN	-	expression tag	UNP Q9NYG8-2
B	104	GLN	ASN	engineered mutation	UNP Q9NYG8-2
B	108	GLN	ASN	engineered mutation	UNP Q9NYG8-2
B	198	GLU	ALA	engineered mutation	UNP Q9NYG8-2
B	291	SER	-	expression tag	UNP Q9NYG8-2
B	292	ASN	-	expression tag	UNP Q9NYG8-2
B	293	SER	-	expression tag	UNP Q9NYG8-2
B	294	LEU	-	expression tag	UNP Q9NYG8-2
B	295	GLU	-	expression tag	UNP Q9NYG8-2
B	296	VAL	-	expression tag	UNP Q9NYG8-2
B	297	LEU	-	expression tag	UNP Q9NYG8-2
B	298	PHE	-	expression tag	UNP Q9NYG8-2
B	299	GLN	-	expression tag	UNP Q9NYG8-2

- Molecule 2 is a protein called ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	211	1616	1003	271	333	9	0	0	0
2	F	211	1616	1003	271	333	9	0	0	0

- Molecule 3 is a protein called ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	211	1614	1026	261	319	8	0	0	0
3	G	210	1605	1022	260	315	8	0	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
4	A	4	4	4	0	0
4	B	3	3	3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	2	2	2	0	0
5	G	1	1	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	39	39	39	0	0
6	B	38	38	38	0	0
6	D	34	34	34	0	0

Continued on next page...

Continued from previous page...

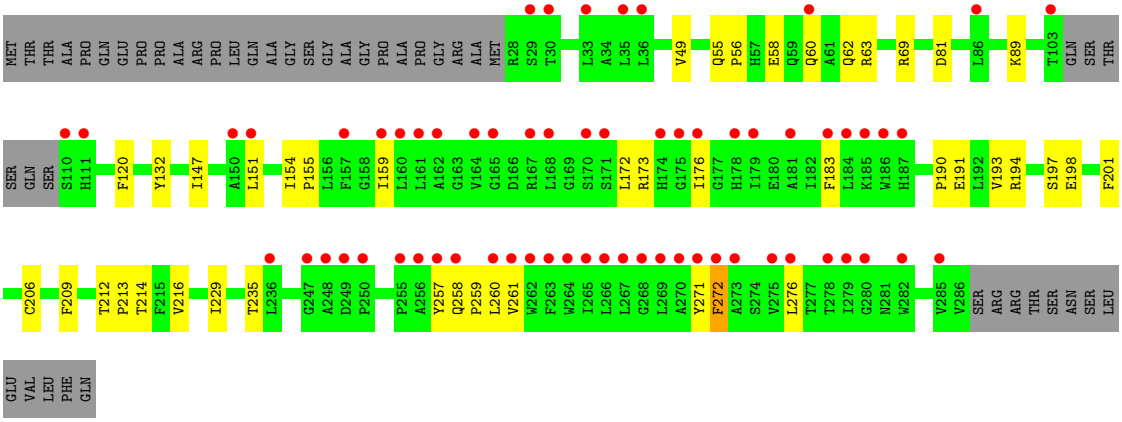
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	E	50	50	50	0	0
			Total	O		
6	F	44	44	44	0	0
			Total	O		
6	G	43	43	43	0	0

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.

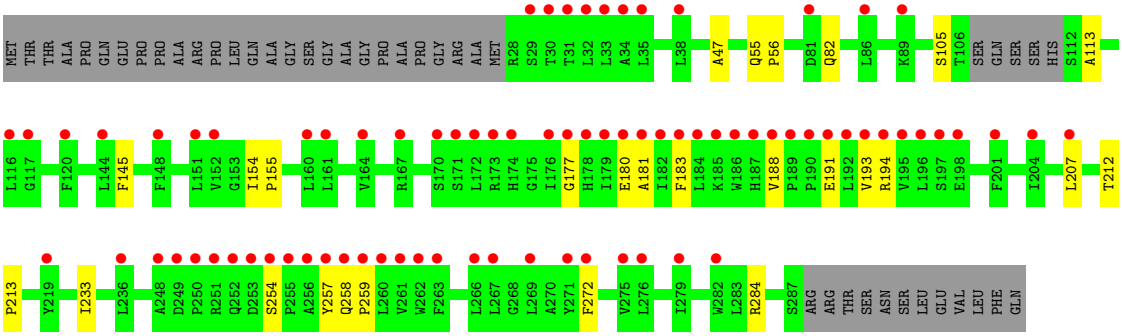
• Molecule 1: Isoform 2 of Potassium channel subfamily K member 4

Chain A:



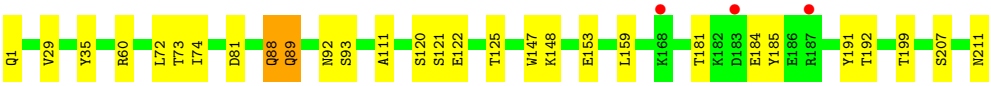
• Molecule 1: Isoform 2 of Potassium channel subfamily K member 4

Chain B:



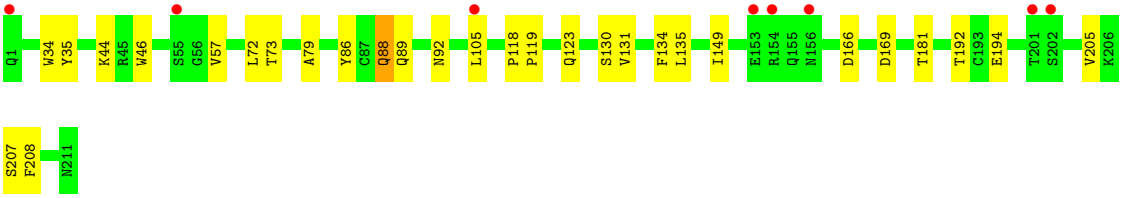
• Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN

Chain D:



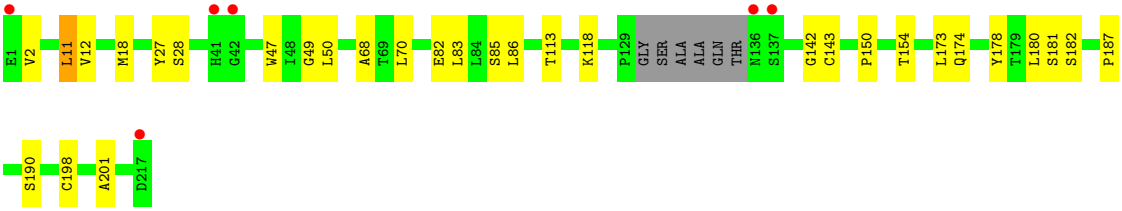
• Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN

Chain F:



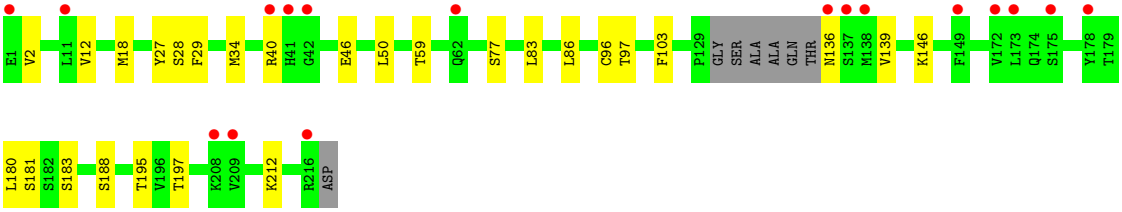
• Molecule 3: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT HEAVY CHAIN

Chain E:



• Molecule 3: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT HEAVY CHAIN

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.16Å 136.98Å 95.74Å 90.00° 94.47° 90.00°	Depositor
Resolution (Å)	95.45 – 2.26 95.45 – 2.26	Depositor EDS
% Data completeness (in resolution range)	60.3 (95.45-2.26) 60.3 (95.45-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.220 , 0.252 0.221 , 0.251	Depositor DCC
R_{free} test set	2846 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	55.1	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.9	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	0.91	EDS
Total number of atoms	10660	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: K, CA

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	0.66	0/2017	0.74	0/2750
1	B	0.66	0/2034	0.72	0/2773
2	D	0.65	0/1655	0.81	0/2247
2	F	0.67	0/1655	0.83	0/2247
3	E	0.66	0/1656	0.82	0/2260
3	G	0.65	0/1647	0.84	0/2249
All	All	0.66	0/10664	0.79	0/14526

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1967	0	1986	33	1
1	B	1984	0	2004	21	0
2	D	1616	0	1542	26	1
2	F	1616	0	1542	21	0
3	E	1614	0	1586	21	0
3	G	1605	0	1582	22	0
4	A	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	3	0	0	0	0
5	A	2	0	0	0	0
5	G	1	0	0	0	0
6	A	39	0	0	7	0
6	B	38	0	0	0	0
6	D	34	0	0	1	0
6	E	50	0	0	1	0
6	F	44	0	0	1	0
6	G	43	0	0	2	0
All	All	10660	0	10242	131	1

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 6.

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)
2:D:35:TYR:HE2	2:D:88:GLN:HG2	1.45	0.81
1:A:69:ARG:HD2	6:A:402:HOH:O	1.86	0.76
1:A:198:GLU:O	1:A:201:PHE:HB3	1.86	0.76
1:A:81:ASP:OD1	6:A:401:HOH:O	2.03	0.76
3:E:28:SER:HB2	3:G:28:SER:HB2	1.69	0.72
2:F:35:TYR:HE1	2:F:88:GLN:HG2	1.56	0.70
1:A:81:ASP:OD2	6:A:402:HOH:O	2.09	0.70
1:A:212:THR:HB	1:A:213:PRO:HD3	1.73	0.69
1:A:81:ASP:HB3	6:A:418:HOH:O	1.92	0.68
2:D:181:THR:HG23	2:D:184:GLU:H	1.57	0.68
3:E:12:VAL:HG21	3:E:86:LEU:CD1	2.24	0.67
2:D:35:TYR:CE2	2:D:88:GLN:HG2	2.29	0.67
1:B:191:GLU:HA	1:B:194:ARG:HE	1.59	0.66
3:G:12:VAL:HG21	3:G:86:LEU:HD12	1.77	0.66
1:A:60:GLN:OE1	1:A:63:ARG:NH2	2.29	0.66
1:B:180:GLU:HG3	1:B:193:VAL:CG1	2.27	0.65
1:B:183:PHE:O	1:B:188:VAL:HG22	1.96	0.65
2:F:35:TYR:CE1	2:F:88:GLN:HG2	2.33	0.64
2:D:1:GLN:HA	2:D:1:GLN:OE1	1.95	0.64
2:D:159:LEU:HD11	3:E:174:GLN:CD	2.18	0.63
1:A:176:ILE:HD11	1:A:201:PHE:CD1	2.34	0.62
2:D:192:THR:HG22	2:D:207:SER:OG	2.00	0.61
2:D:29:VAL:HG11	2:D:89:GLN:HG3	1.82	0.61
3:E:12:VAL:HG21	3:E:86:LEU:HD12	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:180:LEU:C	3:E:180:LEU:HD12	2.23	0.58
3:G:139:VAL:HG23	3:G:188:SER:HA	1.85	0.58
1:A:172:LEU:HD13	1:A:201:PHE:CE1	2.39	0.58
2:F:149:ILE:HG13	2:F:149:ILE:O	2.04	0.57
2:F:89:GLN:HE21	2:F:92:ASN:H	1.52	0.57
2:F:194:GLU:HG3	2:F:205:VAL:HG22	1.86	0.57
2:D:60:ARG:NH1	2:D:81:ASP:OD1	2.38	0.57
2:D:89:GLN:HE21	2:D:92:ASN:H	1.53	0.56
1:A:258:GLN:HB2	1:A:259:PRO:HD3	1.87	0.55
3:G:12:VAL:HG21	3:G:86:LEU:CD1	2.36	0.55
1:A:206:CYS:HB2	1:A:271:TYR:OH	2.07	0.54
3:E:187:PRO:O	3:E:190:SER:HB2	2.07	0.54
2:D:121:SER:O	2:D:125:THR:HG23	2.08	0.54
2:F:79:ALA:HA	2:F:105:LEU:HD11	1.90	0.53
1:A:257:TYR:CD2	1:A:260:LEU:HD22	2.44	0.53
3:G:34:MET:CE	3:G:96:CYS:HB2	2.39	0.53
1:A:257:TYR:CZ	1:A:261:VAL:HG12	2.43	0.52
2:D:147:TRP:O	2:D:153:GLU:HA	2.10	0.52
3:E:12:VAL:HG21	3:E:86:LEU:HD13	1.90	0.52
2:F:166:ASP:HB3	2:F:169:ASP:OD2	2.10	0.51
2:F:89:GLN:NE2	2:F:92:ASN:H	2.08	0.51
1:A:58:GLU:OE2	1:B:113:ALA:N	2.43	0.51
1:A:197:SER:O	1:A:201:PHE:N	2.42	0.50
3:G:34:MET:HE1	3:G:96:CYS:HB2	1.92	0.50
1:A:214:THR:HG21	1:A:229:ILE:HG12	1.93	0.50
1:B:191:GLU:HA	1:B:194:ARG:NE	2.26	0.50
3:E:83:LEU:HB3	3:E:86:LEU:HD21	1.92	0.50
3:E:154:THR:OG1	3:E:201:ALA:HB3	2.12	0.50
3:G:139:VAL:CG2	3:G:188:SER:HA	2.42	0.50
2:D:185:TYR:HA	2:D:191:TYR:OH	2.12	0.49
1:B:212:THR:HB	1:B:213:PRO:HD3	1.95	0.49
3:G:197:THR:HG22	3:G:212:LYS:HA	1.94	0.48
1:B:207:LEU:HD13	1:B:207:LEU:C	2.34	0.48
2:F:135:LEU:HD12	2:F:135:LEU:N	2.28	0.48
3:E:28:SER:HB2	3:G:28:SER:CB	2.41	0.48
2:F:46:TRP:O	2:F:57:VAL:HG21	2.14	0.48
2:F:192:THR:HG22	2:F:207:SER:OG	2.14	0.48
1:A:62:GLN:NE2	6:A:405:HOH:O	2.47	0.47
3:E:143:CYS:O	3:E:181:SER:HA	2.15	0.47
2:D:72:LEU:HD23	2:D:73:THR:N	2.29	0.47
1:A:272:PHE:O	1:A:276:LEU:HD23	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ILE:N	1:B:155:PRO:HD2	2.29	0.47
3:E:11:LEU:HD12	3:E:113:THR:HB	1.95	0.47
1:A:154:ILE:N	1:A:155:PRO:HD2	2.29	0.47
1:B:180:GLU:CG	1:B:193:VAL:CG1	2.91	0.47
3:G:2:VAL:HG13	3:G:27:TYR:CD2	2.50	0.47
1:B:191:GLU:HB2	1:B:194:ARG:HH21	1.80	0.47
2:F:72:LEU:HD23	2:F:73:THR:N	2.30	0.46
3:G:97:THR:OG1	3:G:103:PHE:HB3	2.15	0.46
3:G:180:LEU:HD12	3:G:180:LEU:C	2.35	0.46
1:A:209:PHE:O	1:A:213:PRO:HG2	2.16	0.46
1:A:190:PRO:O	1:A:194:ARG:HG2	2.15	0.46
2:F:123:GLN:HE22	2:F:130:SER:HB2	1.80	0.46
1:B:188:VAL:HG23	1:B:193:VAL:CG2	2.46	0.46
1:A:89:LYS:NZ	6:A:404:HOH:O	2.41	0.46
1:A:257:TYR:HD2	1:A:260:LEU:HD22	1.79	0.46
1:B:180:GLU:HG3	1:B:193:VAL:HG13	1.99	0.45
1:A:147:ILE:HG23	1:B:233:ILE:HD13	1.99	0.45
3:E:70:LEU:O	6:E:301:HOH:O	2.20	0.45
2:F:44:LYS:HG2	6:F:338:HOH:O	2.17	0.45
3:G:139:VAL:HG23	3:G:188:SER:CA	2.46	0.45
1:B:254:SER:O	1:B:257:TYR:HB3	2.17	0.45
2:D:89:GLN:NE2	2:D:92:ASN:H	2.13	0.45
1:A:183:PHE:HB3	1:A:193:VAL:HG22	1.98	0.44
2:F:34:TRP:HA	2:F:86:TYR:O	2.17	0.44
3:G:29:PHE:CD1	3:G:77:SER:HA	2.52	0.44
2:D:111:ALA:HB2	2:D:199:THR:HG21	1.99	0.44
2:D:148:LYS:HB2	2:D:192:THR:OG1	2.18	0.44
2:F:123:GLN:HE22	2:F:130:SER:CB	2.31	0.44
2:D:159:LEU:HD11	3:E:174:GLN:OE1	2.18	0.43
2:D:199:THR:HG22	2:D:199:THR:O	2.18	0.43
3:E:142:GLY:HA2	3:E:182:SER:O	2.18	0.43
3:G:83:LEU:HB3	3:G:86:LEU:HD21	2.00	0.43
3:G:50:LEU:C	3:G:50:LEU:HD12	2.39	0.43
1:A:120:PHE:HA	1:B:47:ALA:HB2	2.00	0.43
2:D:192:THR:HG22	2:D:207:SER:CB	2.49	0.43
1:A:132:TYR:OH	1:A:235:THR:HG23	2.18	0.43
1:A:159:ILE:HD12	1:B:284:ARG:HD3	2.01	0.43
1:B:177:GLY:O	1:B:181:ALA:N	2.46	0.43
3:E:68:ALA:HA	3:E:82:GLU:O	2.19	0.43
1:B:258:GLN:HB3	1:B:259:PRO:HD3	2.00	0.43
2:D:211:ASN:OD1	2:D:211:ASN:N	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:50:LEU:C	3:E:50:LEU:HD12	2.38	0.42
2:D:72:LEU:HD23	2:D:72:LEU:C	2.40	0.42
2:F:118:PRO:HB3	2:F:208:PHE:CZ	2.54	0.42
2:D:120:SER:HB2	2:D:122:GLU:OE1	2.18	0.42
3:G:29:PHE:HB2	3:G:77:SER:HB2	2.01	0.42
1:A:55:GLN:N	1:A:56:PRO:CD	2.83	0.42
1:A:216:VAL:HG11	1:A:257:TYR:OH	2.19	0.42
2:D:93:SER:HB3	6:D:326:HOH:O	2.19	0.42
3:E:2:VAL:HG13	3:E:27:TYR:CD2	2.55	0.42
2:D:60:ARG:HG3	2:D:74:ILE:HG23	2.01	0.42
2:F:119:PRO:HD3	2:F:131:VAL:HG22	2.01	0.42
3:G:195:THR:HA	6:G:421:HOH:O	2.20	0.42
1:A:214:THR:HG21	1:A:229:ILE:CG1	2.49	0.41
3:E:173:LEU:HG	3:E:178:TYR:CE2	2.55	0.41
1:B:55:GLN:N	1:B:56:PRO:CD	2.83	0.41
1:A:49:VAL:HG11	1:B:145:PHE:CE1	2.55	0.41
6:A:401:HOH:O	2:D:93:SER:N	2.54	0.41
3:E:47:TRP:CZ2	3:E:49:GLY:HA2	2.54	0.41
2:F:134:PHE:CE2	3:G:183:SER:CB	3.03	0.41
3:G:46:GLU:HA	6:G:428:HOH:O	2.21	0.41
1:A:173:ARG:HA	1:A:176:ILE:HB	2.03	0.41
2:D:159:LEU:HD11	3:E:174:GLN:NE2	2.36	0.41
2:F:118:PRO:HB3	2:F:208:PHE:CE1	2.56	0.40
2:F:134:PHE:CE2	3:G:183:SER:HB3	2.56	0.40
1:B:82:GLN:HG3	3:G:59:THR:HG21	2.04	0.40

All (1) 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:191:GLU:OE2	2:D:153:GLU:N[2_645]	2.17	0.03

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	249/299 (83%)	240 (96%)	9 (4%)	0	100	100
1	B	251/299 (84%)	246 (98%)	5 (2%)	0	100	100
2	D	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
2	F	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
3	E	207/217 (95%)	200 (97%)	7 (3%)	0	100	100
3	G	206/217 (95%)	199 (97%)	7 (3%)	0	100	100
All	All	1331/1454 (92%)	1287 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	205/243 (84%)	203 (99%)	2 (1%)	76	84
1	B	208/243 (86%)	206 (99%)	2 (1%)	76	84
2	D	184/184 (100%)	182 (99%)	2 (1%)	73	82
2	F	184/184 (100%)	182 (99%)	2 (1%)	73	82
3	E	187/190 (98%)	181 (97%)	6 (3%)	39	47
3	G	186/190 (98%)	181 (97%)	5 (3%)	44	54
All	All	1154/1234 (94%)	1135 (98%)	19 (2%)	62	73

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	LEU
1	A	272	PHE
1	B	105	SER
1	B	272	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	88	GLN
2	D	89	GLN
3	E	11	LEU
3	E	18	MET
3	E	85	SER
3	E	118	LYS
3	E	150	PRO
3	E	198	CYS
2	F	88	GLN
2	F	181	THR
3	G	18	MET
3	G	40	ARG
3	G	136	ASN
3	G	146	LYS
3	G	181	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	136	ASN
3	E	136	ASN
2	F	88	GLN
2	F	92	ASN
3	G	174	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 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	253/299 (84%)	1.67	64 (25%)	0	0	42, 99, 171, 195	0
1	B	255/299 (85%)	2.05	80 (31%)	0	0	37, 97, 182, 195	0
2	D	211/211 (100%)	0.19	3 (1%)	75	77	35, 56, 93, 111	0
2	F	211/211 (100%)	0.36	8 (3%)	40	43	37, 55, 101, 116	0
3	E	211/217 (97%)	0.22	6 (2%)	53	55	32, 49, 75, 103	0
3	G	210/217 (96%)	0.46	17 (8%)	12	13	35, 54, 90, 131	0
All	All	1351/1454 (92%)	0.89	178 (13%)	3	3	32, 63, 153, 195	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	VAL	19.0
1	A	103	THR	17.5
1	B	184	LEU	15.8
1	A	248	ALA	14.6
1	B	255	PRO	13.7
1	B	192	LEU	13.4
1	B	256	ALA	12.5
1	B	183	PHE	12.4
1	A	282	TRP	12.0
1	A	279	ILE	12.0
1	A	174	HIS	11.9
1	B	34	ALA	11.7
1	B	182	ILE	11.5
1	B	186	TRP	11.1
1	B	116	LEU	10.9
1	B	251	ARG	10.8
1	B	250	PRO	10.3
1	B	189	PRO	9.7
1	A	263	PHE	9.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	178	HIS	9.5
1	B	179	ILE	9.3
1	A	161	LEU	8.8
1	B	181	ALA	8.7
3	G	136	ASN	8.7
1	B	30	THR	8.4
1	A	276	LEU	8.3
1	B	248	ALA	8.1
1	B	188	VAL	7.8
1	A	30	THR	7.7
1	B	262	TRP	7.6
1	A	257	TYR	7.4
1	A	256	ALA	7.4
1	B	190	PRO	7.4
1	B	276	LEU	7.1
1	B	35	LEU	7.1
1	B	31	THR	7.1
1	A	255	PRO	6.9
3	G	41	HIS	6.7
1	A	266	LEU	6.7
1	A	179	ILE	6.4
1	A	249	ASP	6.4
1	B	201	PHE	6.4
2	D	187	ARG	6.1
1	A	267	LEU	6.1
1	A	272	PHE	6.0
1	A	183	PHE	6.0
1	A	270	ALA	5.9
1	B	178	HIS	5.8
1	B	32	LEU	5.8
1	A	261	VAL	5.7
1	B	275	VAL	5.7
1	A	167	ARG	5.6
1	B	219	TYR	5.5
1	A	157	PHE	5.5
1	B	187	HIS	5.4
1	B	263	PHE	5.3
1	A	170	SER	5.2
1	B	253	ASP	5.2
2	F	201	THR	5.1
1	B	252	GLN	5.0
1	B	257	TYR	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	260	LEU	4.9
1	B	254	SER	4.9
1	A	285	VAL	4.9
1	A	186	TRP	4.8
1	A	269	LEU	4.8
1	A	275	VAL	4.8
1	B	259	PRO	4.7
1	B	194	ARG	4.7
1	A	164	VAL	4.6
1	B	266	LEU	4.5
1	B	177	GLY	4.5
1	B	33	LEU	4.5
1	B	180	GLU	4.4
1	B	174	HIS	4.4
1	A	168	LEU	4.4
1	B	148	PHE	4.3
1	A	171	SER	4.3
1	B	171	SER	4.3
1	B	258	GLN	4.3
1	A	250	PRO	4.3
1	A	181	ALA	4.2
1	B	117	GLY	4.2
1	A	110	SER	4.2
1	A	111	HIS	4.1
1	A	159	ILE	4.1
1	B	249	ASP	4.1
1	B	185	LYS	4.1
3	E	41	HIS	4.1
1	B	151	LEU	4.1
1	A	264	TRP	4.0
1	A	262	TRP	3.9
1	B	198	GLU	3.9
1	B	167	ARG	3.8
1	A	278	THR	3.7
3	G	42	GLY	3.7
1	B	282	TRP	3.7
1	B	272	PHE	3.6
3	E	136	ASN	3.6
1	A	162	ALA	3.6
1	A	273	ALA	3.5
3	G	137	SER	3.5
3	G	1	GLU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	247	GLY	3.5
2	F	154	ARG	3.4
1	B	269	LEU	3.3
3	E	1	GLU	3.3
1	A	185	LYS	3.3
1	B	196	LEU	3.3
2	F	202	SER	3.2
1	A	268	GLY	3.2
1	B	279	ILE	3.2
1	A	271	TYR	3.2
3	G	209	VAL	3.2
1	A	176	ILE	3.1
1	A	258	GLN	3.1
1	B	261	VAL	3.1
3	G	175	SER	3.1
1	A	151	LEU	3.1
1	A	280	GLY	3.0
2	F	156	ASN	3.0
3	G	40	ARG	3.0
1	B	120	PHE	3.0
1	B	176	ILE	3.0
1	B	195	VAL	3.0
3	G	216	ARG	2.9
1	A	187	HIS	2.9
1	B	152	VAL	2.9
1	A	236	LEU	2.9
3	E	42	GLY	2.8
3	E	137	SER	2.8
3	G	173	LEU	2.8
1	B	144	LEU	2.7
2	F	153	GLU	2.7
3	G	149	PHE	2.7
1	B	170	SER	2.7
1	B	173	ARG	2.7
1	A	265	ILE	2.7
2	F	1	GLN	2.7
1	B	86	LEU	2.7
1	B	29	SER	2.6
1	A	29	SER	2.6
2	D	168	LYS	2.6
1	A	86	LEU	2.6
1	B	267	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	G	11	LEU	2.5
1	B	164	VAL	2.4
1	A	33	LEU	2.4
1	B	271	TYR	2.4
3	G	178	TYR	2.4
1	B	207	LEU	2.4
1	B	172	LEU	2.3
1	A	184	LEU	2.3
2	D	183	ASP	2.3
1	A	150	ALA	2.3
3	G	172	VAL	2.3
1	B	260	LEU	2.2
1	B	236	LEU	2.2
1	B	204	ILE	2.2
3	G	138	MET	2.2
1	A	60	GLN	2.2
3	G	62	GLN	2.2
1	B	81	ASP	2.1
1	B	160	LEU	2.1
3	G	208	LYS	2.1
1	A	165	GLY	2.1
1	B	197	SER	2.1
2	F	55	SER	2.1
1	A	36	LEU	2.1
1	A	160	LEU	2.1
1	B	89	LYS	2.1
1	B	38	LEU	2.1
1	B	191	GLU	2.1
1	A	175	GLY	2.1
3	E	217	ASP	2.0
1	A	35	LEU	2.0
1	B	161	LEU	2.0
2	F	105	LEU	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)

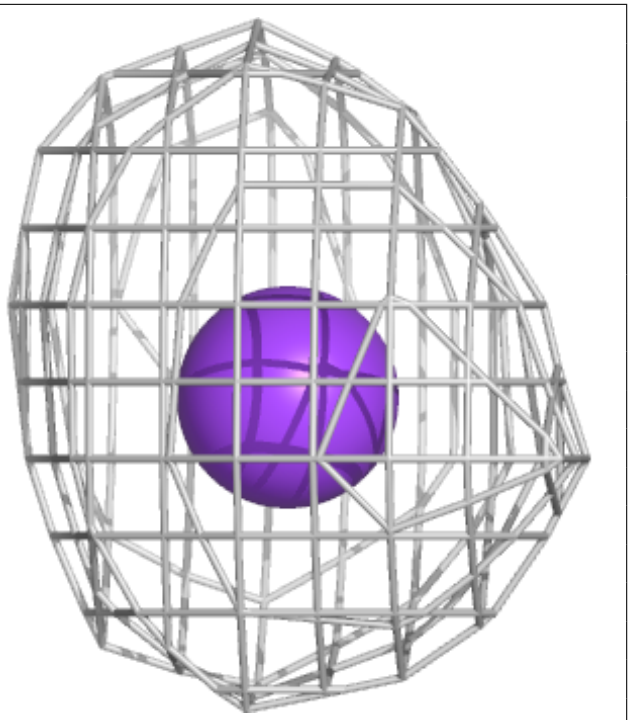
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

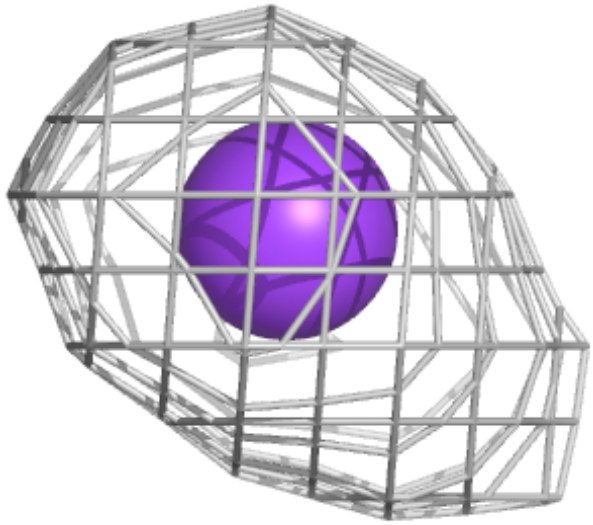
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	K	A	303	1/1	0.86	0.10	101,101,101,101	0
4	K	A	306	1/1	0.86	0.22	87,87,87,87	0
4	K	B	303	1/1	0.87	0.15	94,94,94,94	0
5	CA	A	305	1/1	0.92	0.09	97,97,97,97	0
5	CA	A	304	1/1	0.94	0.08	90,90,90,90	0
4	K	B	302	1/1	0.94	0.12	68,68,68,68	0
4	K	B	301	1/1	0.96	0.07	71,71,71,71	0
4	K	A	302	1/1	0.97	0.06	75,75,75,75	0
4	K	A	301	1/1	0.98	0.12	61,61,61,61	0
5	CA	G	301	1/1	0.98	0.17	52,52,52,52	0

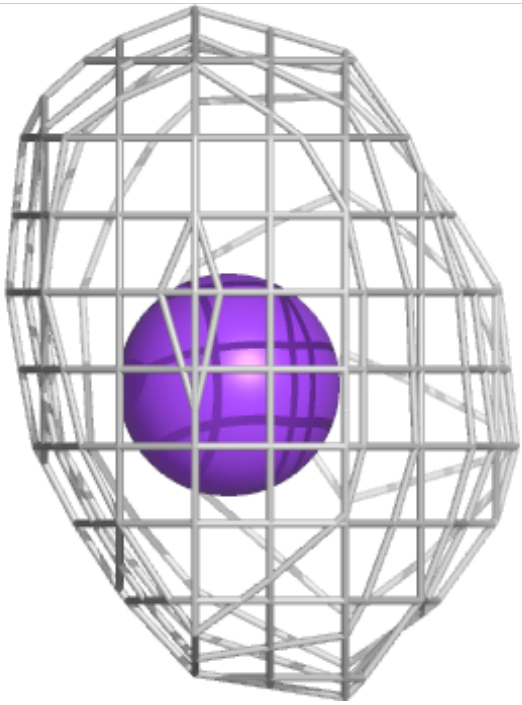
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around K A 303:

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

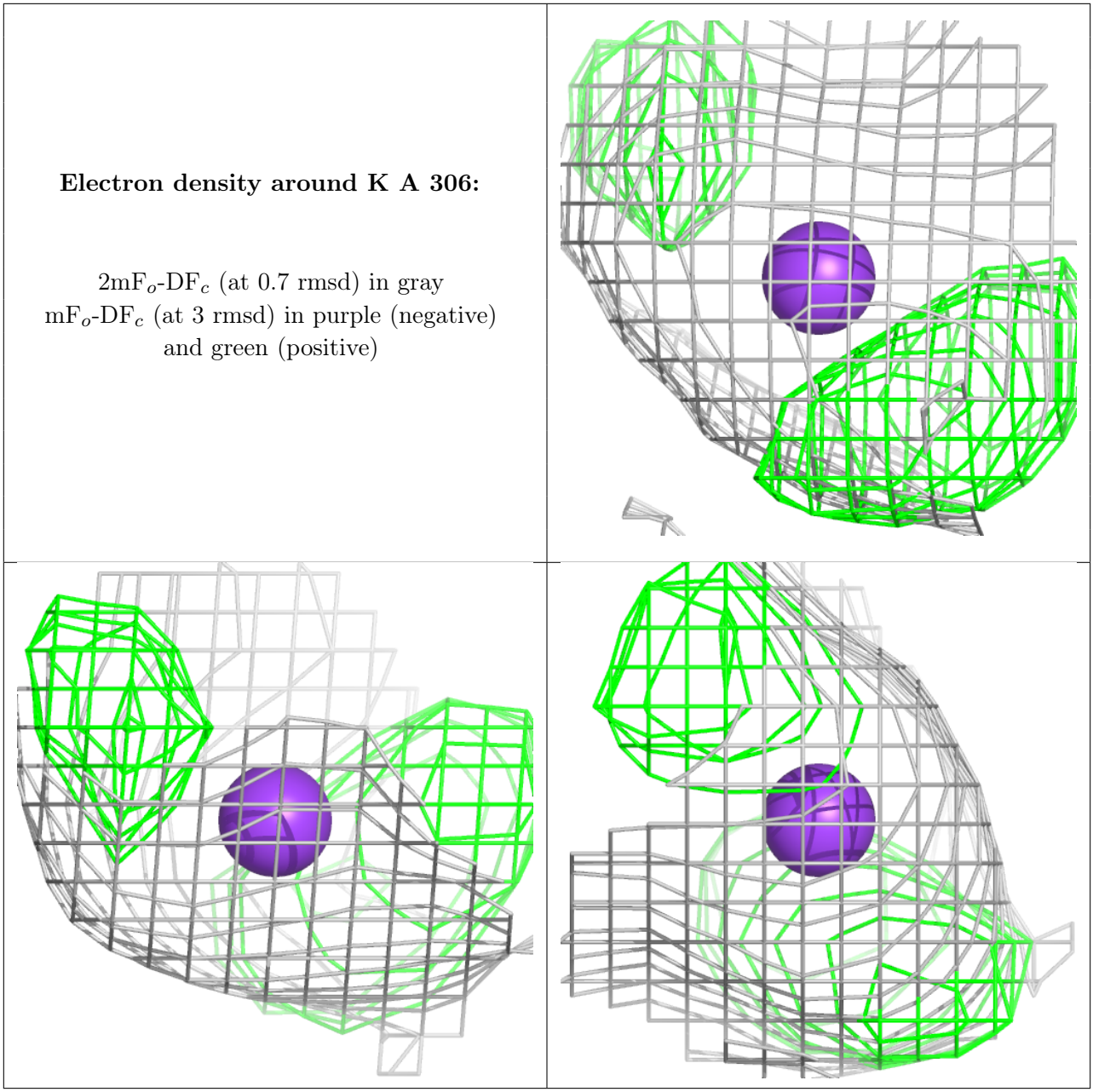






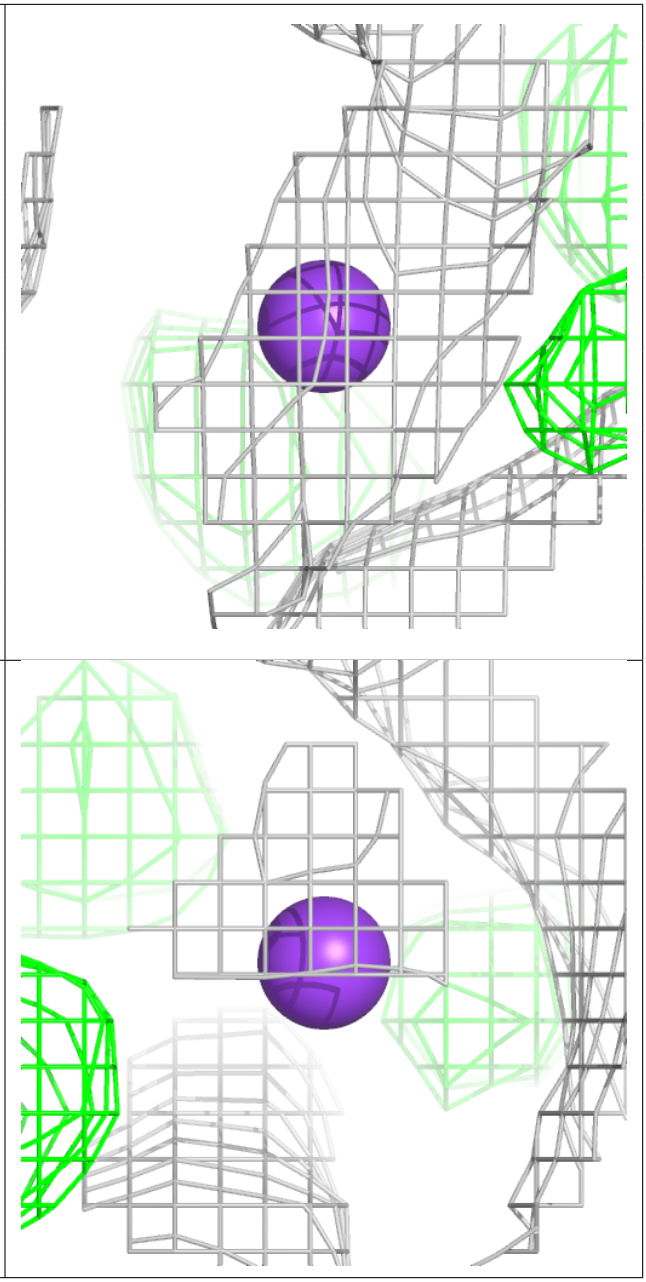
Electron density around K A 306:

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



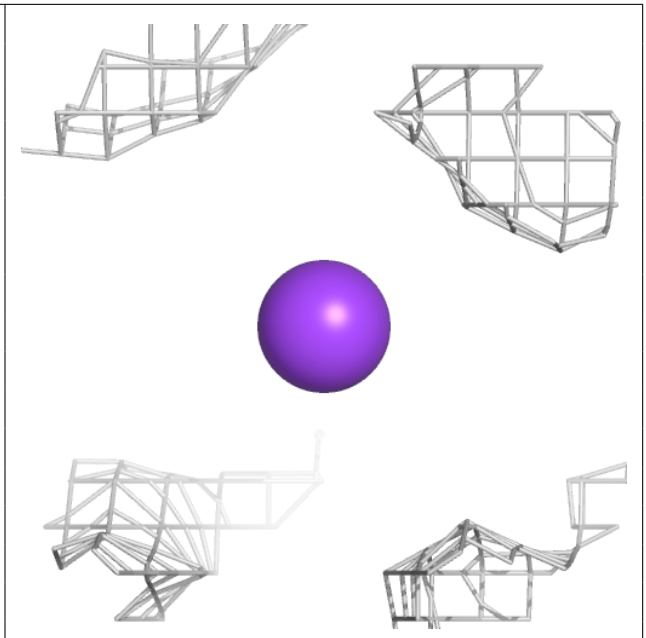
Electron density around K B 303:

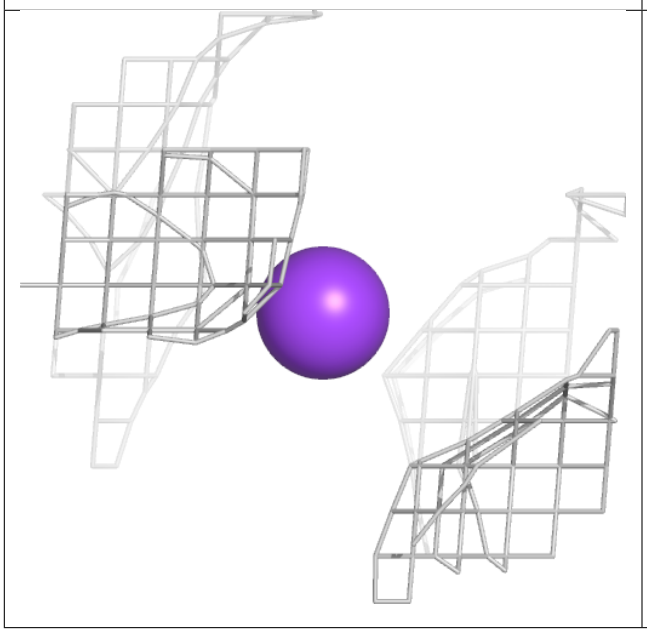
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

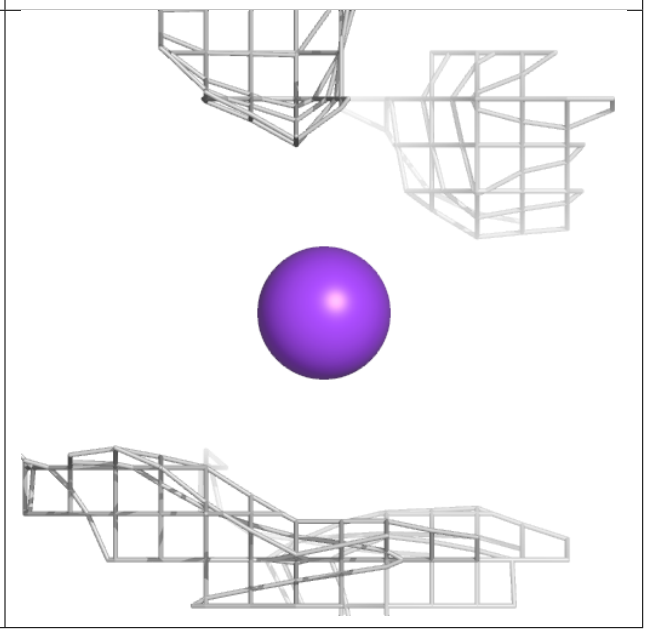


Electron density around K B 302:

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

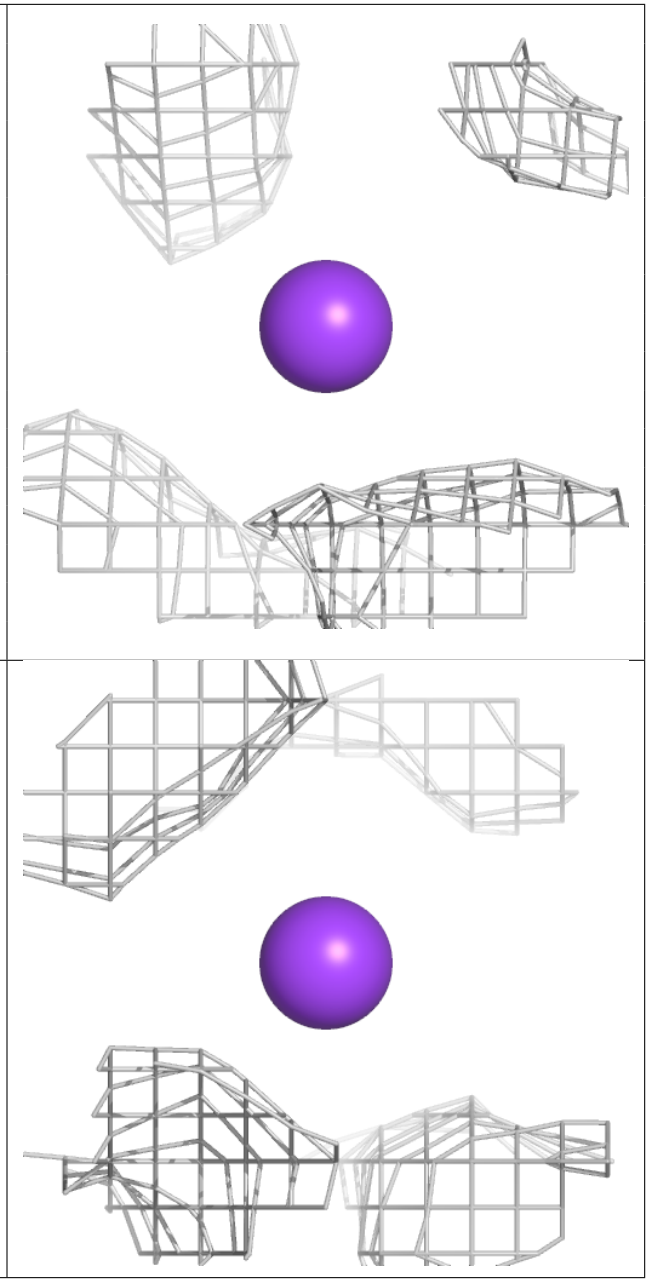






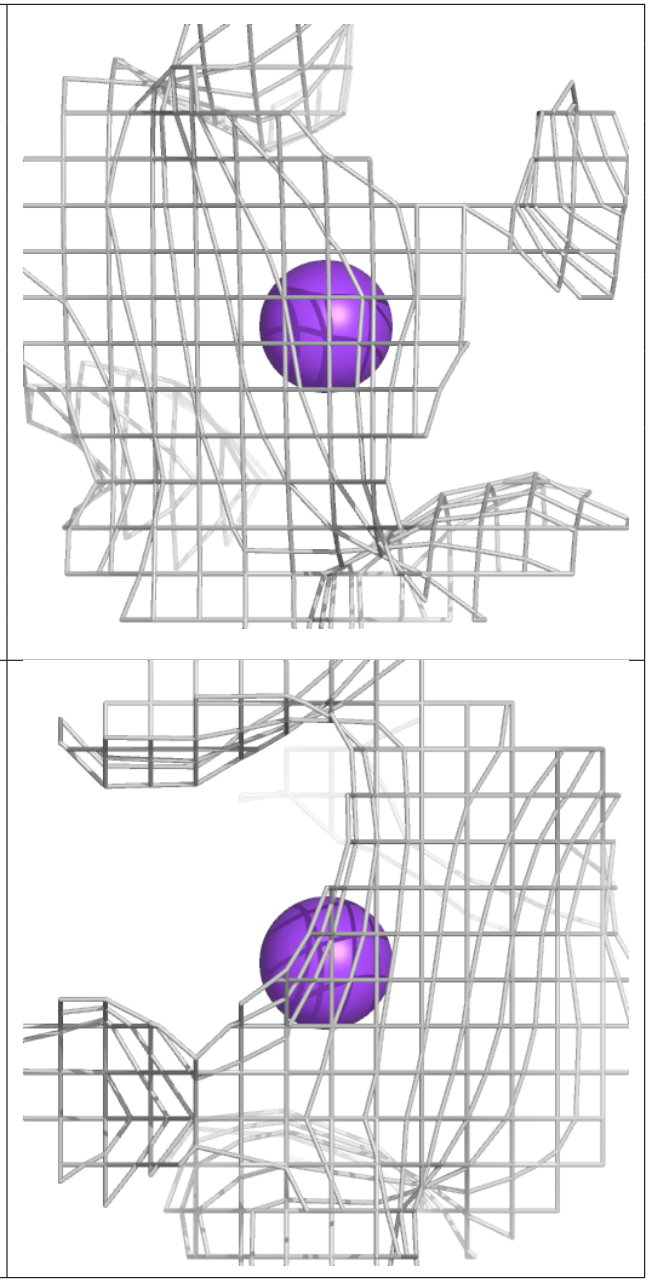
Electron density around K B 301:

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



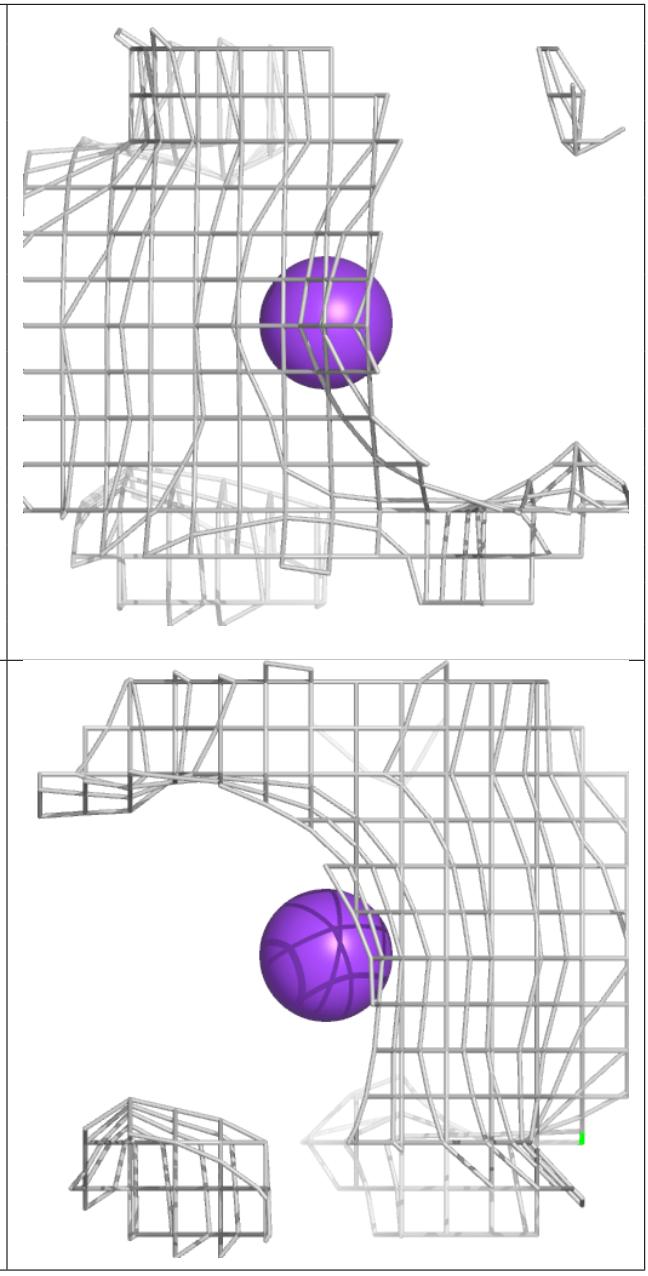
Electron density around K A 302:

$2mF_o$-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 (i)

There are no such residues in this entry.