



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:12 AM UTC

PDB ID : 7LJ5 / pdb_00007lj5
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

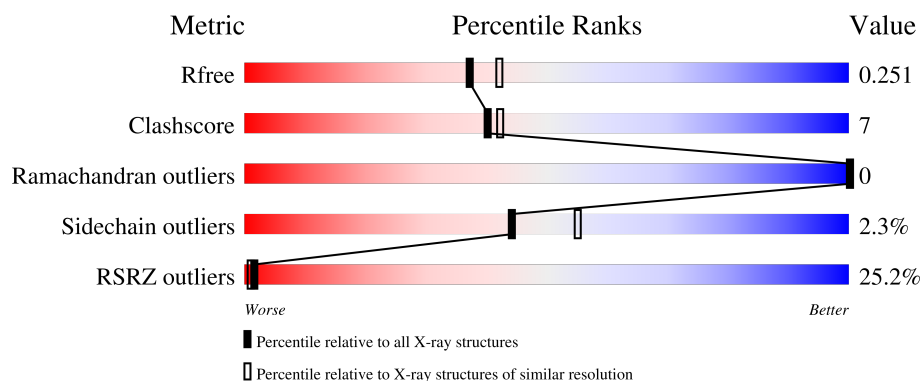
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 $\leq 5\%$. 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	299	40% 68% 17% 15%
1	B	299	40% 75% 11% 15%
2	D	211	10% 85% 13% .
2	F	211	14% 86% 14% .
3	E	217	5% 81% 16% .

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Mol	Chain	Length	Quality of chain
3	G	217	18% 84% 13%

2 Entry composition

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
1	A	253	Total	C	N	O	S	0	0	0
			1967	1301	318	342	6			
1	B	255	Total	C	N	O	S	0	0	0
			1984	1310	321	347	6			

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
2	D	211	Total	C	N	O	S	0	0	0
			1616	1003	271	333	9			
2	F	211	Total	C	N	O	S	0	0	0
			1616	1003	271	333	9			

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

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

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

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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is water.

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

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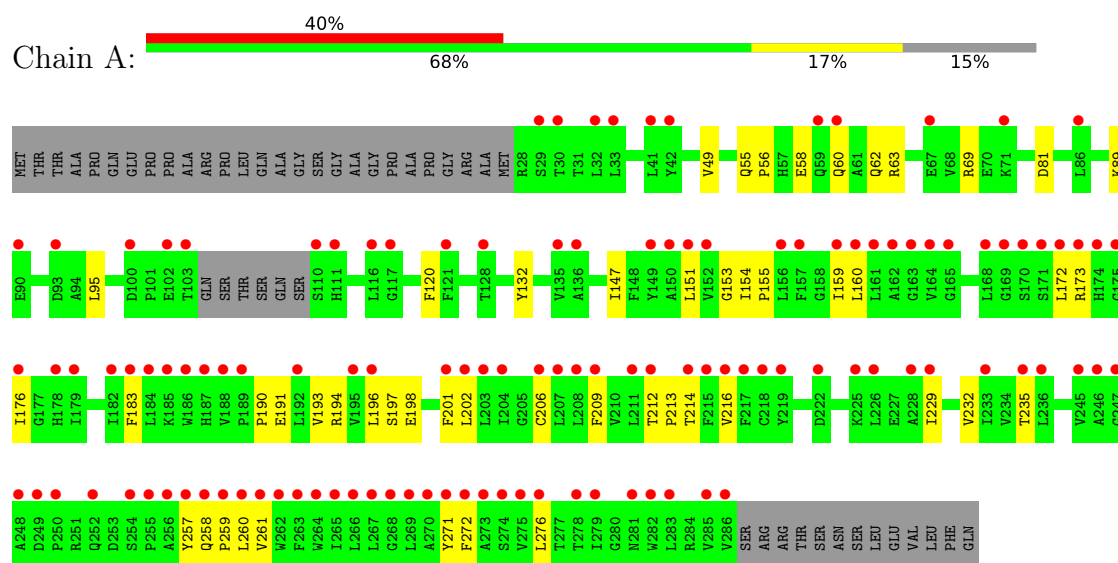
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	50	Total 50	O 50	0	0
6	F	44	Total 44	O 44	0	0
6	G	43	Total 43	O 43	0	0

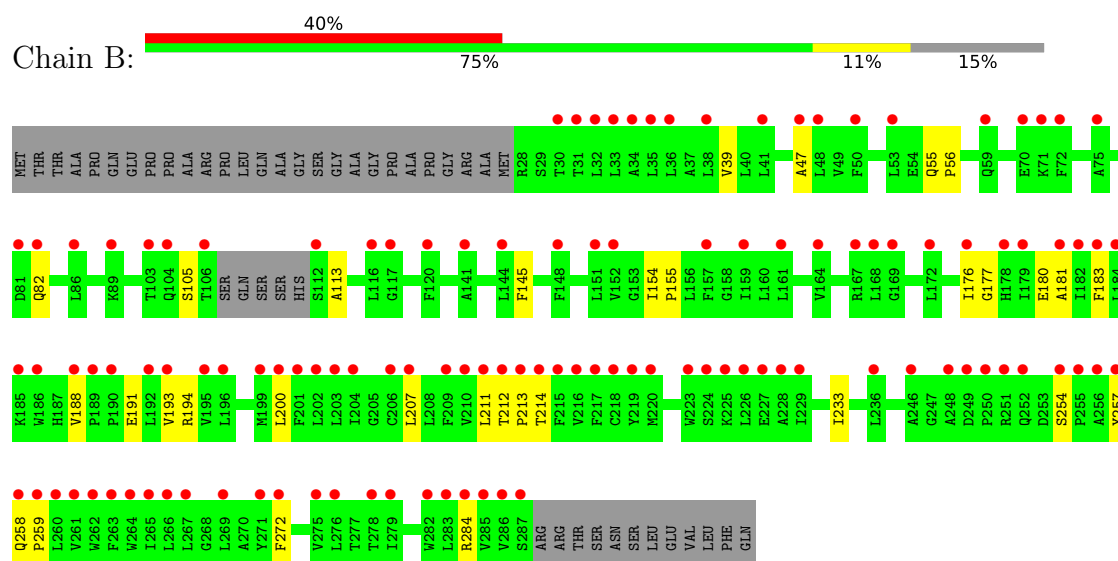
3 Residue-property plots

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.

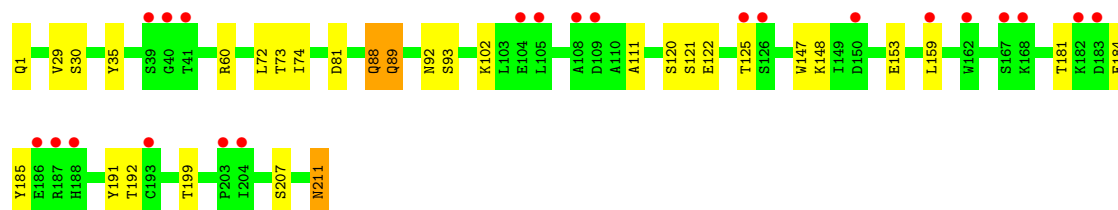
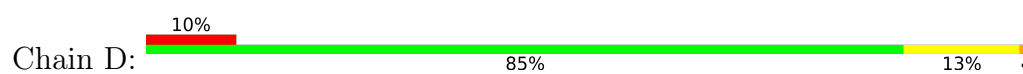
- Molecule 1: Isoform 2 of Potassium channel subfamily K member 4



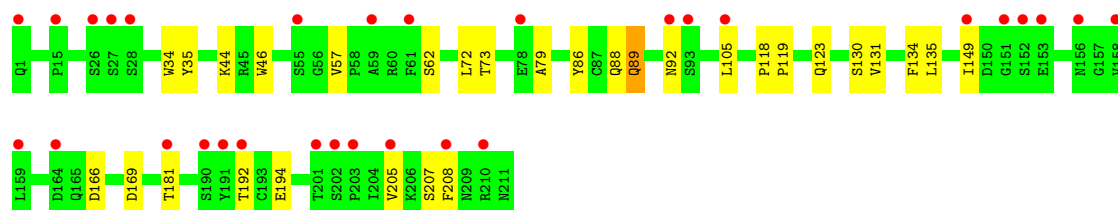
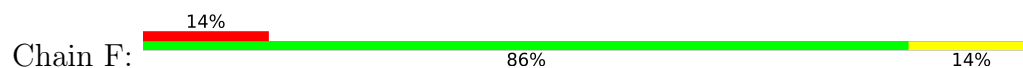
- Molecule 1: Isoform 2 of Potassium channel subfamily K member 4



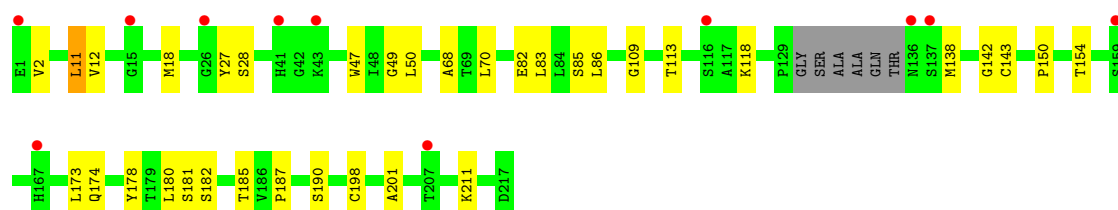
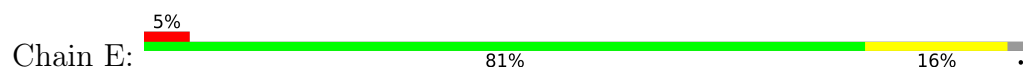
- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



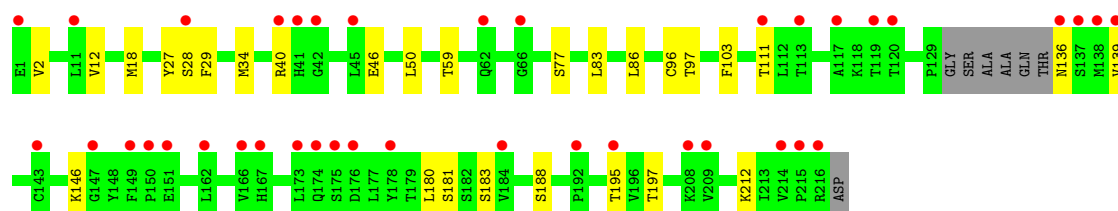
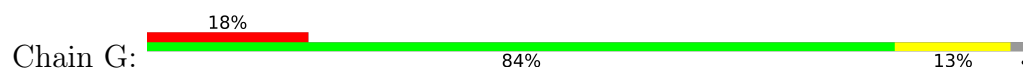
• Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



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



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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (2.97%)	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 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.99	0/2017	1.61	4/2750 (0.1%)
1	B	0.99	0/2034	1.63	2/2773 (0.1%)
2	D	0.97	0/1655	1.28	0/2247
2	F	0.99	0/1655	1.31	2/2247 (0.1%)
3	E	1.00	0/1656	1.27	1/2260 (0.0%)
3	G	1.00	0/1647	1.29	1/2249 (0.0%)
All	All	0.99	0/10664	1.43	10/14526 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	62	SER	CA-C-N	5.49	126.30	121.58
2	F	62	SER	C-N-CA	5.49	126.30	121.58
1	A	153	GLY	CA-C-N	5.42	124.67	120.33
1	A	153	GLY	C-N-CA	5.42	124.67	120.33
1	B	176	ILE	CA-C-N	5.38	126.07	119.99
1	B	176	ILE	C-N-CA	5.38	126.07	119.99
3	E	109	GLY	CA-C-O	-5.20	117.82	121.88
3	G	111	THR	CA-CB-OG1	-5.15	101.87	109.60
1	A	95	LEU	CA-C-N	5.12	125.77	120.03
1	A	95	LEU	C-N-CA	5.12	125.77	120.03

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	1967	0	1986	36	1
1	B	1984	0	2004	23	0
2	D	1616	0	1542	26	1
2	F	1616	0	1542	21	0
3	E	1614	0	1586	22	0
3	G	1605	0	1582	22	0
4	A	4	0	0	0	0
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	137	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 7.

All (137) 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
2:D:159:LEU:HD11	3:E:174:GLN:CD	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:E:180:LEU:C	3:E:180:LEU:HD12	2.23	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
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
1:B:207:LEU:HD13	1:B:207:LEU:C	2.34	0.53
3:G:34:MET:CE	3:G:96:CYS:HB2	2.39	0.53
1:A:89:LYS:NZ	6:A:404:HOH:O	2.41	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:G:180:LEU:HD12	3:G:180:LEU:C	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:83:LEU:HB3	3:E:86:LEU:HD21	1.92	0.50
3:G:34:MET:HE1	3:G:96:CYS:HB2	1.93	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
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
3:G:50:LEU:C	3:G:50:LEU:HD12	2.39	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
3:E:50:LEU:C	3:E:50:LEU:HD12	2.38	0.47
1:A:272:PHE:O	1:A:276:LEU:HD23	2.15	0.47
1:B:154:ILE:N	1:B:155:PRO:HD2	2.29	0.47
2:D:72:LEU:HD23	2:D:72:LEU:C	2.40	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
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: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
3:E:138:MET:HE3	3:E:185:THR:HG22	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:29:PHE:CD1	3:G:77:SER:HA	2.52	0.44
1:A:191:GLU:H	1:A:191:GLU:CD	2.24	0.44
2:D:111:ALA:HB2	2:D:199:THR:HG21	1.99	0.44
1:B:183:PHE:C	1:B:188:VAL:HG22	2.42	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: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
1:A:120:PHE:HA	1:B:47:ALA:HB2	2.00	0.43
1:B:211:LEU:O	1:B:214:THR:OG1	2.35	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
2:D:159:LEU:HD11	3:E:174:GLN:OE1	2.18	0.43
3:E:68:ALA:HA	3:E:82:GLU:O	2.19	0.43
1:A:160:LEU:C	1:A:160:LEU:HD23	2.44	0.43
1:B:258:GLN:HB3	1:B:259:PRO:HD3	2.00	0.43
1:A:202:LEU:C	1:A:202:LEU:HD12	2.43	0.43
2:D:211:ASN:OD1	2:D:211:ASN:N	2.39	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	202 (98%)	3 (2%)	57	68
1	B	208/243 (86%)	204 (98%)	4 (2%)	50	61
2	D	184/184 (100%)	179 (97%)	5 (3%)	39	49
2	F	184/184 (100%)	182 (99%)	2 (1%)	65	75
3	E	187/190 (98%)	180 (96%)	7 (4%)	30	37
3	G	186/190 (98%)	181 (97%)	5 (3%)	39	49
All	All	1154/1234 (94%)	1128 (98%)	26 (2%)	44	55

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	LEU
1	A	196	LEU
1	A	232	VAL
1	B	39	VAL
1	B	105	SER
1	B	200	LEU
1	B	272	PHE
2	D	30	SER
2	D	88	GLN
2	D	89	GLN
2	D	102	LYS
2	D	211	ASN
3	E	11	LEU
3	E	18	MET
3	E	85	SER
3	E	118	LYS
3	E	150	PRO
3	E	198	CYS
3	E	211	LYS
2	F	89	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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	55	GLN
1	B	57	HIS
1	B	281	ASN
2	D	36	GLN
2	D	37	GLN
2	D	136	ASN
3	E	39	GLN
3	E	136	ASN
2	F	88	GLN
2	F	92	ASN
2	F	136	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 oligosaccharides 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

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, 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%)	2.34	120 (47%) 0 0	42, 99, 171, 195	0
1	B	255/299 (85%)	2.23	119 (46%) 0 0	37, 97, 182, 195	0
2	D	211/211 (100%)	0.77	22 (10%) 11 11	35, 56, 93, 111	0
2	F	211/211 (100%)	1.00	30 (14%) 6 5	37, 55, 101, 116	0
3	E	211/217 (97%)	0.42	11 (5%) 33 31	32, 49, 75, 103	0
3	G	210/217 (96%)	0.92	39 (18%) 3 3	35, 54, 90, 131	0
All	All	1351/1454 (92%)	1.34	341 (25%) 1 1	32, 63, 153, 195	0

All (341) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	THR	14.6
1	B	34	ALA	14.3
1	A	161	LEU	11.1
1	A	279	ILE	10.6
1	A	263	PHE	10.1
2	D	187	ARG	9.6
1	A	248	ALA	9.4
1	A	157	PHE	8.6
1	A	272	PHE	8.3
1	A	266	LEU	8.1
1	B	116	LEU	7.9
1	A	282	TRP	7.7
1	A	276	LEU	7.7
1	A	267	LEU	7.6
1	B	275	VAL	7.4
1	A	247	GLY	7.2
1	B	262	TRP	7.1
1	B	251	ARG	7.0
1	B	256	ALA	7.0

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Mol	Chain	Res	Type	RSRZ
1	A	275	VAL	6.9
1	B	276	LEU	6.8
1	B	250	PRO	6.6
1	A	269	LEU	6.5
2	F	201	THR	6.5
1	A	262	TRP	6.4
1	B	148	PHE	6.4
1	A	270	ALA	6.4
1	B	255	PRO	6.3
1	A	256	ALA	6.1
1	A	151	LEU	6.1
1	B	35	LEU	6.0
3	G	136	ASN	5.7
1	B	31	THR	5.6
1	A	164	VAL	5.5
1	A	259	PRO	5.5
1	B	272	PHE	5.5
1	B	179	ILE	5.4
1	A	278	THR	5.4
1	B	182	ILE	5.4
3	G	149	PHE	5.4
1	A	260	LEU	5.3
1	B	219	TYR	5.3
1	B	190	PRO	5.2
3	G	173	LEU	5.2
1	A	273	ALA	5.1
1	B	151	LEU	5.1
1	B	207	LEU	5.1
1	B	257	TYR	5.1
1	A	178	HIS	5.1
2	F	92	ASN	5.1
1	A	250	PRO	5.0
1	B	152	VAL	4.9
1	B	183	PHE	4.9
3	G	178	TYR	4.9
1	B	266	LEU	4.8
1	B	228	ALA	4.8
1	B	192	LEU	4.8
1	B	211	LEU	4.8
3	G	11	LEU	4.8
2	F	27	SER	4.8
1	A	271	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
2	F	78	GLU	4.7
1	A	265	ILE	4.7
1	A	110	SER	4.7
1	B	75	ALA	4.6
1	A	236	LEU	4.6
1	B	172	LEU	4.6
1	B	267	LEU	4.5
2	D	183	ASP	4.5
1	A	257	TYR	4.4
1	B	193	VAL	4.4
1	A	186	TRP	4.4
2	D	39	SER	4.4
1	A	159	ILE	4.4
3	E	137	SER	4.4
1	B	176	ILE	4.3
2	F	202	SER	4.2
3	G	151	GLU	4.2
1	A	264	TRP	4.2
1	A	268	GLY	4.2
1	B	225	LYS	4.2
3	G	137	SER	4.2
1	A	283	LEU	4.2
1	B	117	GLY	4.1
2	D	40	GLY	4.1
2	F	55	SER	4.1
1	B	186	TRP	4.1
1	B	200	LEU	4.1
2	F	1	GLN	4.1
1	B	248	ALA	4.1
1	B	196	LEU	4.1
1	A	179	ILE	4.1
1	B	184	LEU	4.0
1	A	111	HIS	4.0
1	A	215	PHE	4.0
1	A	172	LEU	4.0
1	A	184	LEU	3.9
1	A	185	LYS	3.9
1	A	255	PRO	3.9
1	B	30	THR	3.9
1	B	81	ASP	3.9
1	A	176	ILE	3.9
1	A	182	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
3	G	41	HIS	3.9
1	B	71	LYS	3.9
2	D	168	LYS	3.8
1	A	192	LEU	3.8
1	B	82	GLN	3.8
3	E	136	ASN	3.8
1	A	160	LEU	3.8
1	B	32	LEU	3.8
1	B	269	LEU	3.8
1	B	226	LEU	3.7
1	A	219	TYR	3.7
1	B	218	CYS	3.7
1	B	33	LEU	3.7
1	A	189	PRO	3.7
1	A	163	GLY	3.6
1	B	223	TRP	3.6
1	B	263	PHE	3.6
1	A	218	CYS	3.6
1	B	189	PRO	3.5
1	B	202	LEU	3.5
1	B	215	PHE	3.5
3	E	159	SER	3.5
1	B	86	LEU	3.5
1	A	195	VAL	3.5
1	B	259	PRO	3.4
1	B	285	VAL	3.4
2	F	93	SER	3.4
3	G	175	SER	3.4
1	B	157	PHE	3.4
1	A	30	THR	3.4
1	B	181	ALA	3.4
1	A	102	GLU	3.4
1	A	86	LEU	3.4
1	B	188	VAL	3.4
1	B	120	PHE	3.4
3	G	40	ARG	3.4
3	G	195	THR	3.3
3	G	150	PRO	3.3
1	B	70	GLU	3.3
1	B	203	LEU	3.3
1	B	283	LEU	3.3
1	B	229	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	195	VAL	3.3
1	A	168	LEU	3.3
1	B	178	HIS	3.3
1	B	201	PHE	3.3
1	B	159	ILE	3.2
3	G	143	CYS	3.2
2	D	108	ALA	3.2
1	A	174	HIS	3.2
1	A	150	ALA	3.2
1	A	261	VAL	3.2
1	B	271	TYR	3.2
2	F	158	VAL	3.1
1	B	204	ILE	3.1
3	G	120	THR	3.1
1	A	183	PHE	3.1
1	A	229	ILE	3.1
1	B	89	LYS	3.1
1	A	136	ALA	3.1
1	A	162	ALA	3.1
3	G	184	VAL	3.1
2	D	105	LEU	3.1
1	B	104	GLN	3.0
1	A	207	LEU	3.0
3	G	138	MET	3.0
1	B	103	THR	3.0
3	G	62	GLN	3.0
1	B	287	SER	3.0
1	B	210	VAL	3.0
1	A	187	HIS	3.0
3	E	41	HIS	3.0
2	F	208	PHE	3.0
3	G	192	PRO	3.0
1	A	196	LEU	3.0
1	A	217	PHE	2.9
3	G	208	LYS	2.9
1	B	258	GLN	2.9
1	A	214	THR	2.9
1	B	224	SER	2.9
2	F	156	ASN	2.9
1	B	144	LEU	2.9
1	B	185	LYS	2.9
1	A	173	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	59	GLN	2.9
1	B	279	ILE	2.9
2	F	149	ILE	2.9
2	F	190	SER	2.9
3	G	28	SER	2.9
3	G	176	ASP	2.9
1	A	203	LEU	2.9
1	A	226	LEU	2.9
1	B	260	LEU	2.9
2	F	28	SER	2.8
1	A	32	LEU	2.8
1	A	208	LEU	2.8
3	G	162	LEU	2.8
1	A	233	ILE	2.8
1	B	282	TRP	2.8
2	D	41	THR	2.8
1	B	161	LEU	2.8
2	F	153	GLU	2.8
1	A	246	ALA	2.8
1	A	188	VAL	2.8
3	E	207	THR	2.8
2	D	162	TRP	2.8
2	F	59	ALA	2.8
1	B	286	VAL	2.8
1	A	212	THR	2.7
1	A	121	PHE	2.7
1	A	254	SER	2.7
1	A	286	VAL	2.7
1	B	261	VAL	2.7
1	B	38	LEU	2.7
1	B	236	LEU	2.7
1	A	249	ASP	2.7
1	B	106	THR	2.7
1	A	33	LEU	2.7
1	A	202	LEU	2.7
1	B	168	LEU	2.7
1	A	135	VAL	2.6
1	A	222	ASP	2.6
2	F	164	ASP	2.6
1	A	285	VAL	2.6
2	F	181	THR	2.6
1	B	254	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	41	LEU	2.6
3	G	119	THR	2.6
1	B	213	PRO	2.6
1	A	235	THR	2.6
1	B	217	PHE	2.6
3	G	111	THR	2.6
1	A	274	SER	2.6
1	B	112	SER	2.6
1	A	165	GLY	2.5
1	B	214	THR	2.5
2	F	151	GLY	2.5
2	F	191	TYR	2.5
1	A	41	LEU	2.5
2	F	105	LEU	2.5
2	F	159	LEU	2.5
1	B	47	ALA	2.5
2	D	167	SER	2.5
1	A	156	LEU	2.5
1	A	29	SER	2.5
2	D	182	LYS	2.5
2	D	203	PRO	2.5
3	G	1	GLU	2.4
3	G	209	VAL	2.4
1	A	149	TYR	2.4
1	A	258	GLN	2.4
2	D	186	GLU	2.4
2	D	204	ILE	2.4
1	B	278	THR	2.4
1	B	220	MET	2.4
1	B	36	LEU	2.4
1	A	252	GLN	2.4
1	B	284	ARG	2.4
3	G	174	GLN	2.4
3	G	42	GLY	2.4
2	F	192	THR	2.4
1	A	170	SER	2.4
1	B	164	VAL	2.4
1	A	60	GLN	2.4
1	A	90	GLU	2.4
1	B	264	TRP	2.4
1	A	100	ASP	2.3
3	G	117	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	72	PHE	2.3
1	A	281	ASN	2.3
1	B	249	ASP	2.3
1	A	225	LYS	2.3
1	B	246	ALA	2.3
1	B	199	MET	2.3
1	A	152	VAL	2.3
1	A	209	PHE	2.3
3	E	1	GLU	2.3
1	A	116	LEU	2.3
1	A	211	LEU	2.3
2	F	15	PRO	2.3
1	A	128	THR	2.3
2	F	210	ARG	2.3
1	A	201	PHE	2.3
1	B	212	THR	2.3
3	G	113	THR	2.3
1	B	252	GLN	2.3
1	A	216	VAL	2.3
1	A	245	VAL	2.3
1	B	209	PHE	2.2
2	F	61	PHE	2.2
2	D	126	SER	2.2
2	D	159	LEU	2.2
1	A	206	CYS	2.2
1	A	171	SER	2.2
2	F	26	SER	2.2
1	B	265	ILE	2.2
3	G	214	VAL	2.2
1	B	167	ARG	2.2
2	D	150	ASP	2.2
2	F	203	PRO	2.2
1	A	175	GLY	2.2
2	F	152	SER	2.2
1	A	71	LYS	2.2
3	E	167	HIS	2.2
3	G	147	GLY	2.2
1	B	206	CYS	2.2
1	A	228	ALA	2.2
3	E	116	SER	2.2
1	A	42	TYR	2.1
1	B	216	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	26	GLY	2.1
1	B	48	LEU	2.1
2	D	104	GLU	2.1
3	G	139	VAL	2.1
1	A	59	GLN	2.1
1	A	117	GLY	2.1
1	B	169	GLY	2.1
1	A	204	ILE	2.1
3	G	45	LEU	2.1
3	E	15	GLY	2.1
1	A	93	ASP	2.1
3	G	167	HIS	2.1
2	F	205	VAL	2.1
3	G	166	VAL	2.1
1	B	50	PHE	2.1
3	G	66	GLY	2.1
1	B	141	ALA	2.0
2	D	188	HIS	2.0
1	B	53	LEU	2.0
1	A	169	GLY	2.0
1	A	67	GLU	2.0
1	B	227	GLU	2.0
2	D	125	THR	2.0
2	D	193	CYS	2.0
2	D	109	ASP	2.0
3	G	215	PRO	2.0
3	G	216	ARG	2.0
3	E	43	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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,

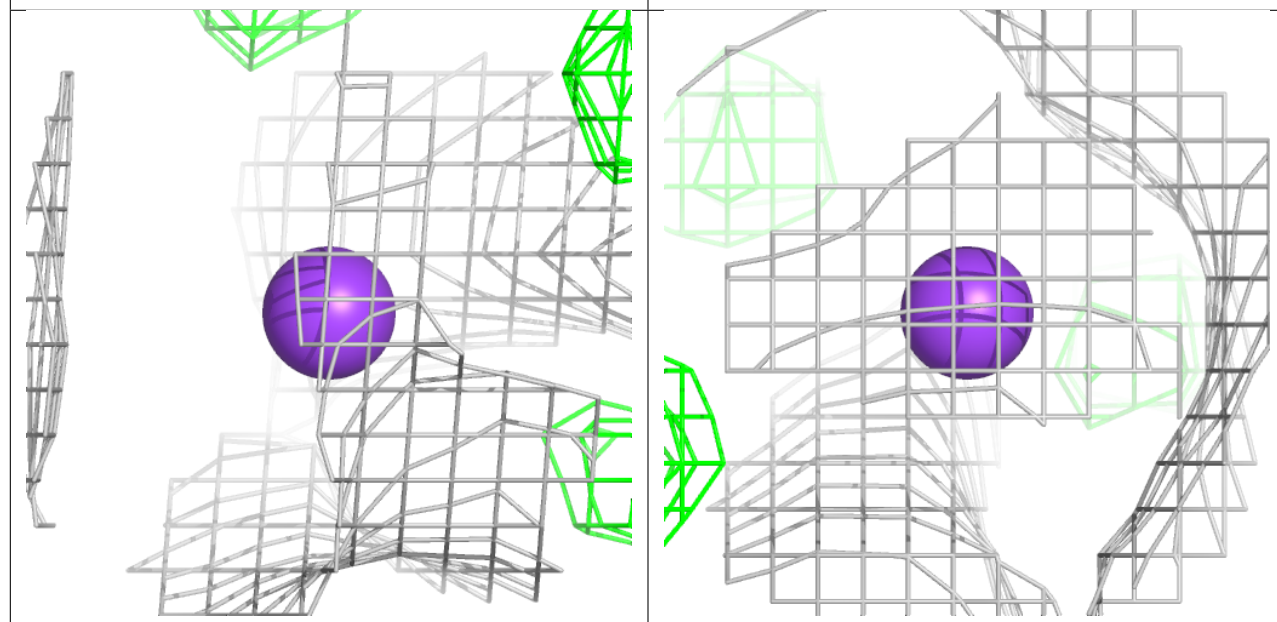
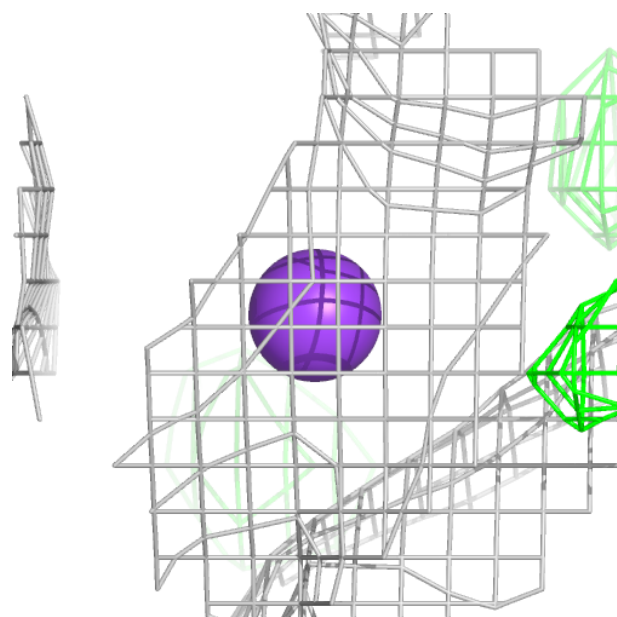
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K	B	303	1/1	0.88	0.15	94,94,94,94	0
4	K	A	306	1/1	0.89	0.19	87,87,87,87	0
4	K	A	303	1/1	0.90	0.10	101,101,101,101	0
5	CA	A	305	1/1	0.91	0.09	97,97,97,97	0
4	K	A	302	1/1	0.96	0.04	75,75,75,75	0
4	K	B	301	1/1	0.97	0.04	71,71,71,71	0
5	CA	A	304	1/1	0.98	0.04	90,90,90,90	0
4	K	B	302	1/1	0.98	0.04	68,68,68,68	0
5	CA	G	301	1/1	0.98	0.03	52,52,52,52	0
4	K	A	301	1/1	0.99	0.04	61,61,61,61	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.

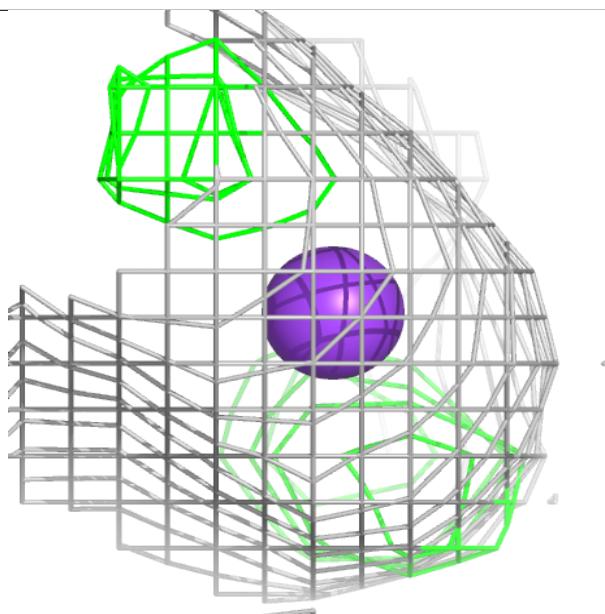
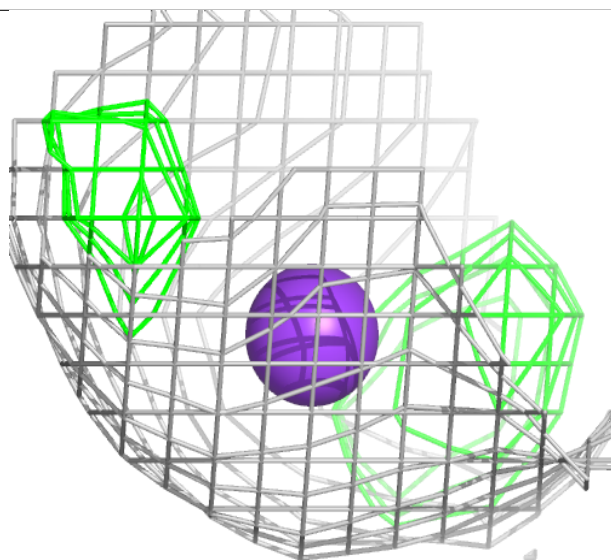
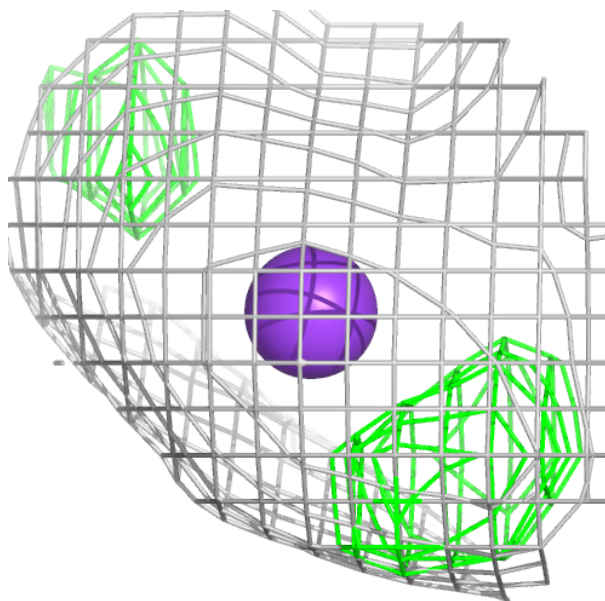
Electron density around K B 303:

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



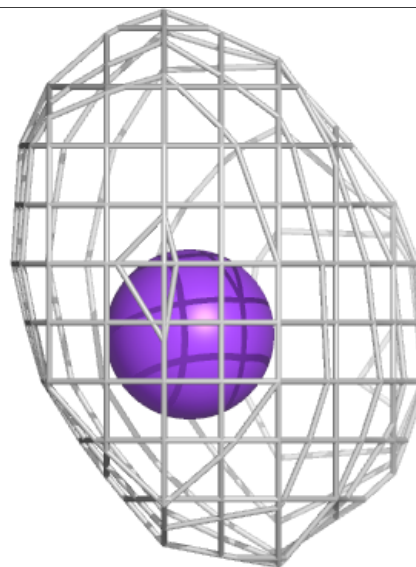
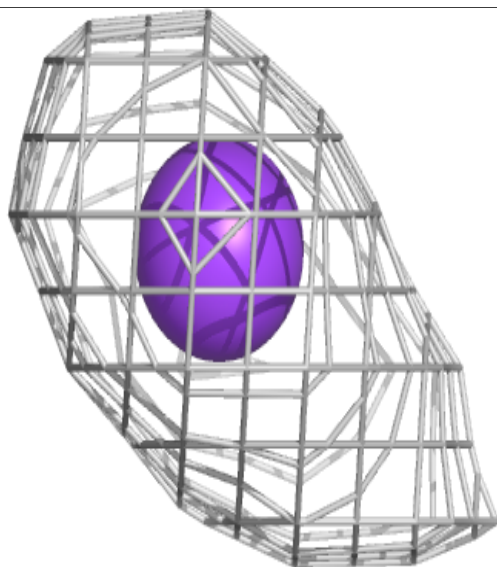
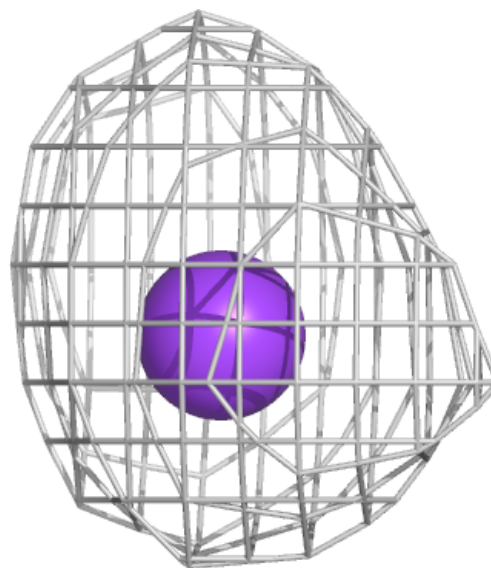
Electron density around K A 306:

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



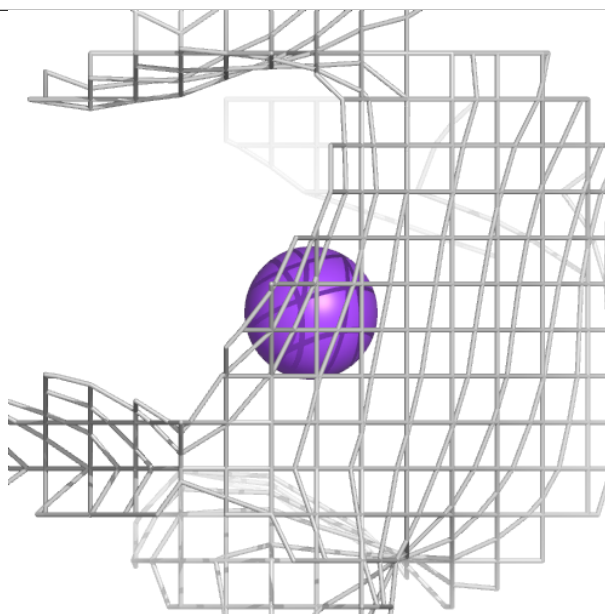
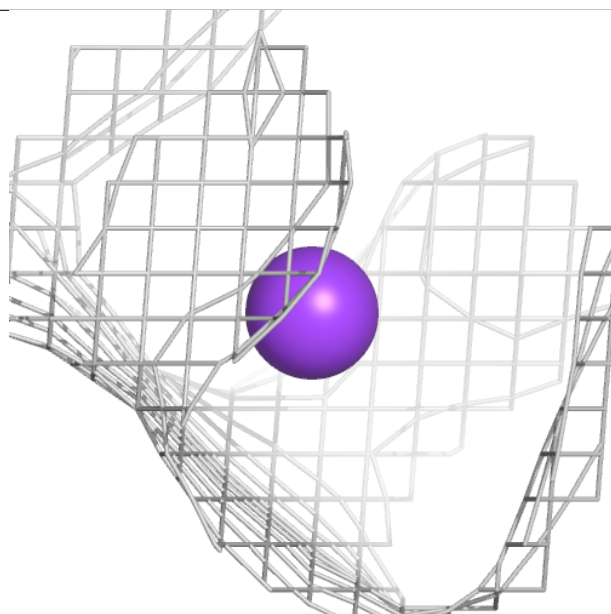
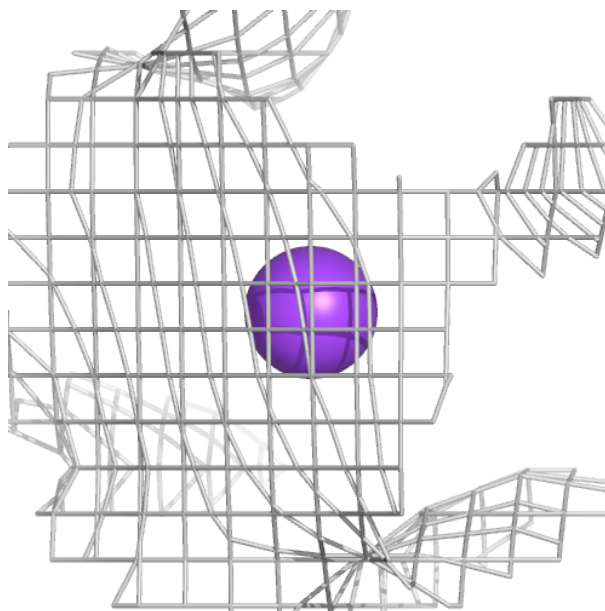
Electron density around K A 303:

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



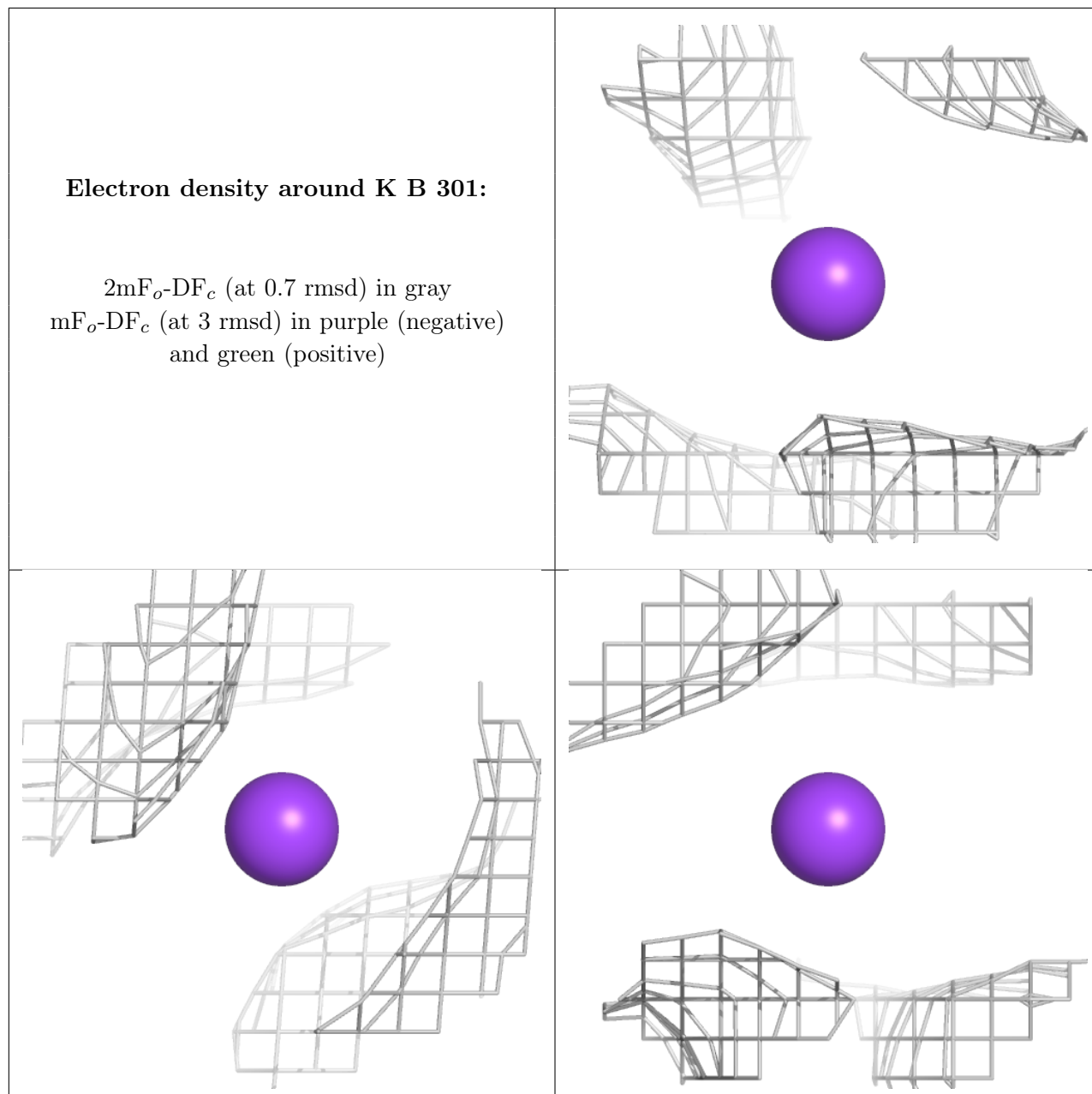
Electron density around K A 302:

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



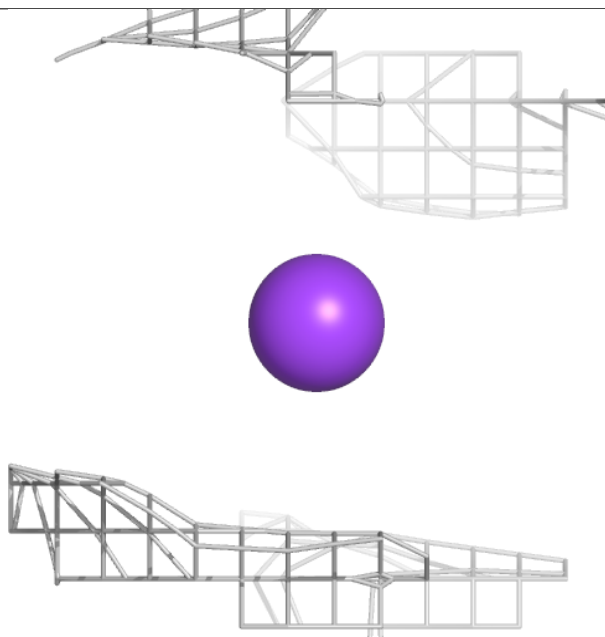
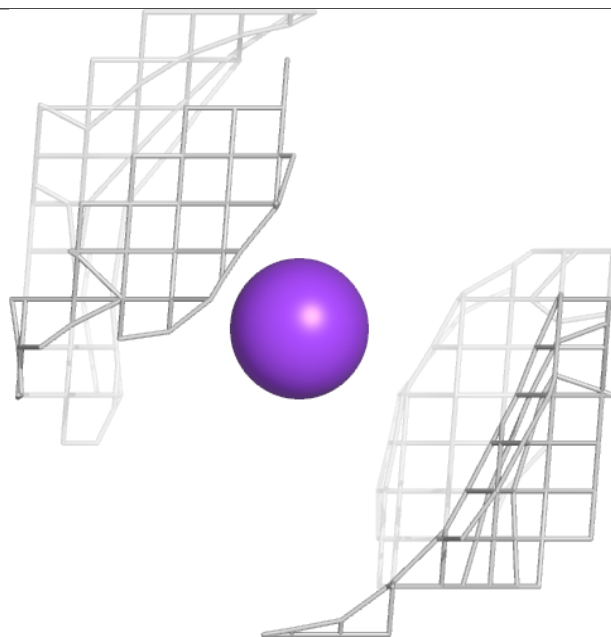
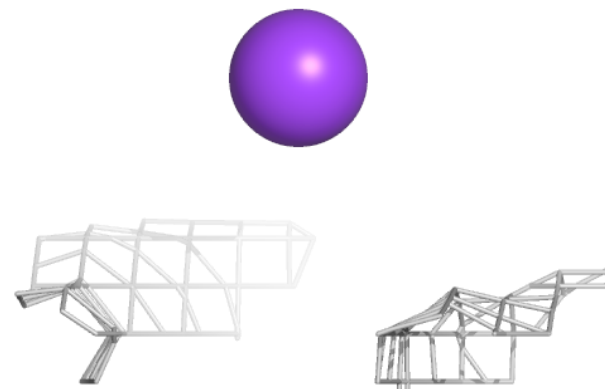
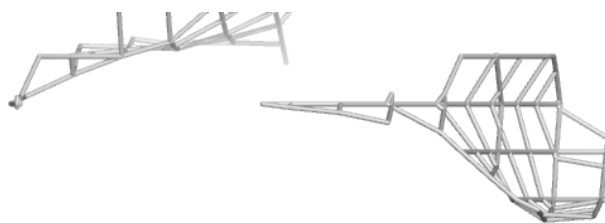
Electron density around K B 301:

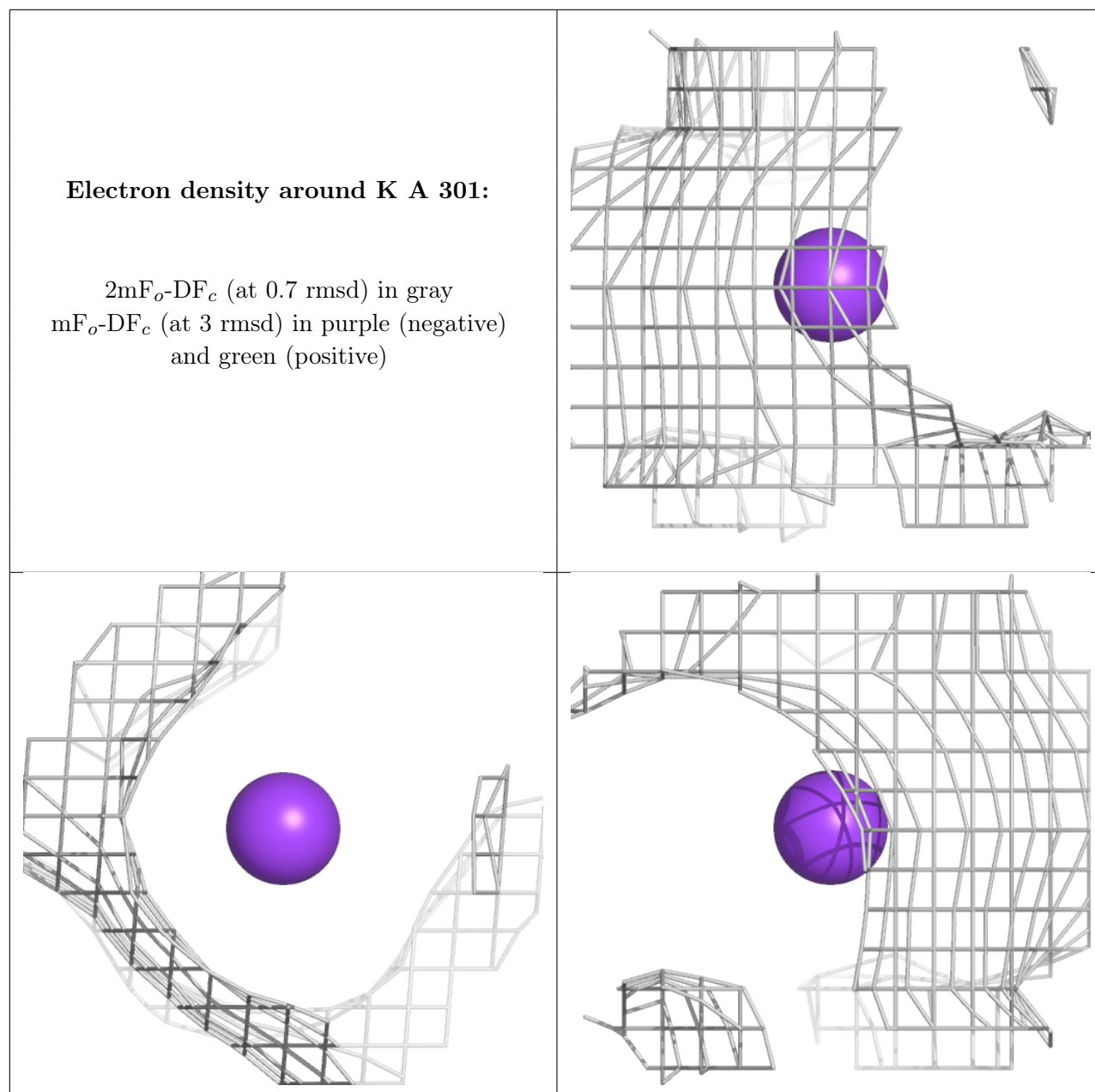
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around K 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.