



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:34 AM UTC

PDB ID : 7LJ4 / pdb_00007lj4
Title : Human TRAAK K⁺ channel FHEIG mutant A270P in a K⁺ bound conductive conformation
Authors : Rietmeijer, R.A.; Brohawn, S.G.
Deposited on : 2021-01-28
Resolution : 2.78 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

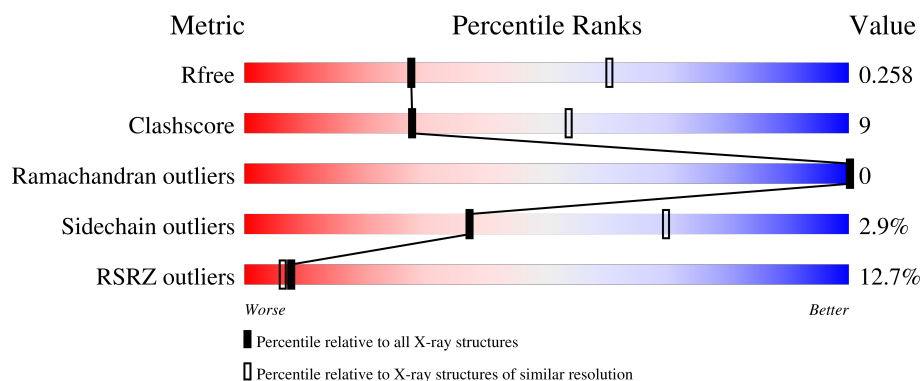
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	27% 65% 19% • 15%
1	B	299	18% 69% 15% • 15%
2	D	211	2% 83% 16% •
2	F	211	4% 83% 16% •
3	E	217	3% 80% 16% • •

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Mol	Chain	Length	Quality of chain
3	G	217	7% 78% 18% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10596 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
			1965	1301	318	340	6			
1	B	255	Total	C	N	O	S	0	0	0
			1982	1310	321	345	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	270	PRO	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	270	PRO	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	5	Total	K	0	0
			5	5		
4	B	2	Total	K	0	0
			2	2		

- 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	33	Total	O	0	0
			33	33		
6	B	31	Total	O	0	0
			31	31		
6	D	24	Total	O	0	0
			24	24		

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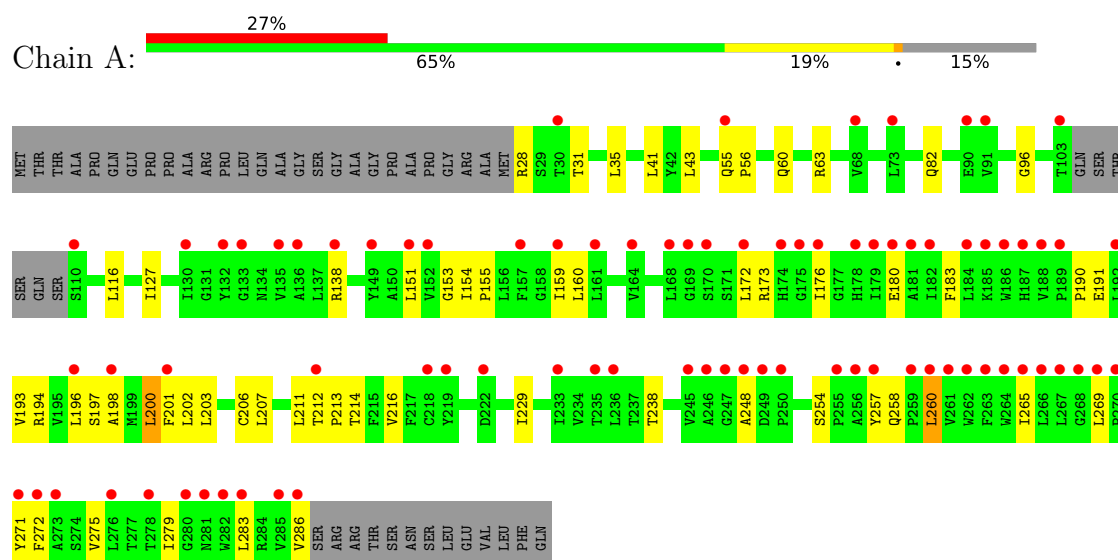
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	37	Total 37	O 37	0	0
6	F	34	Total 34	O 34	0	0
6	G	29	Total 29	O 29	0	0

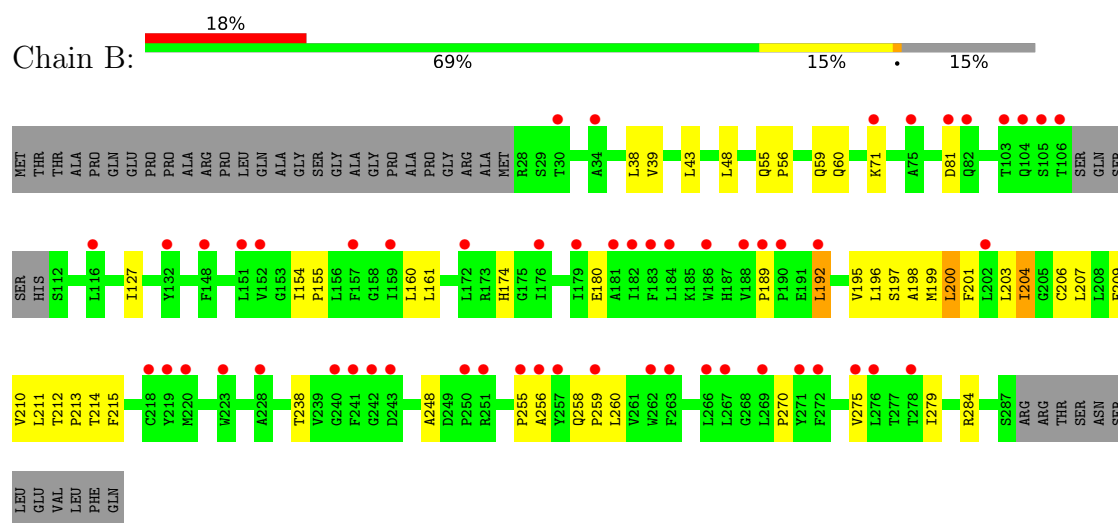
3 Residue-property plots

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.

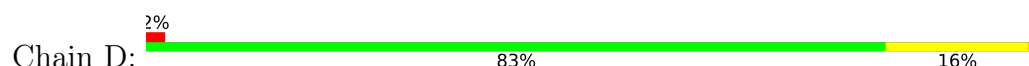
- Molecule 1: Isoform 2 of Potassium channel subfamily K member 4

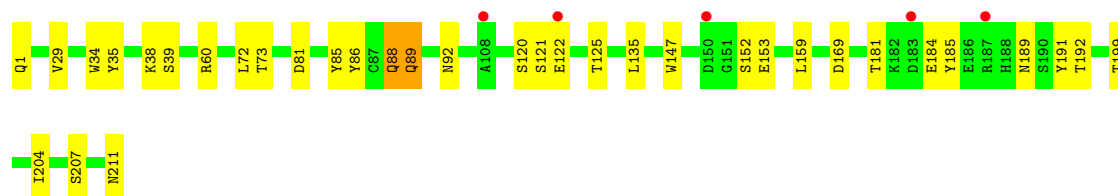


- Molecule 1: Isoform 2 of Potassium channel subfamily K member 4

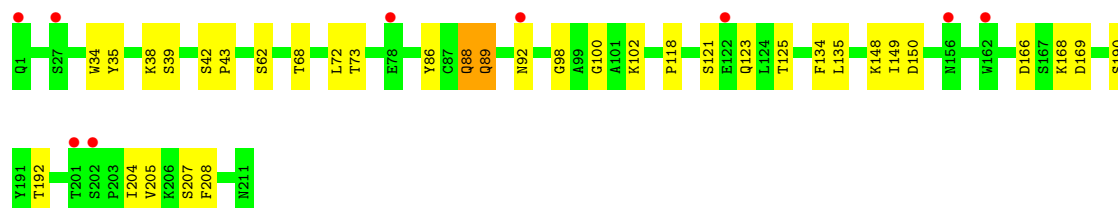
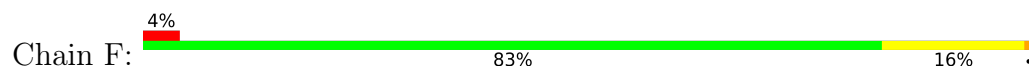


- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN

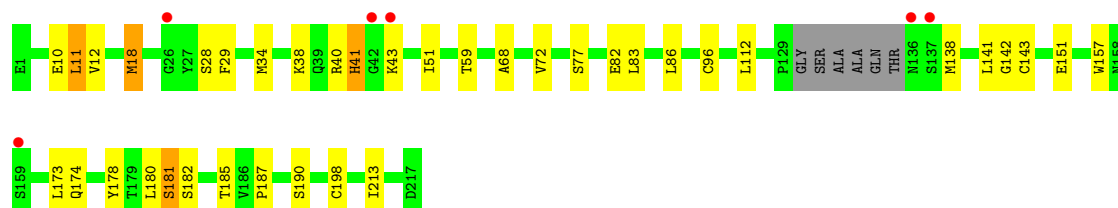
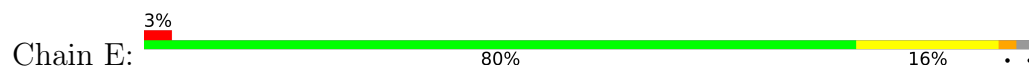




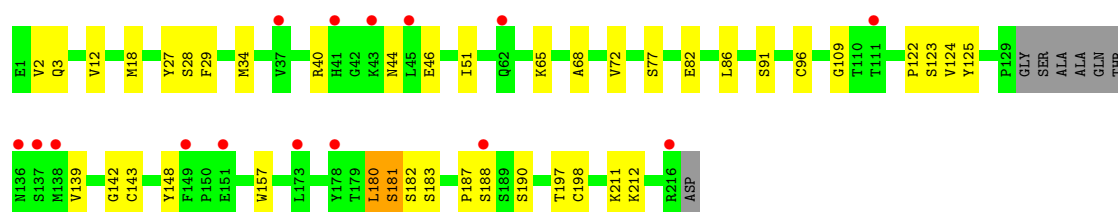
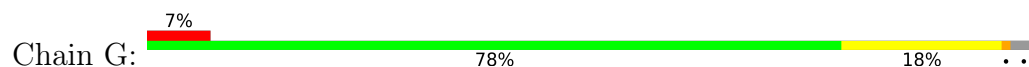
• Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



• 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	80.28Å 136.88Å 95.58Å 90.00° 94.24° 90.00°	Depositor
Resolution (Å)	47.66 – 2.78 47.66 – 2.78	Depositor EDS
% Data completeness (in resolution range)	63.2 (47.66-2.78) 63.2 (47.66-2.78)	Depositor EDS
R_{merge}	0.39	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.214 , 0.258 0.217 , 0.258	Depositor DCC
R_{free} test set	1619 reflections (2.21%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10596	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: CA, K

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	1.04	0/2016	1.65	2/2750 (0.1%)
1	B	1.07	0/2033	1.65	4/2773 (0.1%)
2	D	1.03	0/1655	1.32	0/2247
2	F	1.05	0/1655	1.35	3/2247 (0.1%)
3	E	1.01	0/1656	1.30	1/2260 (0.0%)
3	G	1.02	0/1647	1.30	1/2249 (0.0%)
All	All	1.04	0/10662	1.45	11/14526 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	68	THR	CA-CB-OG1	-6.56	99.76	109.60
1	A	153	GLY	CA-C-N	5.82	124.98	120.33
1	A	153	GLY	C-N-CA	5.82	124.98	120.33
1	B	192	LEU	CA-C-N	5.64	127.67	120.56
1	B	192	LEU	C-N-CA	5.64	127.67	120.56
3	E	41	HIS	CA-CB-CG	5.64	119.44	113.80
2	F	100	GLY	CA-C-O	-5.57	117.39	122.24
3	G	109	GLY	CA-C-O	-5.38	118.52	122.23
1	B	174	HIS	CA-C-N	5.22	125.73	119.94
1	B	174	HIS	C-N-CA	5.22	125.73	119.94
2	F	68	THR	CB-CA-C	5.06	118.72	110.17

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	1965	0	1986	48	1
1	B	1982	0	2005	41	0
2	D	1616	0	1542	23	1
2	F	1616	0	1542	23	0
3	E	1614	0	1586	32	0
3	G	1605	0	1582	33	0
4	A	5	0	0	0	0
4	B	2	0	0	0	0
5	A	2	0	0	0	0
5	G	1	0	0	0	0
6	A	33	0	0	0	0
6	B	31	0	0	1	0
6	D	24	0	0	1	0
6	E	37	0	0	4	0
6	F	34	0	0	5	0
6	G	29	0	0	1	0
All	All	10596	0	10243	186	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 9.

All (186) 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:A:198:ALA:O	1:A:201:PHE:HB3	1.80	0.82
2:F:35:TYR:HE1	2:F:88:GLN:HG2	1.45	0.81
2:D:35:TYR:HE2	2:D:88:GLN:HG2	1.47	0.79
1:B:195:VAL:O	1:B:199:MET:HG2	1.88	0.74
1:A:176:ILE:HD11	1:A:201:PHE:CD1	2.23	0.73
1:B:198:ALA:O	1:B:201:PHE:HB3	1.89	0.72
2:F:35:TYR:CE1	2:F:88:GLN:HG2	2.26	0.70
6:F:301:HOH:O	3:G:44:ASN:HA	1.90	0.70
2:D:181:THR:HG23	2:D:184:GLU:H	1.57	0.69
3:E:10:GLU:OE2	6:E:301:HOH:O	2.09	0.69
3:E:10:GLU:C	3:E:11:LEU:HD12	2.17	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:28:SER:HB2	3:G:28:SER:HB2	1.75	0.68
1:B:200:LEU:C	1:B:200:LEU:HD13	2.19	0.68
2:D:35:TYR:CE2	2:D:88:GLN:HG2	2.28	0.68
1:B:256:ALA:O	1:B:259:PRO:HD2	1.95	0.67
1:A:172:LEU:HD13	1:A:201:PHE:CE1	2.30	0.67
3:E:12:VAL:HG21	3:E:86:LEU:HD12	1.79	0.65
1:A:116:LEU:HD21	1:B:48:LEU:HD23	1.79	0.65
2:F:134:PHE:CE2	3:G:183:SER:HB3	2.31	0.65
1:A:172:LEU:HB3	1:A:201:PHE:HE1	1.62	0.65
3:G:12:VAL:HG21	3:G:86:LEU:HD12	1.78	0.65
3:E:180:LEU:C	3:E:180:LEU:HD12	2.21	0.64
3:G:180:LEU:HD12	3:G:180:LEU:C	2.23	0.64
1:B:189:PRO:HB2	1:B:192:LEU:HD13	1.78	0.64
3:E:83:LEU:HB3	3:E:86:LEU:HD21	1.80	0.63
1:A:214:THR:HG21	1:A:229:ILE:HG12	1.82	0.62
1:B:256:ALA:C	1:B:259:PRO:HD2	2.25	0.61
1:B:211:LEU:O	1:B:215:PHE:HD1	1.83	0.61
1:A:265:ILE:CG2	1:A:269:LEU:HD11	2.29	0.61
1:A:96:GLY:O	1:A:138:ARG:NH2	2.33	0.61
1:A:127:ILE:HD13	1:B:43:LEU:HD21	1.83	0.60
1:A:212:THR:HB	1:A:213:PRO:HD3	1.83	0.60
1:A:191:GLU:H	1:A:191:GLU:CD	2.10	0.59
1:A:265:ILE:HG23	1:A:269:LEU:HD11	1.83	0.59
1:A:200:LEU:C	1:A:200:LEU:HD13	2.28	0.59
1:A:200:LEU:HD13	1:A:200:LEU:O	2.02	0.59
1:A:260:LEU:HD22	1:A:260:LEU:O	2.03	0.58
1:B:206:CYS:SG	1:B:211:LEU:CD2	2.91	0.58
3:E:12:VAL:HG21	3:E:86:LEU:CD1	2.34	0.58
1:A:127:ILE:CD1	1:B:43:LEU:HD21	2.33	0.57
1:A:41:LEU:C	1:A:41:LEU:HD13	2.28	0.57
1:B:212:THR:HB	1:B:213:PRO:HD3	1.86	0.57
2:F:166:ASP:HB3	2:F:169:ASP:OD2	2.05	0.57
2:D:60:ARG:NH1	2:D:81:ASP:OD1	2.38	0.56
3:E:34:MET:CE	3:E:96:CYS:HB2	2.36	0.56
1:A:214:THR:HG21	1:A:229:ILE:CG1	2.34	0.56
1:A:269:LEU:HD12	1:A:269:LEU:N	2.21	0.55
2:D:120:SER:HB2	2:D:122:GLU:OE1	2.05	0.55
3:G:139:VAL:HG23	3:G:188:SER:HB3	1.89	0.55
3:G:34:MET:CE	3:G:96:CYS:HB2	2.37	0.55
1:A:202:LEU:HD12	1:A:203:LEU:N	2.22	0.54
3:G:139:VAL:HG23	3:G:188:SER:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:51:ILE:HD13	3:G:72:VAL:HG13	1.90	0.54
1:A:248:ALA:HA	1:A:258:GLN:HB3	1.89	0.54
2:F:149:ILE:HG13	2:F:149:ILE:O	2.08	0.54
1:A:172:LEU:CB	1:A:201:PHE:HE1	2.21	0.54
1:B:161:LEU:HD11	1:B:270:PRO:HD3	1.89	0.54
1:A:82:GLN:HG3	3:E:59:THR:HG21	1.90	0.53
3:E:138:MET:HE3	3:E:185:THR:HG22	1.89	0.53
3:E:11:LEU:CD1	3:E:11:LEU:N	2.71	0.53
3:G:139:VAL:CG2	3:G:188:SER:HB3	2.38	0.53
1:A:254:SER:HB3	1:A:257:TYR:CD2	2.44	0.53
3:E:51:ILE:HD13	3:E:72:VAL:HG13	1.91	0.53
1:A:160:LEU:C	1:A:160:LEU:HD23	2.33	0.53
1:A:60:GLN:OE1	1:A:63:ARG:NH2	2.42	0.52
3:E:141:LEU:HD22	3:E:213:ILE:HG21	1.90	0.52
1:B:206:CYS:SG	1:B:211:LEU:HD21	2.50	0.52
3:G:28:SER:HA	6:G:410:HOH:O	2.09	0.51
3:G:29:PHE:CD1	3:G:77:SER:HA	2.45	0.51
1:A:159:ILE:HD12	1:B:284:ARG:HD3	1.93	0.51
2:F:72:LEU:HD23	2:F:73:THR:N	2.24	0.51
2:D:147:TRP:O	2:D:153:GLU:HA	2.10	0.51
2:D:29:VAL:HG11	2:D:89:GLN:HG3	1.91	0.51
1:B:198:ALA:HA	1:B:201:PHE:HB3	1.92	0.50
2:F:134:PHE:CE2	3:G:183:SER:CB	2.94	0.50
1:A:197:SER:O	1:A:201:PHE:N	2.43	0.50
3:E:151:GLU:HG3	3:E:178:TYR:CZ	2.47	0.50
1:A:213:PRO:HA	1:A:216:VAL:HB	1.94	0.50
2:F:192:THR:HG22	2:F:207:SER:OG	2.12	0.50
3:G:2:VAL:HG13	3:G:27:TYR:CD2	2.47	0.50
1:A:172:LEU:HB3	1:A:201:PHE:CE1	2.44	0.50
1:A:206:CYS:HB2	1:A:271:TYR:OH	2.11	0.50
2:D:192:THR:HG22	2:D:207:SER:OG	2.12	0.50
3:G:34:MET:HE1	3:G:96:CYS:HB2	1.93	0.49
3:G:139:VAL:HG23	3:G:188:SER:CA	2.41	0.49
3:E:187:PRO:O	3:E:190:SER:HB2	2.11	0.49
1:B:59:GLN:HG2	6:B:405:HOH:O	2.13	0.49
2:F:98:GLY:O	6:F:301:HOH:O	2.20	0.49
2:D:72:LEU:HD23	2:D:73:THR:N	2.28	0.48
3:E:10:GLU:O	3:E:11:LEU:HD12	2.13	0.48
2:D:199:THR:HG22	2:D:199:THR:O	2.12	0.48
3:G:139:VAL:CG2	3:G:188:SER:HA	2.44	0.48
2:D:185:TYR:HA	2:D:191:TYR:OH	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:10:GLU:C	3:E:11:LEU:CD1	2.87	0.48
1:A:207:LEU:HD13	1:A:211:LEU:HD22	1.95	0.47
1:B:200:LEU:C	1:B:200:LEU:CD1	2.87	0.47
3:E:34:MET:HE1	3:E:96:CYS:HB2	1.96	0.47
1:A:283:LEU:O	1:A:286:VAL:HB	2.13	0.47
2:D:159:LEU:HD21	3:E:174:GLN:NE2	2.29	0.47
3:E:68:ALA:HA	3:E:82:GLU:O	2.15	0.47
2:F:43:PRO:O	6:F:302:HOH:O	2.20	0.47
1:B:81:ASP:HB3	6:F:325:HOH:O	2.15	0.47
2:F:62:SER:HB3	6:F:317:HOH:O	2.14	0.47
1:A:154:ILE:N	1:A:155:PRO:HD2	2.29	0.47
1:A:82:GLN:HG2	6:D:307:HOH:O	2.14	0.47
1:B:260:LEU:C	1:B:260:LEU:HD23	2.39	0.47
1:B:258:GLN:HB3	1:B:259:PRO:HD3	1.96	0.47
2:F:135:LEU:HD12	2:F:135:LEU:N	2.30	0.47
1:B:154:ILE:N	1:B:155:PRO:HD2	2.29	0.46
3:G:68:ALA:HA	3:G:82:GLU:O	2.15	0.46
3:G:12:VAL:HG21	3:G:86:LEU:CD1	2.44	0.46
1:B:200:LEU:HD13	1:B:200:LEU:O	2.16	0.46
2:F:118:PRO:HB3	2:F:208:PHE:CZ	2.51	0.46
3:G:2:VAL:O	3:G:3:GLN:HG2	2.16	0.46
3:G:187:PRO:O	3:G:190:SER:HB2	2.16	0.45
1:A:269:LEU:N	1:A:269:LEU:CD1	2.79	0.45
2:D:159:LEU:HD11	3:E:174:GLN:CD	2.42	0.45
3:E:29:PHE:CD2	3:E:77:SER:HA	2.52	0.45
3:E:41:HIS:HE1	3:E:43:LYS:HB2	1.80	0.45
3:E:173:LEU:HG	3:E:178:TYR:CE2	2.52	0.45
3:G:139:VAL:HG23	3:G:188:SER:CB	2.47	0.45
1:B:38:LEU:C	1:B:38:LEU:HD23	2.41	0.45
1:A:190:PRO:O	1:A:194:ARG:HG2	2.17	0.45
2:D:34:TRP:HA	2:D:86:TYR:O	2.17	0.45
2:D:38:LYS:O	2:D:39:SER:C	2.60	0.45
3:E:40:ARG:HD3	6:E:320:HOH:O	2.17	0.45
1:B:55:GLN:N	1:B:56:PRO:CD	2.80	0.44
1:B:209:PHE:O	1:B:213:PRO:HG2	2.17	0.44
1:A:28:ARG:HA	1:A:31:THR:HB	1.99	0.44
3:G:142:GLY:HA2	3:G:182:SER:O	2.18	0.44
1:B:248:ALA:N	1:B:258:GLN:HE22	2.16	0.44
2:F:72:LEU:HD23	2:F:72:LEU:C	2.42	0.44
2:D:169:ASP:OD1	2:D:169:ASP:C	2.60	0.44
1:A:183:PHE:HB3	1:A:193:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:C	1:A:200:LEU:CD1	2.91	0.44
1:A:35:LEU:HD23	1:B:160:LEU:HA	2.00	0.44
3:G:122:PRO:HB3	3:G:148:TYR:HB3	2.00	0.44
1:A:180:GLU:HG2	1:A:193:VAL:HG12	2.00	0.43
1:A:254:SER:CB	1:A:257:TYR:CD2	3.01	0.43
2:D:72:LEU:HD23	2:D:72:LEU:C	2.43	0.43
3:G:197:THR:HG22	3:G:212:LYS:HA	2.01	0.43
1:B:55:GLN:O	1:B:59:GLN:HG3	2.18	0.43
1:B:60:GLN:OE1	1:B:60:GLN:HA	2.18	0.43
1:A:173:ARG:HA	1:A:176:ILE:HB	1.99	0.43
2:F:89:GLN:HE21	2:F:92:ASN:H	1.65	0.43
1:B:197:SER:O	1:B:201:PHE:N	2.47	0.43
2:F:134:PHE:CD2	3:G:183:SER:HB3	2.53	0.43
3:G:40:ARG:NH1	3:G:91:SER:O	2.52	0.43
2:F:34:TRP:HA	2:F:86:TYR:O	2.18	0.43
3:G:124:VAL:HG12	3:G:211:LYS:HG2	2.01	0.43
1:A:260:LEU:C	1:A:260:LEU:HD13	2.44	0.42
2:F:118:PRO:HB3	2:F:208:PHE:CE1	2.54	0.42
1:B:203:LEU:O	1:B:207:LEU:HG	2.20	0.42
1:B:200:LEU:HD11	1:B:204:ILE:CD1	2.49	0.42
2:D:89:GLN:HE21	2:D:92:ASN:H	1.66	0.42
3:E:142:GLY:HA2	3:E:182:SER:O	2.19	0.42
3:E:157:TRP:CZ3	3:E:198:CYS:HB3	2.54	0.42
1:A:275:VAL:O	1:A:279:ILE:HG12	2.18	0.42
3:G:180:LEU:C	3:G:180:LEU:CD1	2.91	0.42
3:E:143:CYS:O	3:E:181:SER:HA	2.20	0.42
1:A:43:LEU:HD21	1:B:127:ILE:CD1	2.50	0.42
1:B:195:VAL:C	1:B:199:MET:HG2	2.44	0.42
1:A:55:GLN:N	1:A:56:PRO:CD	2.83	0.42
1:B:196:LEU:HA	1:B:199:MET:HB2	2.03	0.41
3:E:11:LEU:HD12	3:E:11:LEU:N	2.32	0.41
3:E:38:LYS:NZ	6:E:308:HOH:O	2.53	0.41
2:F:150:ASP:HA	2:F:190:SER:OG	2.20	0.41
3:G:157:TRP:CZ3	3:G:198:CYS:HB3	2.55	0.41
1:B:255:PRO:O	1:B:259:PRO:HD3	2.21	0.41
2:D:35:TYR:O	2:D:85:TYR:HA	2.21	0.41
2:D:121:SER:O	2:D:125:THR:HG23	2.21	0.41
1:B:275:VAL:O	1:B:279:ILE:HG22	2.20	0.41
2:D:189:ASN:ND2	2:D:211:ASN:OD1	2.38	0.41
2:F:121:SER:O	2:F:125:THR:HG23	2.20	0.41
2:D:135:LEU:N	2:D:135:LEU:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:PRO:O	1:B:259:PRO:CD	2.69	0.41
2:F:38:LYS:O	2:F:39:SER:C	2.64	0.41
2:F:148:LYS:HB2	2:F:192:THR:OG1	2.21	0.41
3:G:139:VAL:CG2	3:G:188:SER:CB	2.98	0.41
3:E:11:LEU:HD11	6:E:315:HOH:O	2.20	0.41
2:F:123:GLN:HG3	3:G:125:TYR:CE2	2.56	0.40
3:G:143:CYS:O	3:G:181:SER:HA	2.21	0.40
1:B:210:VAL:O	1:B:214:THR:HG23	2.21	0.40
1:B:197:SER:O	1:B:200:LEU:HB3	2.21	0.40
2:D:192:THR:HG22	2:D:207:SER:CB	2.52	0.40
3:E:18:MET:HE3	3:E:112:LEU:HD13	2.03	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

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	249/299 (83%)	242 (97%)	7 (3%)	0	100	100
1	B	251/299 (84%)	244 (97%)	7 (3%)	0	100	100
2	D	209/211 (99%)	199 (95%)	10 (5%)	0	100	100
2	F	209/211 (99%)	203 (97%)	6 (3%)	0	100	100
3	E	207/217 (95%)	199 (96%)	8 (4%)	0	100	100
3	G	206/217 (95%)	198 (96%)	8 (4%)	0	100	100
All	All	1331/1454 (92%)	1285 (96%)	46 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	205/243 (84%)	199 (97%)	6 (3%)	37	70
1	B	208/243 (86%)	202 (97%)	6 (3%)	37	70
2	D	184/184 (100%)	179 (97%)	5 (3%)	39	71
2	F	184/184 (100%)	177 (96%)	7 (4%)	29	61
3	E	187/190 (98%)	184 (98%)	3 (2%)	55	81
3	G	186/190 (98%)	180 (97%)	6 (3%)	34	67
All	All	1154/1234 (94%)	1121 (97%)	33 (3%)	37	70

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	LEU
1	A	196	LEU
1	A	200	LEU
1	A	238	THR
1	A	260	LEU
1	A	272	PHE
1	B	39	VAL
1	B	71	LYS
1	B	180	GLU
1	B	200	LEU
1	B	204	ILE
1	B	238	THR
2	D	1	GLN
2	D	88	GLN
2	D	89	GLN
2	D	152	SER
2	D	204	ILE
3	E	11	LEU
3	E	18	MET

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Mol	Chain	Res	Type
3	E	181	SER
2	F	42	SER
2	F	88	GLN
2	F	89	GLN
2	F	102	LYS
2	F	168	LYS
2	F	204	ILE
2	F	205	VAL
3	G	18	MET
3	G	46	GLU
3	G	65	LYS
3	G	123	SER
3	G	180	LEU
3	G	181	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	174	HIS
1	A	281	ASN
1	B	258	GLN
1	B	281	ASN
2	D	136	ASN
2	D	144	ASN
2	D	155	GLN
3	E	41	HIS
3	E	44	ASN
3	E	62	GLN
3	E	167	HIS
2	F	88	GLN
3	G	41	HIS
3	G	44	ASN
3	G	174	GLN

5.3.3 RNA ⓘ

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%)	1.61	82 (32%) 1 1	42, 108, 168, 188	0
1	B	255/299 (85%)	1.33	55 (21%) 2 2	40, 100, 179, 223	0
2	D	211/211 (100%)	0.26	5 (2%) 59 52	32, 57, 94, 114	0
2	F	211/211 (100%)	0.32	9 (4%) 40 33	33, 58, 102, 125	0
3	E	211/217 (97%)	0.09	6 (2%) 55 47	30, 50, 77, 112	0
3	G	210/217 (96%)	0.40	15 (7%) 22 17	33, 53, 82, 129	0
All	All	1351/1454 (92%)	0.72	172 (12%) 8 6	30, 64, 154, 223	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	136	ASN	6.2
1	A	256	ALA	6.2
1	A	151	LEU	6.0
1	A	179	ILE	5.9
1	A	248	ALA	5.7
1	A	265	ILE	5.7
1	A	269	LEU	5.7
3	G	137	SER	5.5
1	A	262	TRP	5.4
1	B	34	ALA	5.4
2	D	187	ARG	5.3
1	A	161	LEU	5.3
3	G	41	HIS	5.2
1	B	276	LEU	5.2
1	A	272	PHE	4.9
1	A	157	PHE	4.8
1	A	270	PRO	4.7
1	B	257	TYR	4.6
1	B	275	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	192	LEU	4.3
1	B	75	ALA	4.3
1	A	103	THR	4.2
1	B	159	ILE	4.2
1	B	104	GLN	4.2
1	B	278	THR	4.2
1	B	251	ARG	4.1
1	A	247	GLY	4.1
1	A	186	TRP	4.0
1	B	152	VAL	4.0
1	A	273	ALA	3.9
1	A	267	LEU	3.9
1	A	250	PRO	3.9
1	A	176	ILE	3.9
1	B	242	GLY	3.9
1	A	178	HIS	3.9
1	B	272	PHE	3.8
1	A	236	LEU	3.7
1	B	182	ILE	3.7
1	B	219	TYR	3.7
1	B	189	PRO	3.7
1	A	185	LYS	3.6
3	G	151	GLU	3.6
1	B	148	PHE	3.6
2	F	156	ASN	3.6
1	A	135	VAL	3.6
1	B	151	LEU	3.5
1	A	263	PHE	3.5
1	A	174	HIS	3.5
3	G	178	TYR	3.4
3	E	159	SER	3.4
2	F	201	THR	3.4
1	A	259	PRO	3.4
2	F	92	ASN	3.4
3	G	149	PHE	3.3
1	A	266	LEU	3.3
3	G	188	SER	3.3
1	A	192	LEU	3.2
1	B	267	LEU	3.2
3	G	62	GLN	3.2
1	A	271	TYR	3.2
1	A	246	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	260	LEU	3.1
1	B	190	PRO	3.1
3	E	26	GLY	3.1
1	B	179	ILE	3.1
1	B	181	ALA	3.1
1	A	136	ALA	3.1
1	A	182	ILE	3.1
1	B	266	LEU	3.0
1	A	132	TYR	3.0
2	F	1	GLN	3.0
1	A	286	VAL	3.0
3	G	173	LEU	2.9
1	B	186	TRP	2.9
2	F	202	SER	2.9
1	B	176	ILE	2.9
1	B	30	THR	2.9
1	A	218	CYS	2.9
1	B	116	LEU	2.9
1	A	187	HIS	2.9
1	A	282	TRP	2.8
1	B	132	TYR	2.8
1	A	235	THR	2.8
1	A	189	PRO	2.8
1	A	170	SER	2.8
3	E	43	LYS	2.8
1	B	256	ALA	2.8
1	B	271	TYR	2.8
1	A	152	VAL	2.8
1	A	285	VAL	2.8
1	B	82	GLN	2.8
1	A	196	LEU	2.8
1	B	106	THR	2.8
3	G	45	LEU	2.7
1	B	157	PHE	2.7
1	B	262	TRP	2.7
1	A	222	ASP	2.7
1	A	55	GLN	2.6
1	B	103	THR	2.6
1	A	257	TYR	2.6
1	A	110	SER	2.6
1	A	172	LEU	2.6
1	A	168	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	261	VAL	2.5
1	A	233	ILE	2.5
3	G	43	LYS	2.5
1	B	188	VAL	2.5
1	B	240	GLY	2.5
1	B	71	LYS	2.4
1	B	218	CYS	2.4
1	B	81	ASP	2.4
1	A	30	THR	2.4
1	A	159	ILE	2.4
1	A	181	ALA	2.4
1	B	241	PHE	2.4
1	A	149	TYR	2.3
1	A	184	LEU	2.3
1	A	283	LEU	2.3
1	B	105	SER	2.3
1	A	133	GLY	2.3
1	A	68	VAL	2.3
1	A	91	VAL	2.3
1	A	201	PHE	2.3
2	D	108	ALA	2.3
1	B	220	MET	2.3
1	A	281	ASN	2.3
2	D	122	GLU	2.3
1	B	255	PRO	2.3
2	D	183	ASP	2.3
1	A	164	VAL	2.3
1	A	198	ALA	2.3
3	E	137	SER	2.3
1	B	223	TRP	2.3
1	B	184	LEU	2.3
1	B	263	PHE	2.3
3	E	136	ASN	2.2
2	F	27	SER	2.2
1	A	264	TRP	2.2
1	A	130	ILE	2.2
1	A	249	ASP	2.2
1	B	172	LEU	2.2
2	F	162	TRP	2.2
3	G	111	THR	2.2
1	A	276	LEU	2.2
1	A	280	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	G	216	ARG	2.2
1	A	268	GLY	2.2
2	F	122	GLU	2.1
1	A	169	GLY	2.1
1	A	175	GLY	2.1
1	A	188	VAL	2.1
2	D	150	ASP	2.1
1	B	228	ALA	2.1
2	F	78	GLU	2.1
1	A	278	THR	2.1
1	A	255	PRO	2.1
1	A	219	TYR	2.1
3	E	42	GLY	2.1
1	A	180	GLU	2.1
1	B	250	PRO	2.1
1	A	245	VAL	2.1
1	A	73	LEU	2.1
3	G	37	VAL	2.1
1	B	183	PHE	2.1
1	B	243	ASP	2.0
1	A	90	GLU	2.0
1	A	212	THR	2.0
1	B	259	PRO	2.0
3	G	138	MET	2.0
1	A	138	ARG	2.0
1	B	202	LEU	2.0
1	B	269	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 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,

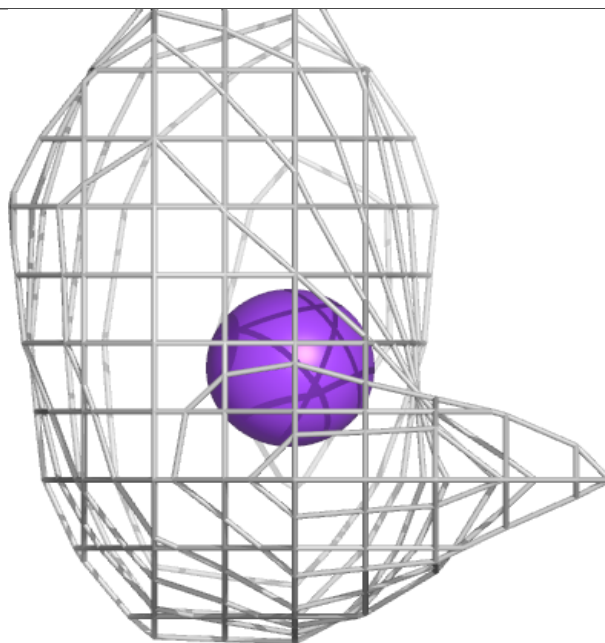
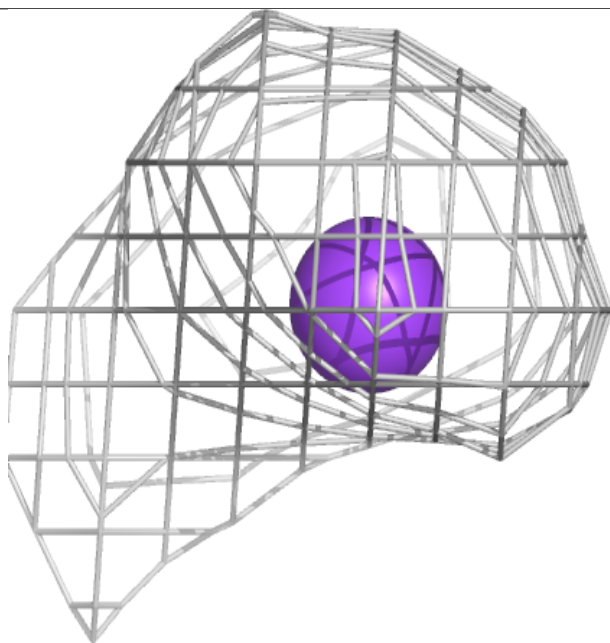
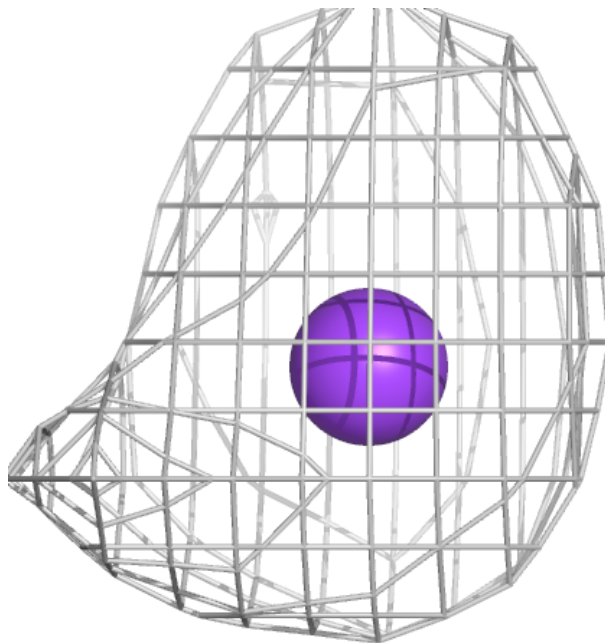
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K	A	304	1/1	0.83	0.10	88,88,88,88	0
4	K	B	301	1/1	0.90	0.18	70,70,70,70	0
4	K	B	302	1/1	0.90	0.22	86,86,86,86	0
5	CA	A	306	1/1	0.92	0.09	118,118,118,118	0
5	CA	A	305	1/1	0.93	0.06	120,120,120,120	0
5	CA	G	301	1/1	0.98	0.03	50,50,50,50	0
4	K	A	307	1/1	0.99	0.10	37,37,37,37	0
4	K	A	303	1/1	0.99	0.08	36,36,36,36	0
4	K	A	301	1/1	0.99	0.10	29,29,29,29	0
4	K	A	302	1/1	1.00	0.08	27,27,27,27	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.

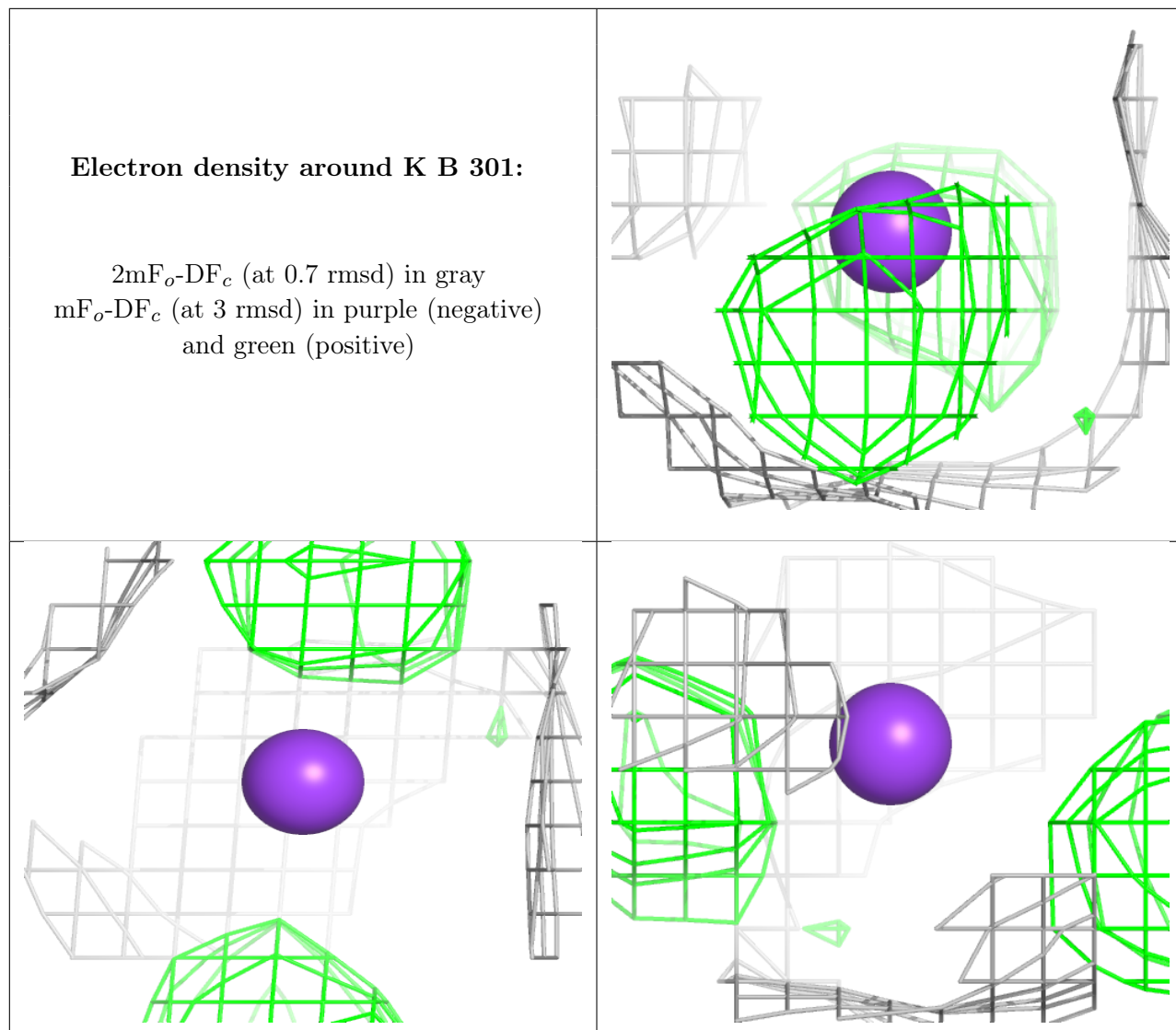
Electron density around K A 304:

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



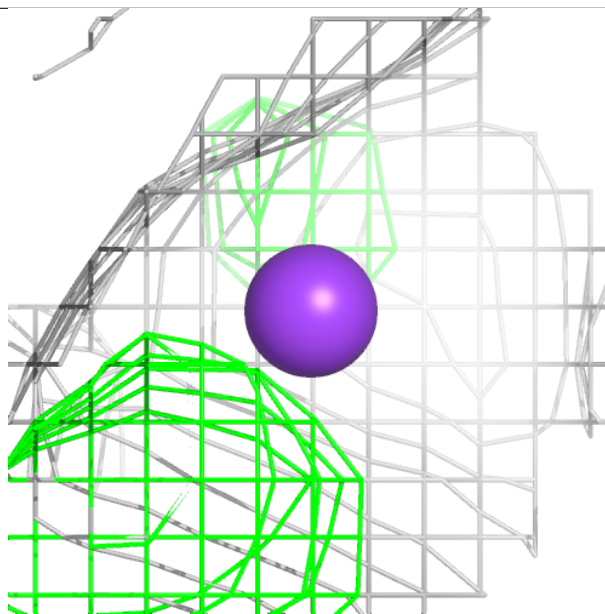
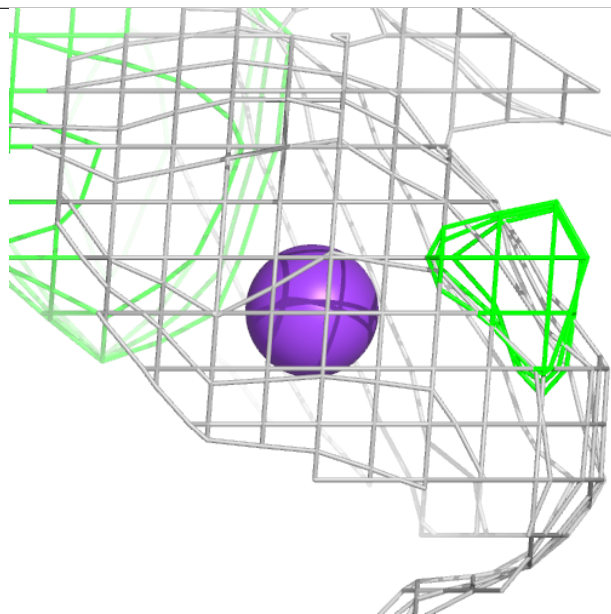
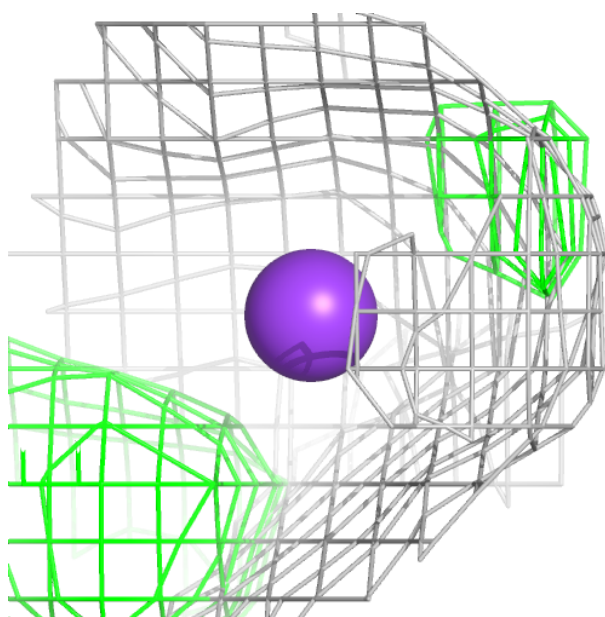
Electron density around K B 301:

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



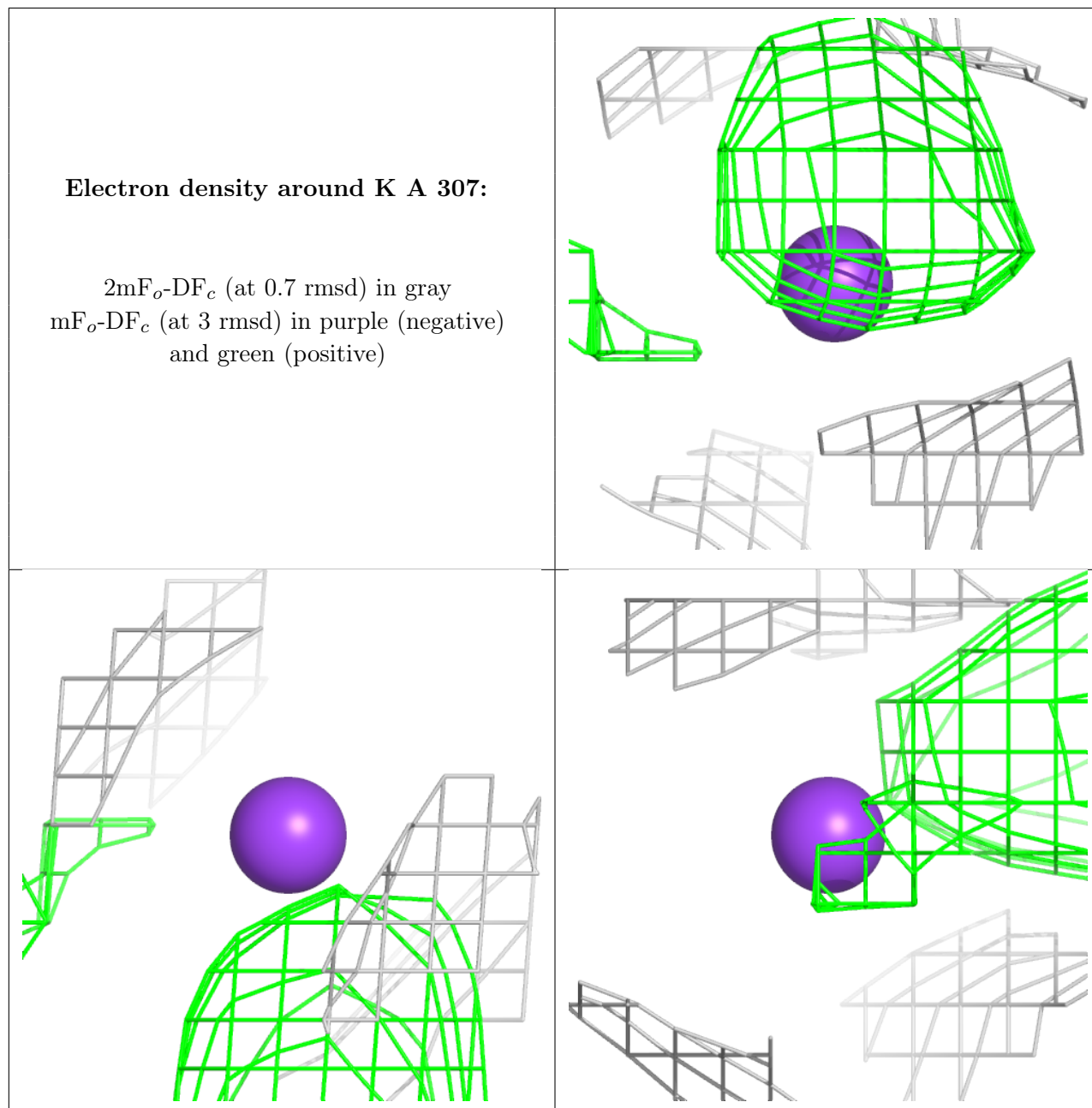
Electron density around K B 302:

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



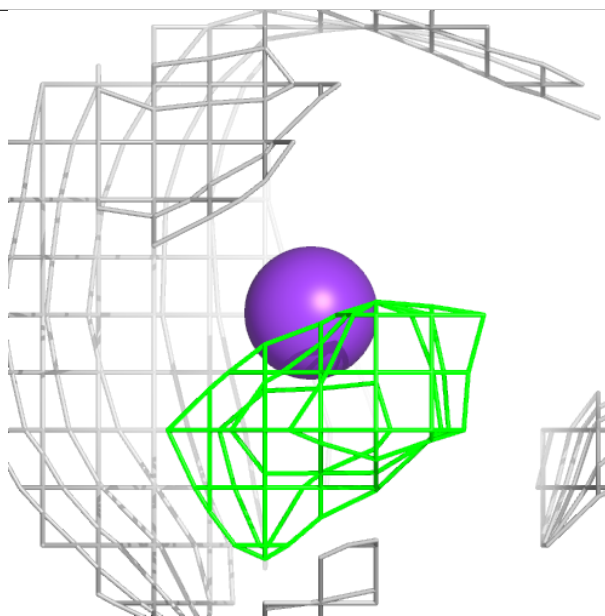
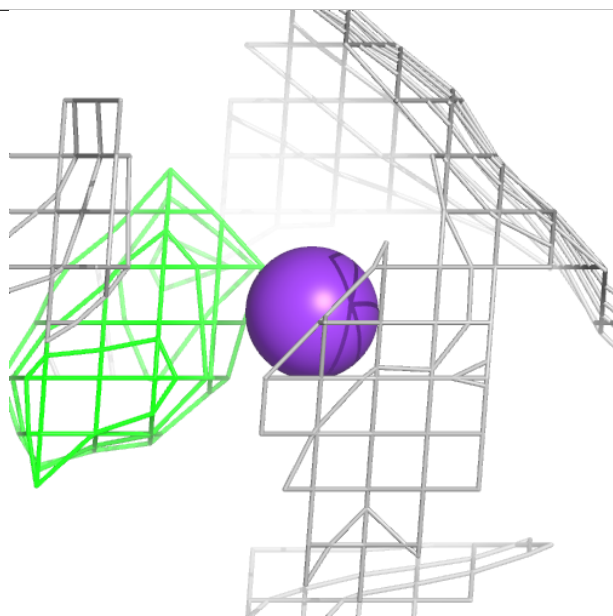
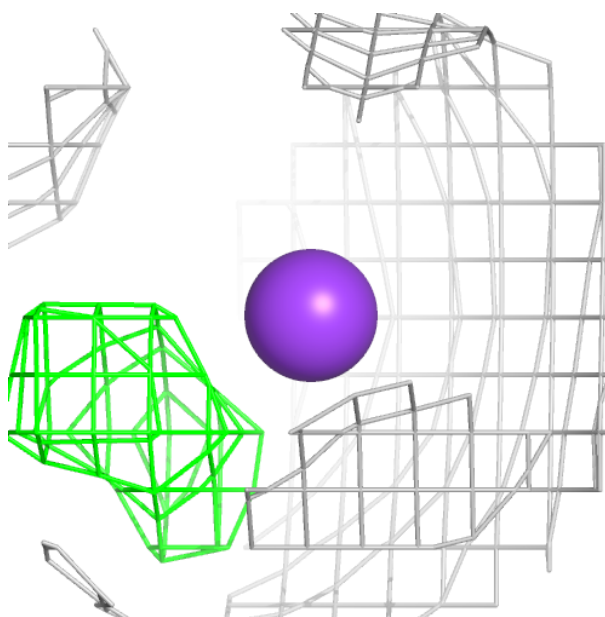
Electron density around K A 307:

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



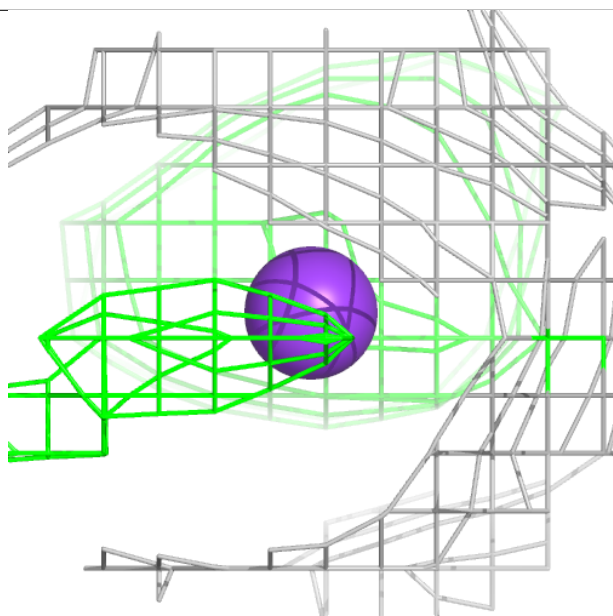
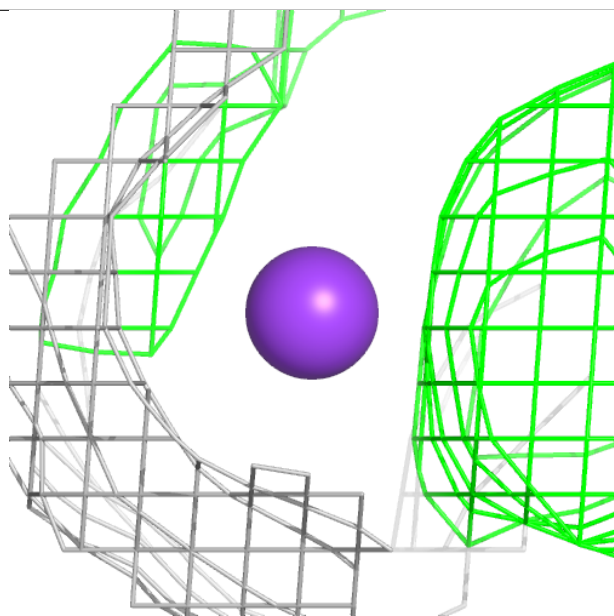
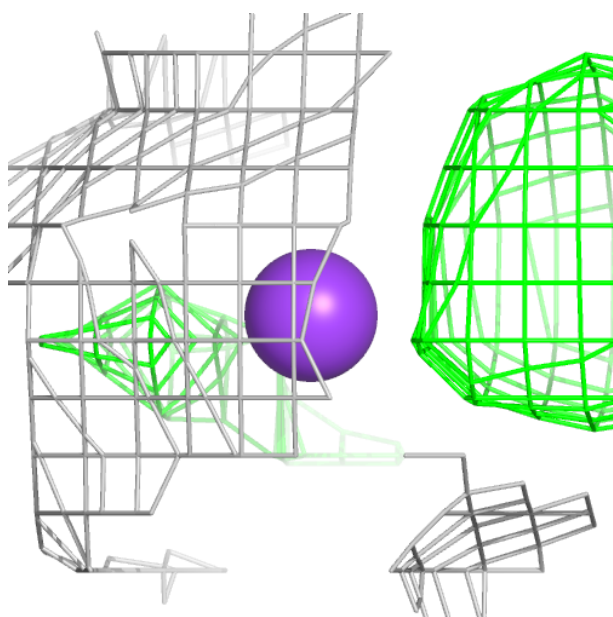
Electron density around K A 303:

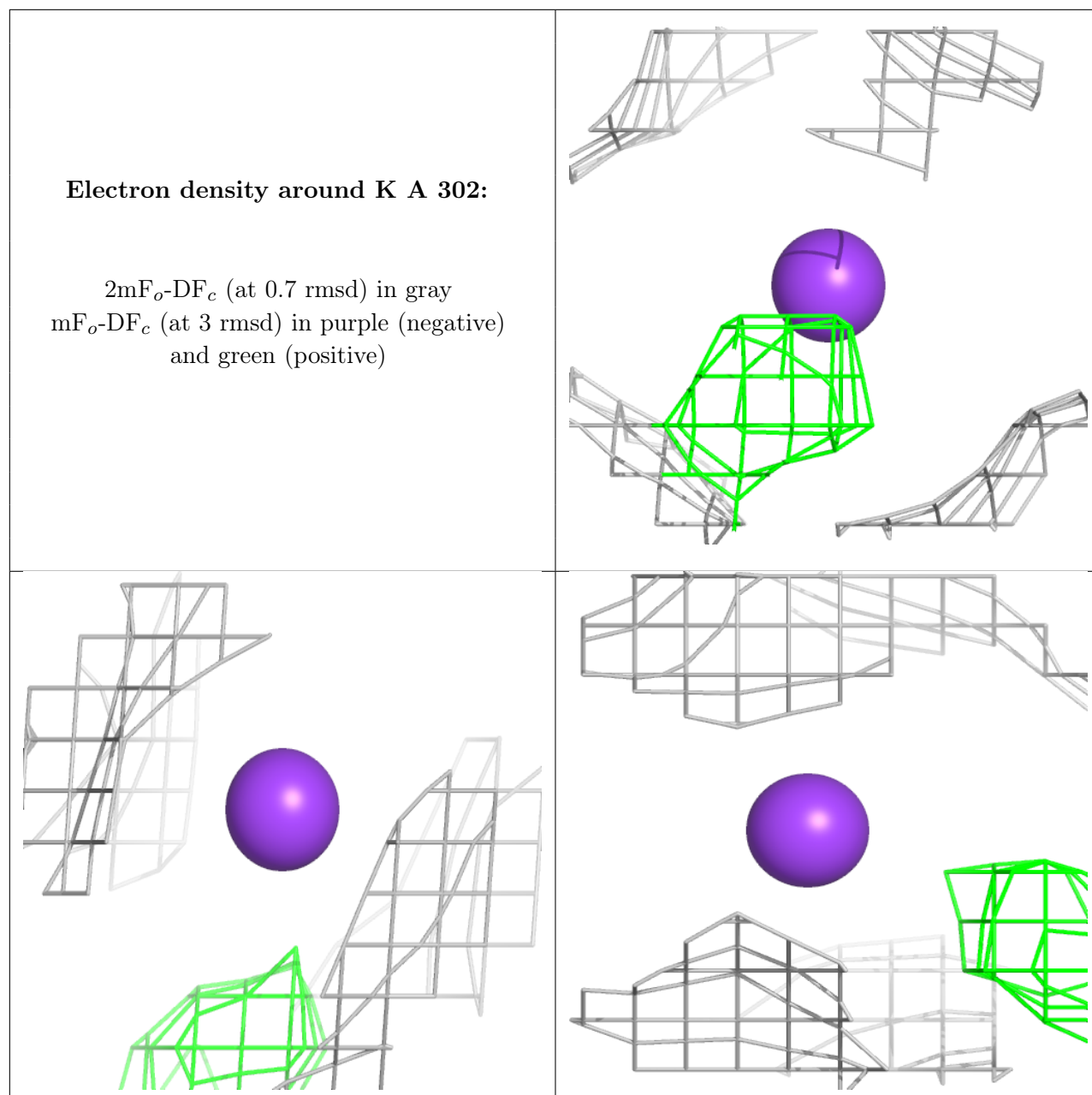
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around K A 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.