



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:42 AM UTC

PDB ID : 7LJA / pdb_00007lja
Title : Human TRAAK K⁺ channel FHEIG mutant A198E in a Tl⁺ bound conductive conformation
Authors : Rietmeijer, R.A.; Brohawn, S.G.
Deposited on : 2021-01-28
Resolution : 2.77 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

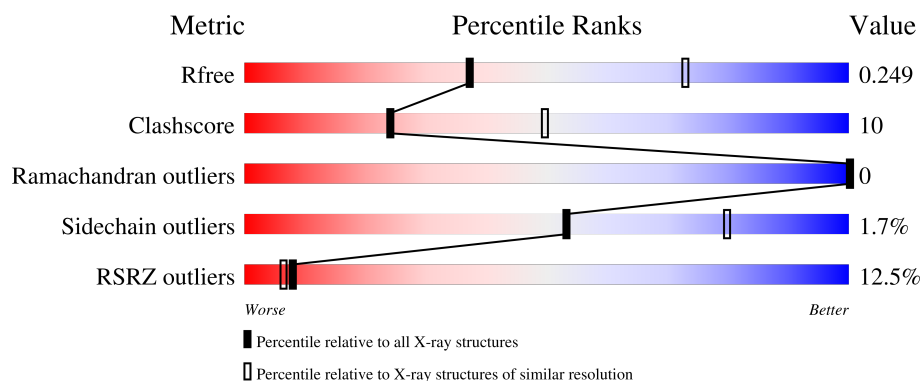
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	22% 66% 18% 15%
1	B	299	20% 73% 12% 15%
2	D	211	6% 83% 17%
2	F	211	3% 80% 18%
3	E	217	5% 71% 25%

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Mol	Chain	Length	Quality of chain
3	G	217	7% 71% 24% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10651 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
			1985	1310	321	348	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 THALLIUM (I) ION (CCD ID: TL) (formula: Tl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Tl	0	0
			5	5		
4	B	3	Total	Tl	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	31	Total	O	0	0
			31	31		
6	B	38	Total	O	0	0
			38	38		
6	D	35	Total	O	0	0
			35	35		

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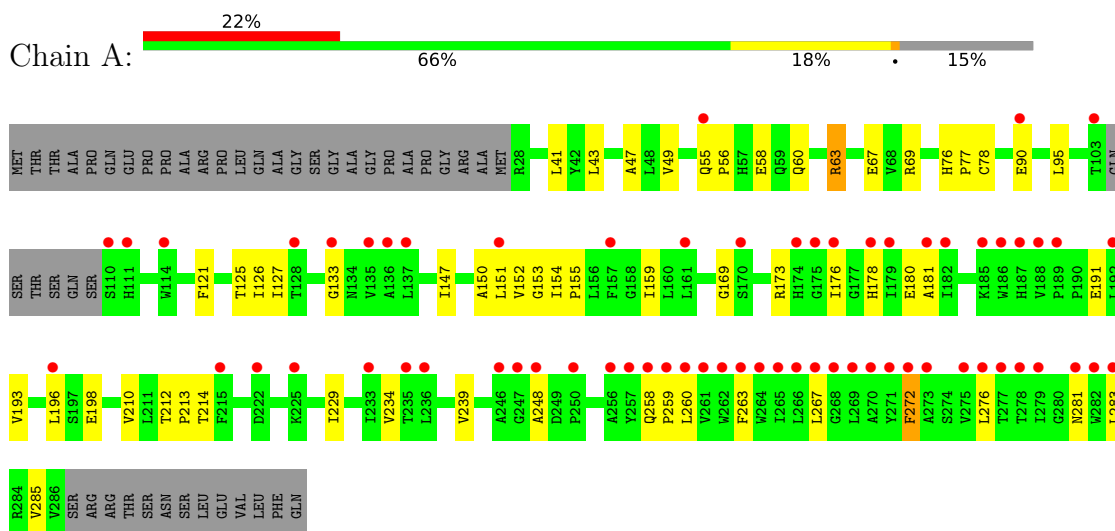
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	51	Total 51	O 51	0	0
6	F	43	Total 43	O 43	0	0
6	G	39	Total 39	O 39	0	0

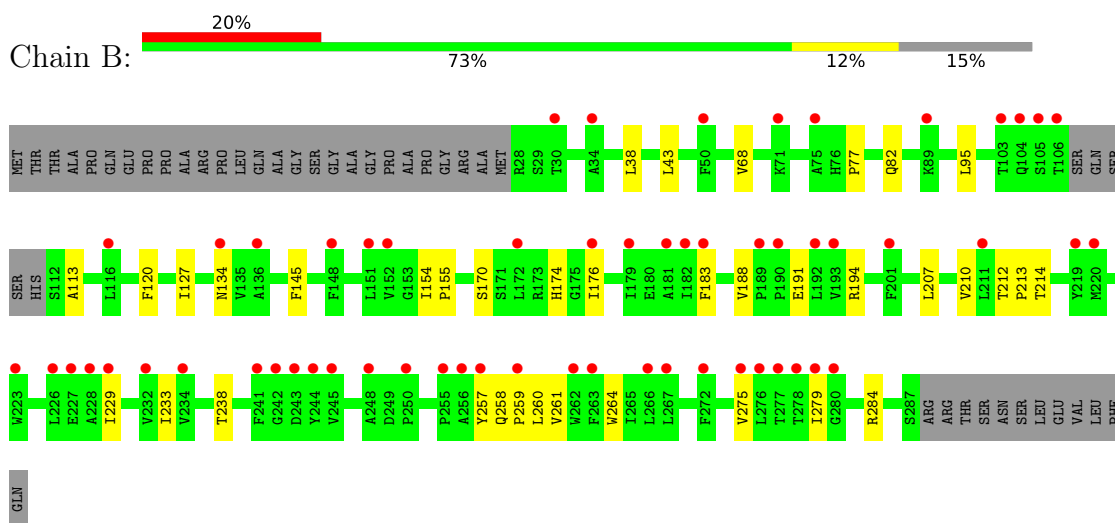
3 Residue-property plots [i](#)

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.

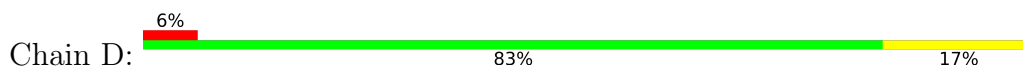
- Molecule 1: Isoform 2 of Potassium channel subfamily K member 4

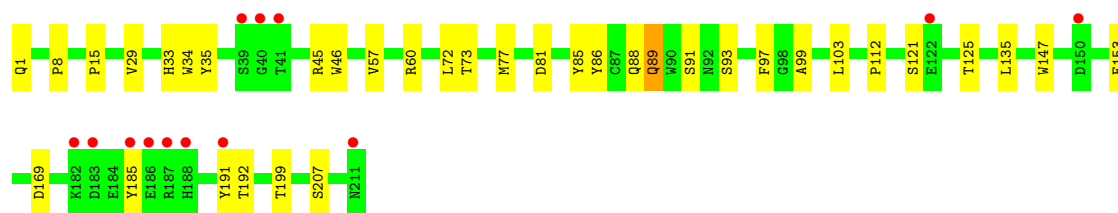


- Molecule 1: Isoform 2 of Potassium channel subfamily K member 4

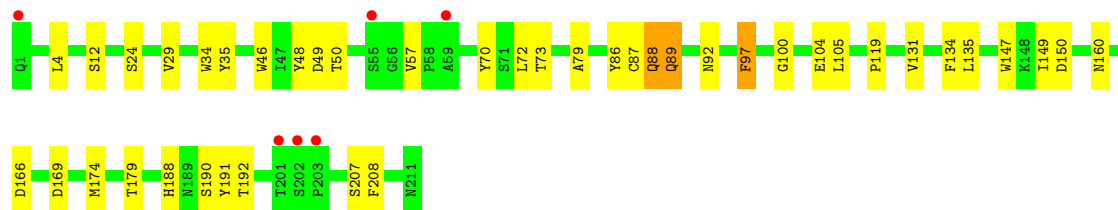
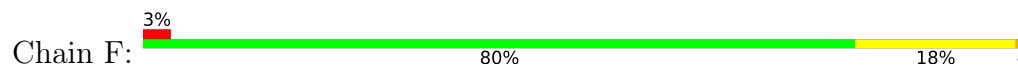


- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN

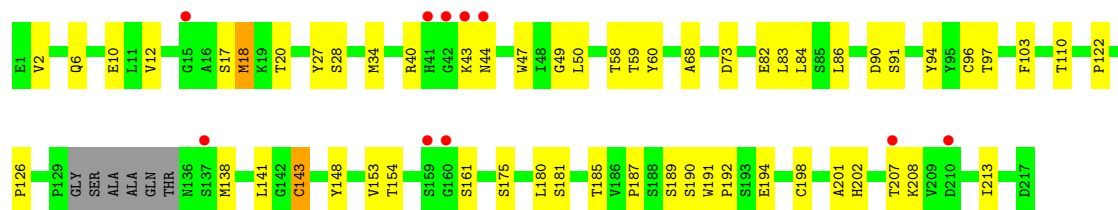




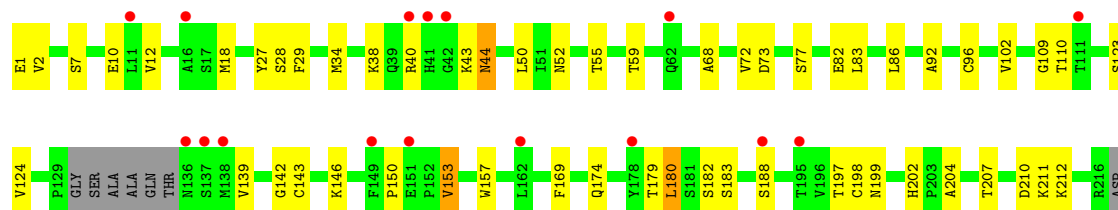
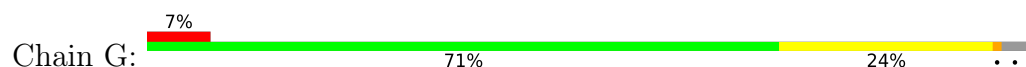
● Molecule 2: ANTI-TRAACK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



● Molecule 3: ANTI-TRAACK ANTIBODY 13E9 FAB FRAGMENT HEAVY CHAIN



● Molecule 3: ANTI-TRAACK 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	80.23Å 136.53Å 95.28Å 90.00° 94.54° 90.00°	Depositor
Resolution (Å)	47.54 – 2.77 47.54 – 2.77	Depositor EDS
% Data completeness (in resolution range)	68.6 (47.54-2.77) 68.6 (47.54-2.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.201 , 0.243 0.207 , 0.249	Depositor DCC
R_{free} test set	1755 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10651	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.08	1/2017 (0.0%)	1.67	10/2750 (0.4%)
1	B	1.10	1/2035 (0.0%)	1.69	8/2774 (0.3%)
2	D	1.08	1/1655 (0.1%)	1.35	2/2247 (0.1%)
2	F	1.14	0/1655	1.37	2/2247 (0.1%)
3	E	1.06	1/1656 (0.1%)	1.35	1/2260 (0.0%)
3	G	1.08	0/1647	1.37	3/2249 (0.1%)
All	All	1.09	4/10665 (0.0%)	1.49	26/14527 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	112	PRO	C-O	-5.55	1.17	1.23
3	E	126	PRO	C-O	-5.52	1.18	1.23
1	A	77	PRO	C-O	-5.24	1.17	1.24
1	B	77	PRO	C-O	-5.00	1.17	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	109	GLY	CA-C-O	-7.80	116.85	122.23
3	E	161	SER	N-CA-C	-6.15	105.26	112.89
1	B	176	ILE	CA-C-N	6.14	126.93	119.99
1	B	176	ILE	C-N-CA	6.14	126.93	119.99
2	F	100	GLY	CA-C-O	-5.72	118.50	122.22
2	F	97	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	95	LEU	CA-C-N	5.62	126.33	120.03
1	B	95	LEU	C-N-CA	5.62	126.33	120.03
1	A	95	LEU	CA-C-N	5.42	126.10	120.03
1	A	95	LEU	C-N-CA	5.42	126.10	120.03
1	A	153	GLY	CA-C-N	5.38	124.63	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	GLY	C-N-CA	5.38	124.63	120.33
3	G	153	VAL	CA-C-O	-5.24	116.11	121.67
2	D	8	PRO	CA-C-N	5.15	127.43	120.38
2	D	8	PRO	C-N-CA	5.15	127.43	120.38
1	B	174	HIS	CA-C-N	5.12	125.52	119.94
1	B	174	HIS	C-N-CA	5.12	125.52	119.94
3	G	169	PHE	CB-CA-C	5.07	116.71	109.11
1	A	133	GLY	CA-C-N	5.06	127.77	120.38
1	A	133	GLY	C-N-CA	5.06	127.77	120.38
1	A	169	GLY	CA-C-N	5.02	126.96	120.44
1	A	169	GLY	C-N-CA	5.02	126.96	120.44
1	A	67	GLU	CB-CG-CD	5.02	121.13	112.60
1	A	239	VAL	N-CA-C	-5.00	105.83	110.53
1	B	170	SER	CA-C-N	5.00	126.94	120.44
1	B	170	SER	C-N-CA	5.00	126.94	120.44

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	1985	49	0
1	B	1985	0	2007	28	0
2	D	1616	0	1542	28	0
2	F	1616	0	1542	35	0
3	E	1614	0	1586	41	1
3	G	1605	0	1582	46	1
4	A	5	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	31	0	0	4	0
6	B	38	0	0	1	0
6	D	35	0	0	1	0
6	E	51	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	43	0	0	1	0
6	G	39	0	0	0	0
All	All	10651	0	10244	207	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 10.

All (207) 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)
3:G:198:CYS:O	3:G:198:CYS:SG	2.36	0.83
2:D:99:ALA:HA	3:E:44:ASN:HB3	1.61	0.81
1:A:69:ARG:HD2	6:A:408:HOH:O	1.81	0.80
1:A:263:PHE:CZ	1:A:267:LEU:HD11	2.15	0.80
2:D:35:TYR:CD1	2:D:45:ARG:HA	2.18	0.78
3:G:199:ASN:HD22	3:G:210:ASP:CG	1.93	0.76
3:G:40:ARG:NH1	3:G:43:LYS:HE3	2.00	0.76
2:D:88:GLN:HB3	2:D:97:PHE:CD1	2.21	0.75
2:F:131:VAL:HG12	2:F:147:TRP:CH2	2.24	0.73
2:D:35:TYR:HD1	2:D:45:ARG:HA	1.54	0.72
3:E:10:GLU:OE2	6:E:301:HOH:O	2.09	0.70
3:G:199:ASN:ND2	3:G:210:ASP:CG	2.51	0.69
3:G:12:VAL:HG21	3:G:86:LEU:HD12	1.75	0.69
2:F:79:ALA:HA	2:F:105:LEU:HD11	1.77	0.66
2:F:88:GLN:HB3	2:F:97:PHE:CD1	2.30	0.66
3:G:1:GLU:HG3	3:G:1:GLU:O	1.94	0.66
1:A:248:ALA:HA	1:A:258:GLN:O	1.96	0.65
1:A:212:THR:HB	1:A:213:PRO:HD3	1.79	0.65
2:F:49:ASP:O	2:F:50:THR:HG22	1.97	0.65
2:D:29:VAL:HG11	2:D:89:GLN:HG3	1.78	0.64
2:F:150:ASP:HA	2:F:190:SER:HG	1.62	0.64
3:E:208:LYS:NZ	6:E:303:HOH:O	2.30	0.64
1:A:76:HIS:CE1	6:A:415:HOH:O	2.51	0.63
3:G:2:VAL:HG13	3:G:27:TYR:CD2	2.32	0.63
1:A:258:GLN:HB2	1:A:259:PRO:HD3	1.80	0.63
1:A:272:PHE:O	1:A:276:LEU:HD23	1.98	0.62
3:E:12:VAL:HG21	3:E:86:LEU:CD1	2.29	0.62
2:F:150:ASP:HA	2:F:190:SER:OG	1.99	0.62
2:F:35:TYR:HE1	2:F:88:GLN:HG2	1.65	0.61
2:F:35:TYR:CE1	2:F:88:GLN:HG2	2.36	0.61
3:G:38:LYS:HE2	3:G:40:ARG:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLU:HG2	1:A:193:VAL:HG12	1.84	0.59
1:A:41:LEU:C	1:A:41:LEU:HD13	2.28	0.58
3:G:180:LEU:HD12	3:G:180:LEU:C	2.28	0.58
1:B:207:LEU:O	1:B:212:THR:OG1	2.20	0.58
3:E:34:MET:CE	3:E:96:CYS:HB2	2.33	0.58
3:G:44:ASN:N	3:G:44:ASN:OD1	2.36	0.58
3:E:202:HIS:HB3	3:E:207:THR:HG22	1.84	0.58
1:A:49:VAL:HG11	1:B:145:PHE:CE1	2.38	0.57
1:B:38:LEU:C	1:B:38:LEU:HD23	2.29	0.57
3:E:34:MET:HE2	3:E:96:CYS:HB2	1.85	0.57
2:D:185:TYR:HA	2:D:191:TYR:OH	2.04	0.57
2:D:81:ASP:O	2:D:103:LEU:HD23	2.04	0.57
3:E:138:MET:HE3	3:E:185:THR:HG22	1.86	0.57
2:F:166:ASP:HB3	2:F:169:ASP:OD2	2.05	0.57
1:A:263:PHE:CE2	1:A:267:LEU:HD11	2.39	0.57
3:G:40:ARG:HG2	3:G:92:ALA:HB2	1.87	0.57
2:D:1:GLN:HA	2:D:1:GLN:OE1	2.05	0.56
3:E:50:LEU:C	3:E:50:LEU:HD12	2.29	0.56
3:E:180:LEU:C	3:E:180:LEU:HD12	2.30	0.56
1:A:263:PHE:CE2	1:A:267:LEU:CD1	2.89	0.56
3:E:50:LEU:HG	3:E:59:THR:HG22	1.87	0.56
2:F:29:VAL:O	2:F:70:TYR:OH	2.20	0.56
1:B:257:TYR:O	1:B:260:LEU:HB3	2.06	0.56
3:E:18:MET:HE2	3:E:20:THR:HB	1.88	0.56
2:F:46:TRP:O	2:F:57:VAL:HG21	2.06	0.55
1:A:260:LEU:O	1:A:263:PHE:N	2.34	0.55
2:F:149:ILE:HG13	2:F:149:ILE:O	2.05	0.55
1:B:183:PHE:O	1:B:188:VAL:HG22	2.07	0.55
2:F:149:ILE:HG22	2:F:191:TYR:CE2	2.42	0.55
1:B:212:THR:HB	1:B:213:PRO:HD3	1.88	0.55
1:A:78:CYS:HB2	6:A:414:HOH:O	2.07	0.54
3:G:34:MET:CE	3:G:96:CYS:HB2	2.37	0.54
1:A:90:GLU:OE1	1:B:68:VAL:HG22	2.08	0.54
1:A:214:THR:HG21	1:A:229:ILE:HG12	1.90	0.53
2:F:192:THR:HG22	2:F:207:SER:OG	2.08	0.53
1:A:283:LEU:C	1:A:283:LEU:HD13	2.33	0.53
1:A:147:ILE:HG23	1:B:233:ILE:HD13	1.91	0.53
2:F:134:PHE:CE2	3:G:183:SER:CB	2.91	0.53
3:G:153:VAL:CG2	3:G:180:LEU:HD21	2.38	0.53
3:E:175:SER:HB3	6:E:343:HOH:O	2.08	0.52
1:A:178:HIS:O	1:A:181:ALA:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:TYR:CE1	2:D:45:ARG:HA	2.44	0.52
3:E:187:PRO:O	3:E:190:SER:HB2	2.10	0.52
1:B:82:GLN:HG3	3:G:59:THR:HG21	1.91	0.52
2:F:135:LEU:HD12	2:F:135:LEU:N	2.25	0.52
3:E:12:VAL:HG21	3:E:86:LEU:HD13	1.91	0.52
3:E:12:VAL:HG21	3:E:86:LEU:HD12	1.91	0.51
3:E:191:TRP:C	6:E:316:HOH:O	2.53	0.51
3:G:197:THR:HG22	3:G:212:LYS:HA	1.91	0.51
2:D:72:LEU:C	2:D:72:LEU:HD23	2.36	0.51
3:E:90:ASP:O	3:E:94:TYR:OH	2.22	0.51
1:A:272:PHE:HD1	1:A:276:LEU:HD21	1.76	0.51
2:D:88:GLN:CB	2:D:97:PHE:CD1	2.92	0.51
3:E:68:ALA:HA	3:E:82:GLU:O	2.11	0.50
2:F:131:VAL:HG12	2:F:147:TRP:CZ3	2.45	0.50
2:F:179:THR:OG1	3:G:174:GLN:NE2	2.44	0.50
2:F:34:TRP:CZ3	2:F:87:CYS:HB3	2.47	0.50
2:F:119:PRO:HD3	2:F:131:VAL:HG22	1.93	0.50
3:E:2:VAL:HG13	3:E:27:TYR:CD2	2.46	0.50
2:F:72:LEU:HD23	2:F:73:THR:N	2.26	0.49
3:E:83:LEU:HB3	3:E:86:LEU:HD21	1.94	0.48
2:D:192:THR:HG22	2:D:207:SER:OG	2.14	0.48
3:G:50:LEU:C	3:G:50:LEU:HD12	2.38	0.48
3:E:143:CYS:O	3:E:181:SER:HA	2.13	0.48
1:A:154:ILE:N	1:A:155:PRO:HD2	2.28	0.48
1:A:260:LEU:C	1:A:260:LEU:HD23	2.39	0.48
3:E:50:LEU:HG	3:E:59:THR:CG2	2.44	0.48
1:A:272:PHE:O	1:A:276:LEU:CD2	2.61	0.48
1:B:258:GLN:HB3	1:B:259:PRO:HD3	1.94	0.48
3:G:146:LYS:HB3	3:G:179:THR:HG23	1.96	0.47
3:E:154:THR:OG1	3:E:201:ALA:HB3	2.14	0.47
2:F:134:PHE:CD2	3:G:183:SER:HB2	2.50	0.47
1:A:260:LEU:O	1:A:263:PHE:HB3	2.15	0.47
2:F:131:VAL:CG1	2:F:147:TRP:CZ3	2.98	0.47
3:G:150:PRO:HD2	3:G:204:ALA:CB	2.45	0.47
3:E:40:ARG:NH1	3:E:91:SER:O	2.41	0.47
2:D:46:TRP:CD2	2:D:57:VAL:HG22	2.51	0.46
1:A:55:GLN:N	1:A:56:PRO:HD2	2.30	0.46
1:A:159:ILE:HG21	1:B:284:ARG:HH11	1.80	0.46
2:D:60:ARG:NH1	2:D:81:ASP:OD1	2.49	0.46
2:F:72:LEU:HD23	2:F:72:LEU:C	2.40	0.46
1:A:58:GLU:OE2	1:B:113:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLN:OE1	1:A:63:ARG:NH2	2.48	0.46
3:G:83:LEU:HB3	3:G:86:LEU:HD21	1.98	0.46
1:B:210:VAL:O	1:B:214:THR:HG23	2.16	0.46
1:B:214:THR:HG21	1:B:229:ILE:CG1	2.45	0.46
1:A:272:PHE:CD1	1:A:276:LEU:HD21	2.51	0.46
3:E:47:TRP:CH2	3:E:49:GLY:HA2	2.52	0.45
1:B:134:ASN:HA	6:B:429:HOH:O	2.16	0.45
3:E:122:PRO:HB3	3:E:148:TYR:HB3	1.98	0.45
2:F:134:PHE:CE2	3:G:183:SER:HB3	2.51	0.45
1:A:214:THR:HG21	1:A:229:ILE:CG1	2.45	0.45
1:B:38:LEU:HD23	1:B:38:LEU:O	2.17	0.45
1:B:261:VAL:O	1:B:264:TRP:HB3	2.16	0.45
1:B:154:ILE:N	1:B:155:PRO:HD2	2.32	0.45
2:D:33:HIS:HD2	2:D:88:GLN:NE2	2.15	0.45
3:G:52:ASN:HB3	3:G:55:THR:OG1	2.17	0.45
3:G:12:VAL:CG2	3:G:86:LEU:HD12	2.46	0.45
2:D:35:TYR:O	2:D:85:TYR:HA	2.17	0.45
1:B:260:LEU:C	1:B:260:LEU:HD23	2.41	0.44
3:G:146:LYS:CB	3:G:179:THR:HG23	2.48	0.44
3:G:2:VAL:HG13	3:G:27:TYR:CE2	2.52	0.44
1:A:198:GLU:HA	1:A:198:GLU:OE1	2.17	0.44
3:G:153:VAL:HG22	3:G:180:LEU:HD21	1.99	0.44
2:D:99:ALA:HA	3:E:44:ASN:CB	2.41	0.44
3:G:29:PHE:CE1	3:G:72:VAL:HB	2.53	0.44
2:D:72:LEU:HD23	2:D:73:THR:N	2.33	0.43
3:E:97:THR:OG1	3:E:103:PHE:HB3	2.18	0.43
2:F:48:TYR:HB3	3:G:102:VAL:HG21	1.99	0.43
2:F:89:GLN:CD	2:F:89:GLN:C	2.86	0.43
1:B:275:VAL:O	1:B:279:ILE:HG22	2.18	0.43
1:A:281:ASN:O	1:A:285:VAL:HG23	2.18	0.43
2:D:15:PRO:HA	2:D:77:MET:O	2.17	0.43
3:E:73:ASP:OD1	3:E:73:ASP:C	2.61	0.43
2:D:93:SER:HB3	6:D:334:HOH:O	2.18	0.43
3:E:141:LEU:HD22	3:E:213:ILE:HG21	2.00	0.43
3:G:139:VAL:HG23	3:G:188:SER:HA	2.00	0.43
2:F:4:LEU:HA	2:F:24:SER:O	2.18	0.43
3:E:28:SER:HB2	3:G:28:SER:HB2	2.01	0.43
3:G:157:TRP:CZ3	3:G:198:CYS:HB3	2.54	0.43
3:G:34:MET:HE1	3:G:96:CYS:HB2	2.00	0.43
1:A:55:GLN:N	1:A:56:PRO:CD	2.82	0.43
2:D:60:ARG:HD2	2:D:81:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:110:THR:O	3:G:110:THR:HG23	2.18	0.43
2:D:135:LEU:N	2:D:135:LEU:HD12	2.33	0.43
3:G:142:GLY:HA2	3:G:182:SER:O	2.19	0.43
1:A:152:VAL:O	1:A:152:VAL:HG12	2.19	0.42
1:A:43:LEU:HD21	1:B:127:ILE:HD13	2.01	0.42
1:A:127:ILE:CD1	1:B:43:LEU:HD21	2.49	0.42
3:G:68:ALA:HA	3:G:82:GLU:O	2.19	0.42
1:A:234:VAL:HG11	6:A:403:HOH:O	2.18	0.42
2:F:12:SER:HB3	2:F:104:GLU:CG	2.49	0.42
2:F:160:ASN:ND2	2:F:174:MET:HE1	2.35	0.42
3:G:124:VAL:HG12	3:G:211:LYS:CG	2.50	0.42
3:G:2:VAL:HG13	3:G:27:TYR:HD2	1.81	0.42
2:D:147:TRP:O	2:D:153:GLU:HA	2.20	0.42
3:G:12:VAL:HG21	3:G:86:LEU:CD1	2.46	0.42
1:A:173:ARG:HA	1:A:176:ILE:HD12	2.02	0.42
1:B:284:ARG:NE	1:B:284:ARG:HA	2.35	0.42
2:D:46:TRP:O	2:D:57:VAL:HG21	2.20	0.42
3:E:58:THR:HG21	3:E:60:TYR:CZ	2.54	0.42
3:G:29:PHE:HB2	3:G:77:SER:HB2	2.01	0.42
1:A:151:LEU:HD12	1:A:151:LEU:HA	1.92	0.41
1:A:191:GLU:OE1	1:A:191:GLU:N	2.29	0.41
1:A:210:VAL:O	1:A:214:THR:HG23	2.21	0.41
2:F:191:TYR:HB2	2:F:208:PHE:CZ	2.55	0.41
2:D:34:TRP:HA	2:D:86:TYR:O	2.21	0.41
3:G:29:PHE:CD1	3:G:77:SER:HA	2.55	0.41
1:A:263:PHE:CE2	1:A:267:LEU:HD12	2.55	0.41
3:E:2:VAL:HG13	3:E:27:TYR:HD2	1.85	0.41
1:A:126:ILE:CG2	1:A:150:ALA:HB2	2.51	0.41
2:F:134:PHE:CD2	3:G:183:SER:CB	3.03	0.41
2:F:34:TRP:HA	2:F:86:TYR:O	2.20	0.41
1:A:43:LEU:HD21	1:B:127:ILE:CD1	2.50	0.41
2:F:134:PHE:CE2	3:G:183:SER:HB2	2.55	0.41
3:G:202:HIS:HB3	3:G:207:THR:HB	2.03	0.41
3:E:6:GLN:HE22	3:E:110:THR:HG22	1.86	0.41
3:E:50:LEU:CG	3:E:59:THR:HG22	2.49	0.41
3:E:148:TYR:CE2	3:E:153:VAL:HG13	2.56	0.41
3:E:191:TRP:CG	3:E:192:PRO:HA	2.56	0.41
1:A:248:ALA:HA	1:A:258:GLN:C	2.45	0.41
1:B:194:ARG:CZ	1:B:194:ARG:HB2	2.51	0.41
3:E:17:SER:HB2	3:E:84:LEU:HD23	2.02	0.41
2:D:121:SER:O	2:D:125:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:73:ASP:C	3:G:73:ASP:OD1	2.64	0.40
3:E:50:LEU:CD1	3:E:59:THR:HG22	2.50	0.40
3:E:58:THR:HG21	3:E:60:TYR:OH	2.21	0.40
1:A:47:ALA:HB2	1:B:120:PHE:HA	2.03	0.40
2:D:169:ASP:C	2:D:169:ASP:OD1	2.64	0.40
1:A:121:PHE:O	1:A:125:THR:HG23	2.22	0.40
1:A:248:ALA:HB1	1:A:259:PRO:HA	2.04	0.40
2:F:188:HIS:CE1	6:F:311:HOH:O	2.74	0.40
1:A:147:ILE:O	1:A:151:LEU:HB2	2.21	0.40
1:B:191:GLU:HA	1:B:194:ARG:HE	1.87	0.40
1:B:214:THR:HG21	1:B:229:ILE:HG12	2.04	0.40
2:D:89:GLN:HG2	2:D:91:SER:H	1.86	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)
3:E:194:GLU:OE2	3:G:10:GLU:OE1[2_556]	1.72	0.48

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%)	235 (94%)	14 (6%)	0	100	100
1	B	251/299 (84%)	245 (98%)	6 (2%)	0	100	100
2	D	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
2	F	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
3	E	207/217 (95%)	203 (98%)	4 (2%)	0	100	100
3	G	206/217 (95%)	200 (97%)	6 (3%)	0	100	100
All	All	1331/1454 (92%)	1286 (97%)	45 (3%)	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%)	202 (98%)	3 (2%)	57	81
1	B	209/243 (86%)	208 (100%)	1 (0%)	81	92
2	D	184/184 (100%)	182 (99%)	2 (1%)	65	85
2	F	184/184 (100%)	181 (98%)	3 (2%)	55	81
3	E	187/190 (98%)	182 (97%)	5 (3%)	39	71
3	G	186/190 (98%)	180 (97%)	6 (3%)	34	67
All	All	1155/1234 (94%)	1135 (98%)	20 (2%)	53	80

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	196	LEU
1	A	272	PHE
1	B	238	THR
2	D	89	GLN
2	D	199	THR
3	E	18	MET
3	E	43	LYS
3	E	143	CYS
3	E	189	SER
3	E	198	CYS
2	F	88	GLN
2	F	89	GLN
2	F	92	ASN
3	G	7	SER
3	G	18	MET
3	G	44	ASN
3	G	123	SER
3	G	143	CYS

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Mol	Chain	Res	Type
3	G	180	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	258	GLN
1	B	59	GLN
2	D	88	GLN
2	D	136	ASN
2	D	137	ASN
2	D	144	ASN
2	D	155	GLN
2	D	209	ASN
3	E	136	ASN
2	F	88	GLN
2	F	188	HIS
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 11 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	1.34	65 (25%) 1 1	46, 106, 174, 197	0
1	B	255/299 (85%)	1.25	59 (23%) 2 1	45, 107, 179, 199	0
2	D	211/211 (100%)	0.26	13 (6%) 26 21	38, 64, 104, 125	0
2	F	211/211 (100%)	0.21	6 (2%) 55 47	38, 64, 111, 127	0
3	E	211/217 (97%)	-0.05	10 (4%) 36 31	34, 55, 85, 124	0
3	G	210/217 (96%)	0.33	16 (7%) 20 16	37, 60, 96, 156	0
All	All	1351/1454 (92%)	0.60	169 (12%) 8 6	34, 71, 164, 199	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	TRP	8.0
2	D	187	ARG	7.0
3	G	136	ASN	6.9
1	A	263	PHE	6.8
1	A	269	LEU	6.7
1	B	276	LEU	6.2
2	F	201	THR	6.1
1	B	275	VAL	5.8
1	B	34	ALA	5.7
1	A	265	ILE	5.6
1	A	272	PHE	5.6
1	A	266	LEU	5.5
1	A	161	LEU	5.4
1	A	136	ALA	5.4
3	G	41	HIS	5.3
1	B	151	LEU	5.3
1	B	242	GLY	5.0
1	A	248	ALA	5.0
1	A	157	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	243	ASP	4.8
2	F	202	SER	4.8
1	B	262	TRP	4.7
3	G	151	GLU	4.6
1	B	152	VAL	4.5
1	A	178	HIS	4.4
1	B	267	LEU	4.4
1	A	247	GLY	4.4
1	A	179	ILE	4.4
1	B	75	ALA	4.3
3	G	178	TYR	4.3
2	F	1	GLN	4.2
1	A	270	ALA	4.2
1	A	273	ALA	4.2
1	B	228	ALA	4.1
1	A	110	SER	4.1
1	B	193	VAL	4.1
1	A	135	VAL	4.1
3	E	159	SER	4.0
2	D	211	ASN	4.0
2	D	183	ASP	3.9
1	A	268	GLY	3.9
1	A	103	THR	3.8
1	B	278	THR	3.6
1	B	257	TYR	3.6
1	B	266	LEU	3.6
1	A	259	PRO	3.6
1	B	104	GLN	3.6
2	D	150	ASP	3.5
1	A	256	ALA	3.5
3	G	137	SER	3.5
1	B	106	THR	3.5
1	A	267	LEU	3.4
1	B	219	TYR	3.4
1	B	248	ALA	3.4
1	A	186	TRP	3.4
1	A	137	LEU	3.4
1	A	222	ASP	3.4
1	B	192	LEU	3.3
1	A	264	TRP	3.3
1	B	244	TYR	3.3
1	B	89	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	176	ILE	3.3
1	A	276	LEU	3.2
1	A	278	THR	3.2
2	D	186	GLU	3.2
1	A	257	TYR	3.2
1	B	245	VAL	3.1
1	A	185	LYS	3.1
1	A	250	PRO	3.1
1	B	256	ALA	3.1
1	A	275	VAL	3.1
1	B	272	PHE	3.1
1	A	279	ILE	3.1
1	B	182	ILE	3.1
1	B	263	PHE	3.1
1	A	260	LEU	3.0
1	A	235	THR	3.0
1	A	271	TYR	3.0
1	B	190	PRO	3.0
3	G	40	ARG	3.0
3	E	41	HIS	2.9
1	B	103	THR	2.9
3	G	195	THR	2.9
2	D	188	HIS	2.9
1	A	133	GLY	2.9
3	G	149	PHE	2.9
2	D	122	GLU	2.8
1	B	172	LEU	2.8
1	B	148	PHE	2.8
1	B	241	PHE	2.8
1	B	277	THR	2.8
1	A	281	ASN	2.7
1	B	176	ILE	2.7
3	G	11	LEU	2.7
1	A	90	GLU	2.7
1	A	175	GLY	2.7
1	A	282	TRP	2.7
1	B	280	GLY	2.7
3	E	160	GLY	2.7
1	B	181	ALA	2.7
1	A	192	LEU	2.6
1	B	211	LEU	2.6
2	D	182	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	41	THR	2.6
3	E	207	THR	2.6
3	G	42	GLY	2.5
1	A	170	SER	2.5
1	B	179	ILE	2.5
2	D	40	GLY	2.5
1	A	182	ILE	2.5
1	B	223	TRP	2.5
1	B	279	ILE	2.5
1	A	55	GLN	2.5
1	B	234	VAL	2.5
1	A	181	ALA	2.5
1	A	187	HIS	2.5
1	A	261	VAL	2.5
1	A	174	HIS	2.4
3	E	43	LYS	2.4
1	B	255	PRO	2.4
1	A	283	LEU	2.4
1	A	128	THR	2.4
1	B	71	LYS	2.4
3	E	210	ASP	2.3
1	A	151	LEU	2.3
1	A	196	LEU	2.3
3	G	188	SER	2.3
1	B	250	PRO	2.3
1	A	236	LEU	2.3
1	B	105	SER	2.3
2	D	39	SER	2.3
1	A	258	GLN	2.3
1	B	30	THR	2.3
2	D	185	TYR	2.3
1	B	227	GLU	2.3
1	B	259	PRO	2.3
2	F	55	SER	2.3
3	E	15	GLY	2.3
3	E	137	SER	2.2
1	A	246	ALA	2.2
1	B	136	ALA	2.2
3	G	16	ALA	2.2
1	A	189	PRO	2.2
1	B	220	MET	2.2
1	A	188	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	229	ILE	2.2
1	B	50	PHE	2.2
2	F	59	ALA	2.1
3	E	44	ASN	2.1
2	D	191	TYR	2.1
3	G	138	MET	2.1
3	E	42	GLY	2.1
3	G	162	LEU	2.1
1	A	111	HIS	2.1
1	A	114	TRP	2.1
1	A	277	THR	2.1
1	B	189	PRO	2.1
1	B	116	LEU	2.1
1	B	232	VAL	2.1
1	B	183	PHE	2.1
1	A	215	PHE	2.1
1	B	201	PHE	2.1
1	A	225	LYS	2.0
1	B	226	LEU	2.0
3	G	62	GLN	2.0
1	A	233	ILE	2.0
2	F	203	PRO	2.0
3	G	111	THR	2.0
1	B	134	ASN	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](#)

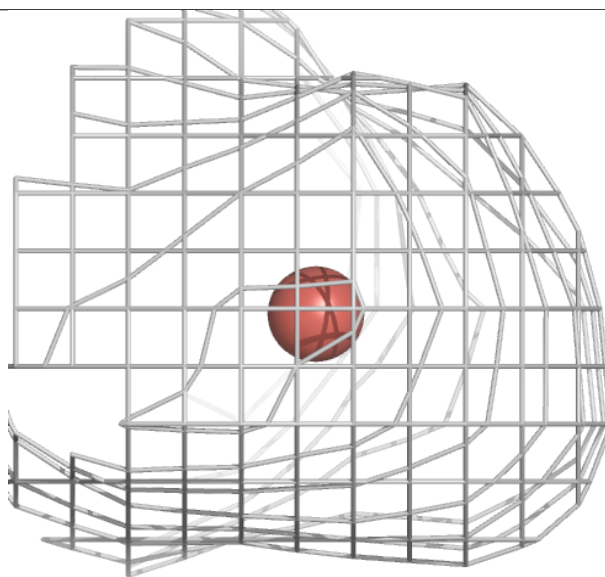
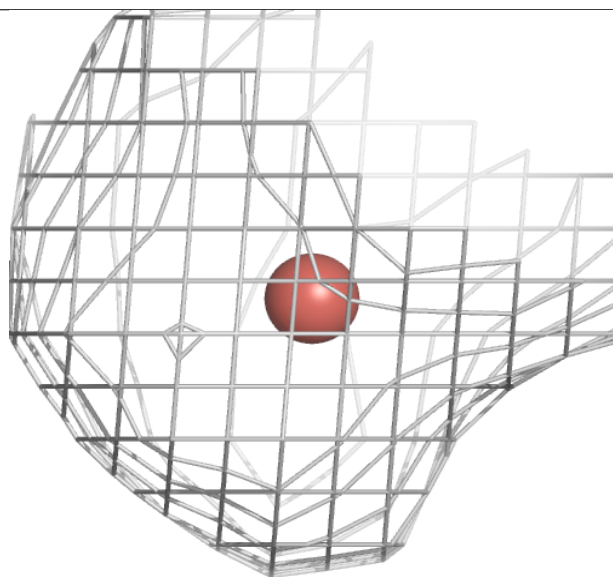
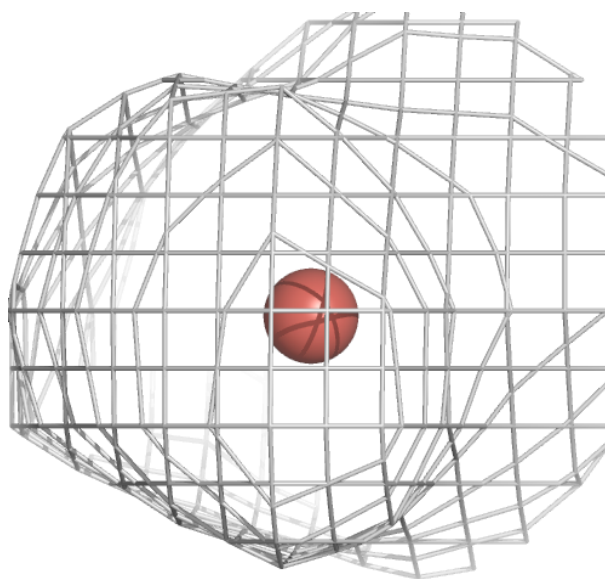
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	TL	A	306	1/1	0.71	0.14	220,220,220,220	0
4	TL	B	303	1/1	0.82	0.10	245,245,245,245	0
4	TL	A	307	1/1	0.87	0.14	225,225,225,225	0
4	TL	B	302	1/1	0.91	0.08	183,183,183,183	0
5	CA	A	304	1/1	0.94	0.09	102,102,102,102	0
5	CA	A	303	1/1	0.95	0.05	107,107,107,107	0
4	TL	A	302	1/1	0.99	0.02	88,88,88,88	0
4	TL	B	301	1/1	0.99	0.02	89,89,89,89	0
5	CA	G	301	1/1	0.99	0.03	63,63,63,63	0
4	TL	A	301	1/1	1.00	0.02	85,85,85,85	0
4	TL	A	305	1/1	1.00	0.01	88,88,88,88	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.

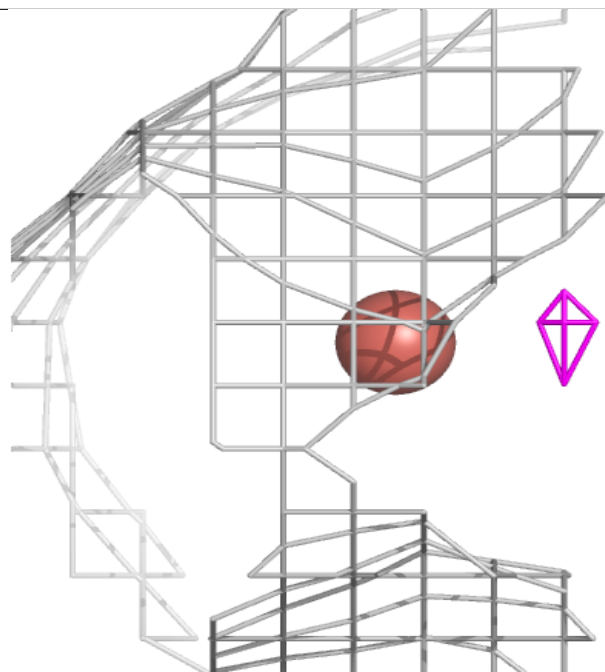
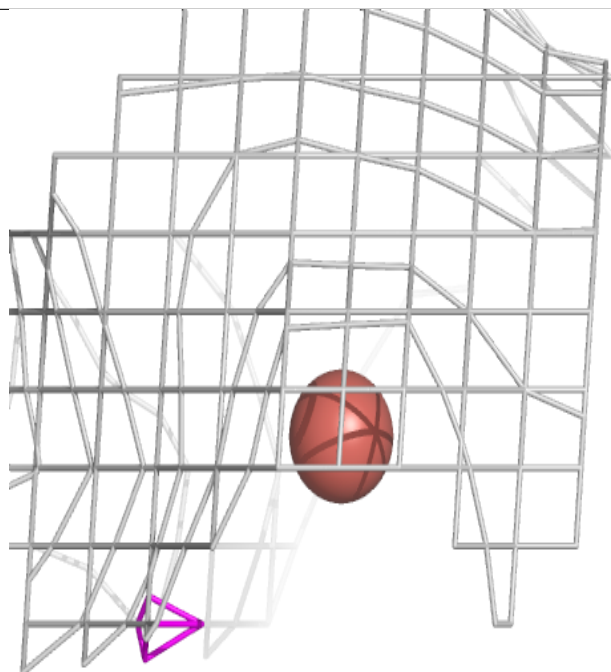
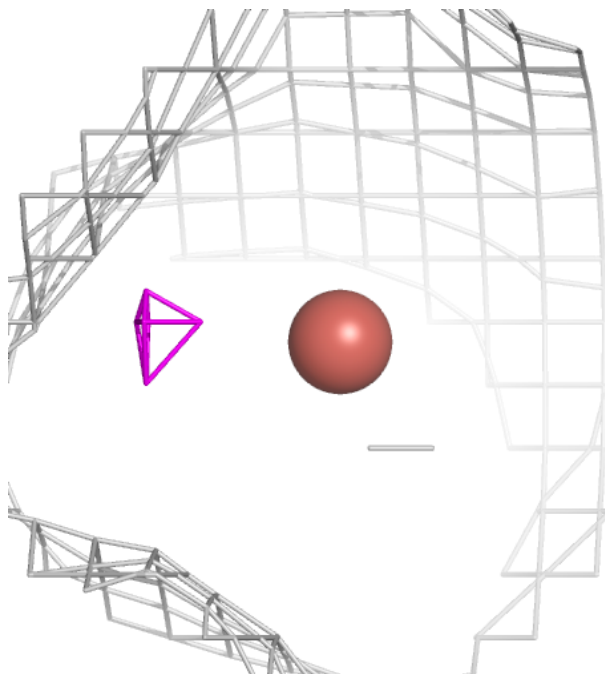
Electron density around TL A 306:

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



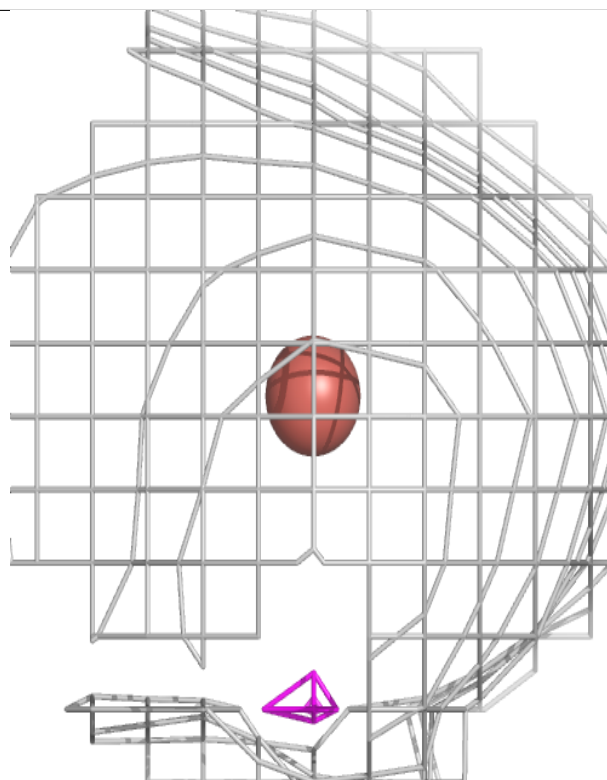
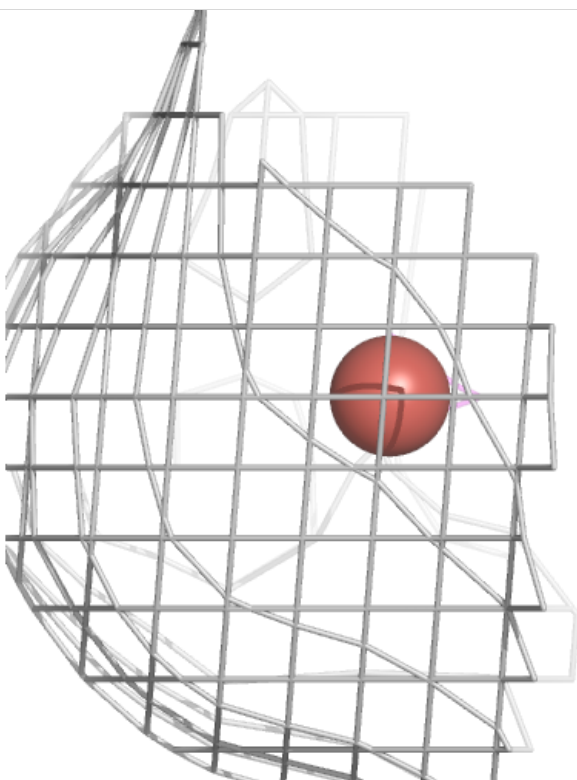
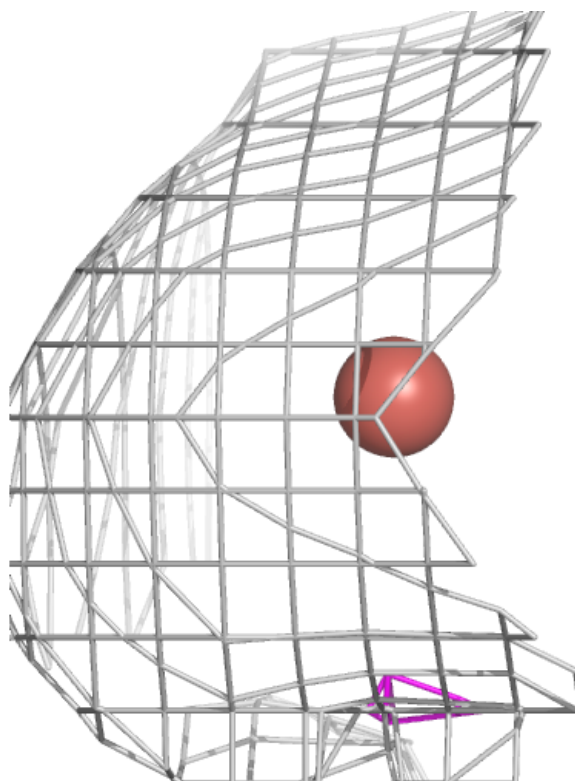
Electron density around TL B 303:

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



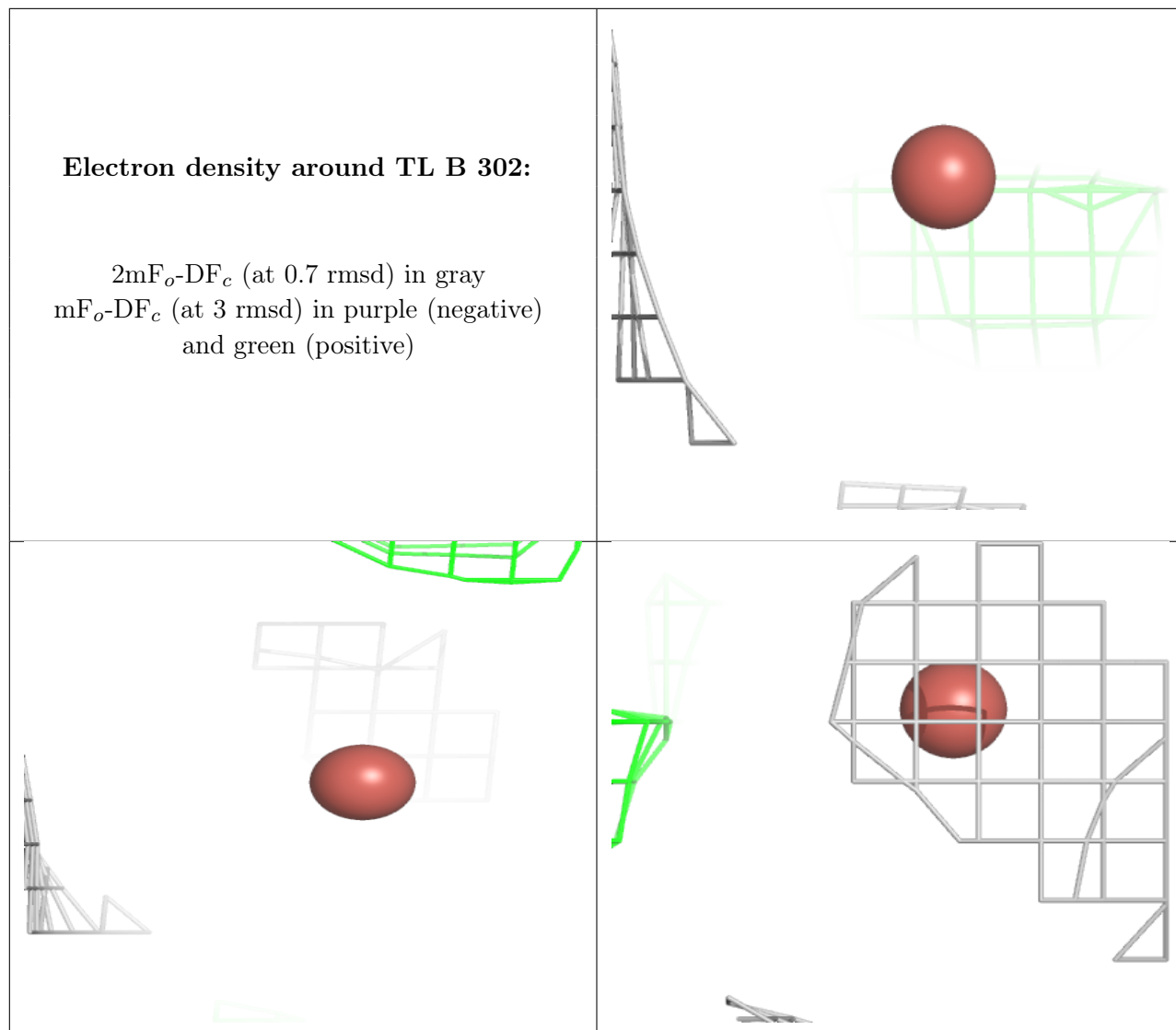
Electron density around TL A 307:

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



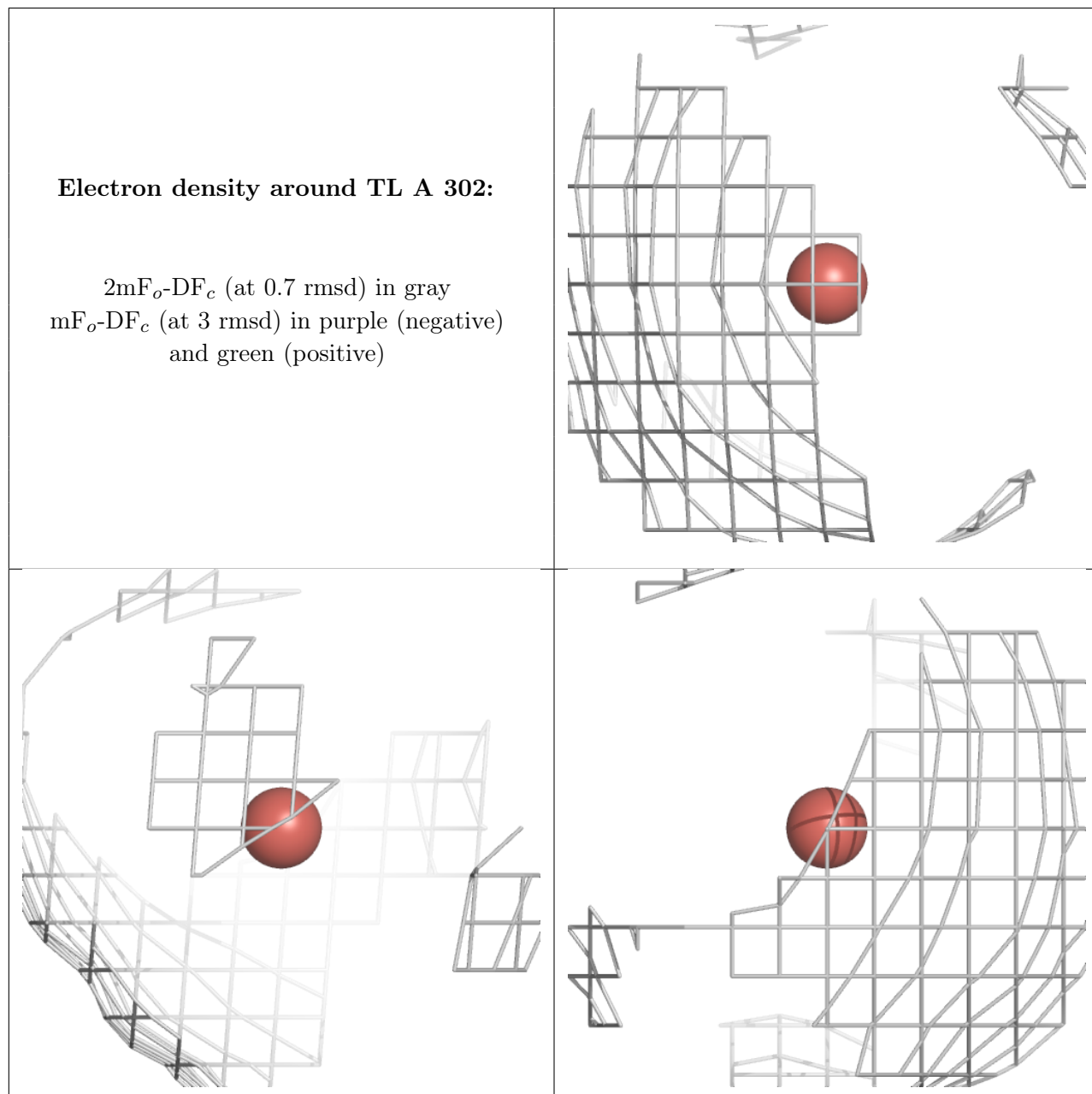
Electron density around TL B 302:

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



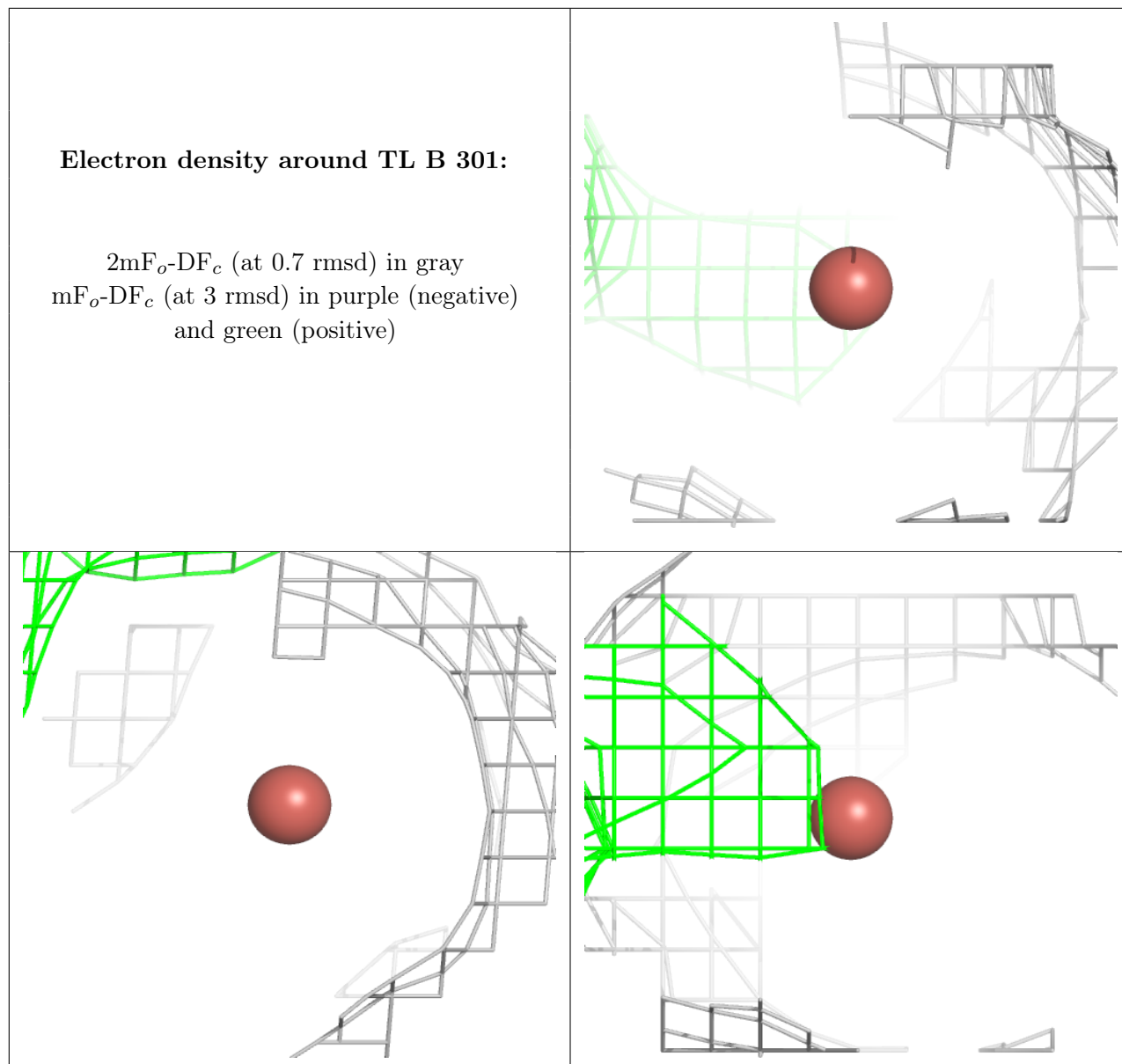
Electron density around TL A 302:

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



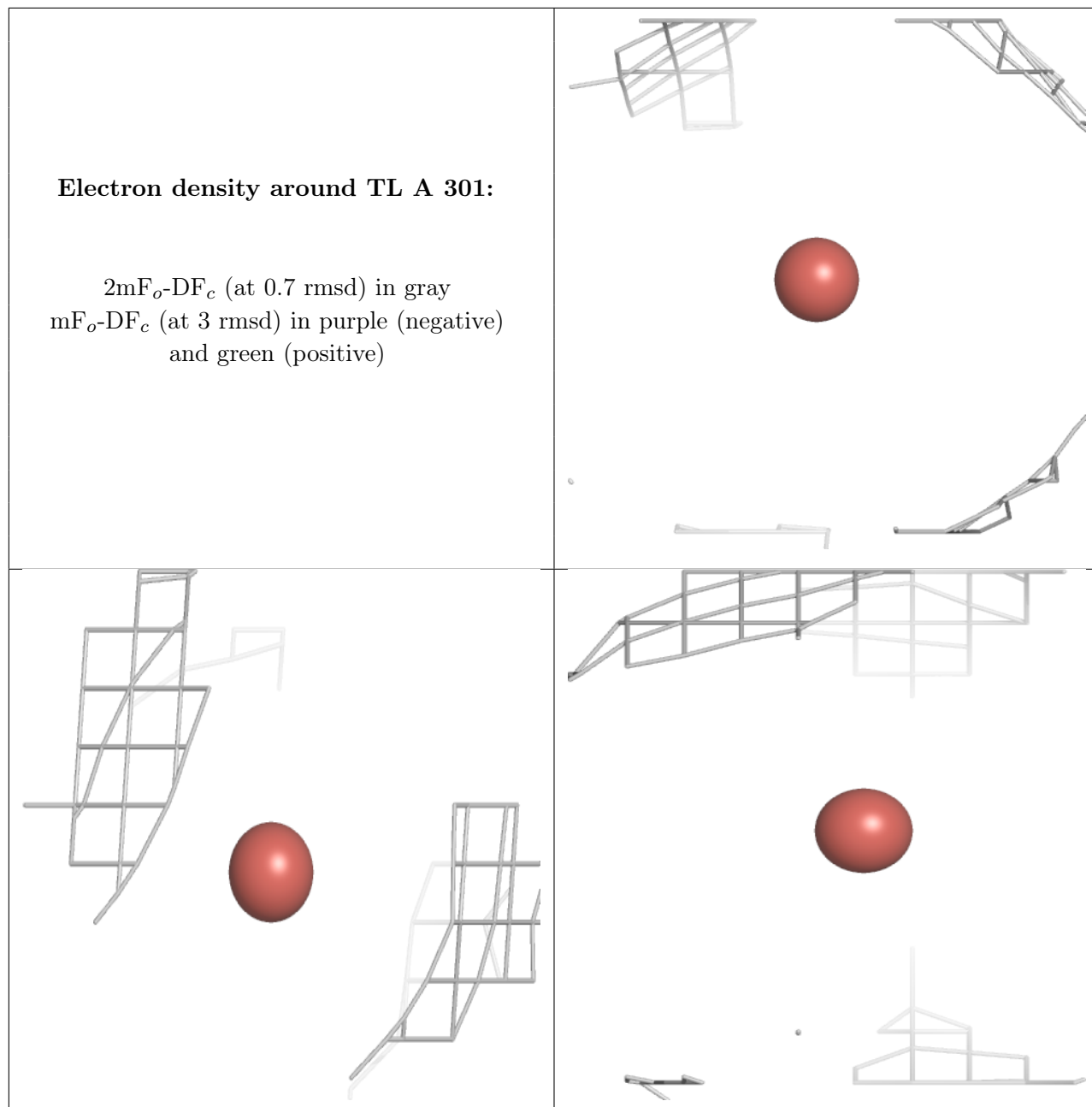
Electron density around TL B 301:

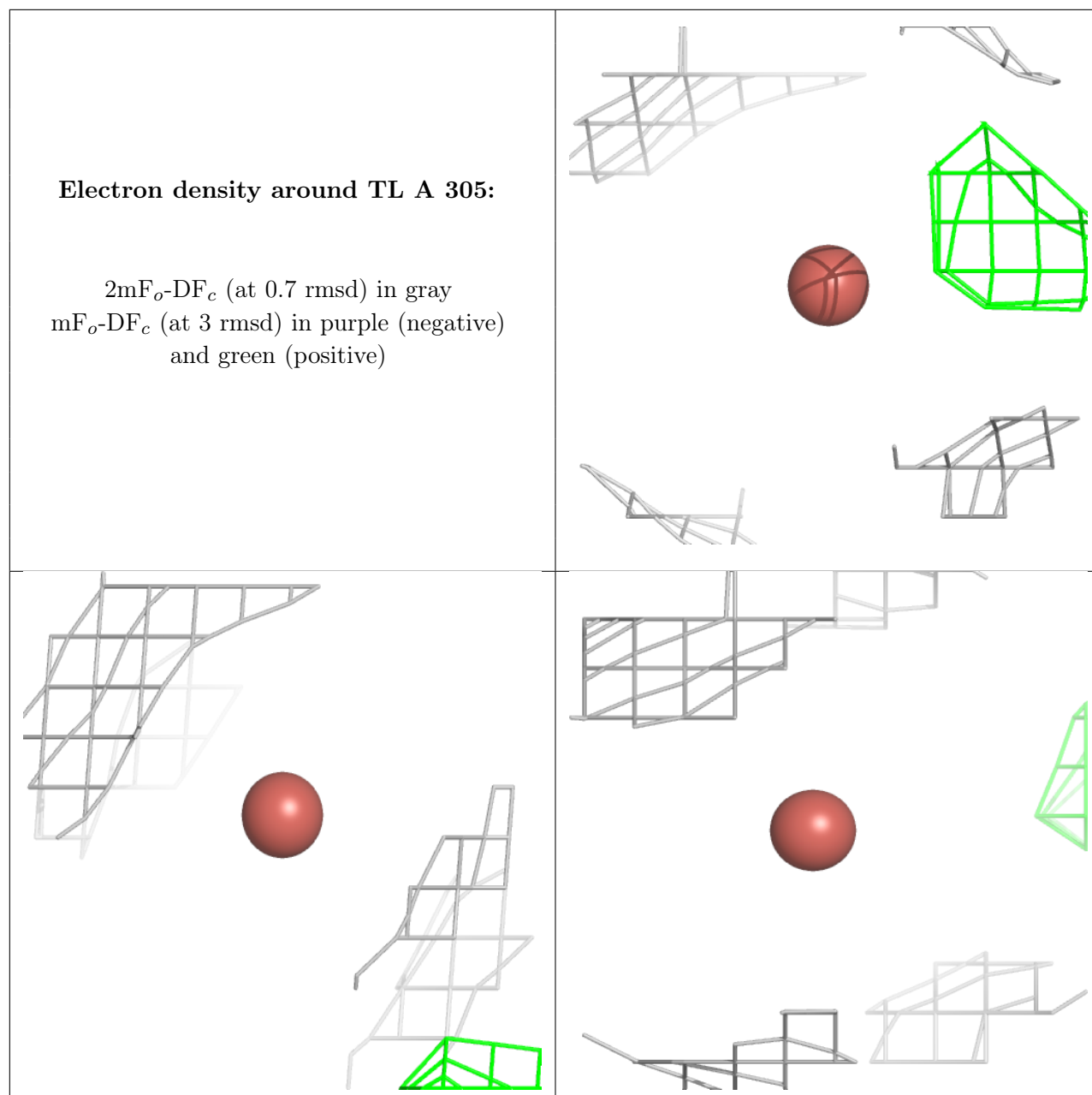
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TL 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.