Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 09:27 AM EDT

PDB ID	:	7LJA
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:

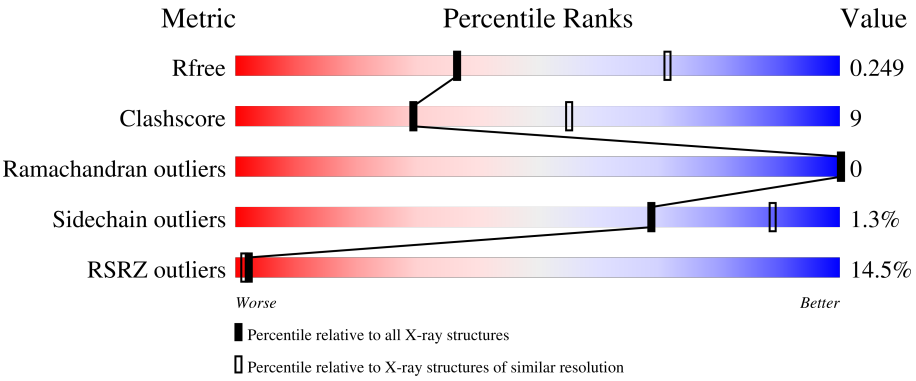
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.77 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}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	299	21% 68% 16% 15%
1	B	299	28% 75% 10% 15%
2	D	211	5% 84% 15%
2	F	211	6% 81% 18%
3	E	217	5% 75% 22%

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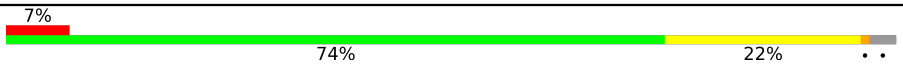
Mol	Chain	Length	Quality of chain
3	G	217	

2 Entry composition (i)

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 (three-letter code: 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 (three-letter code: 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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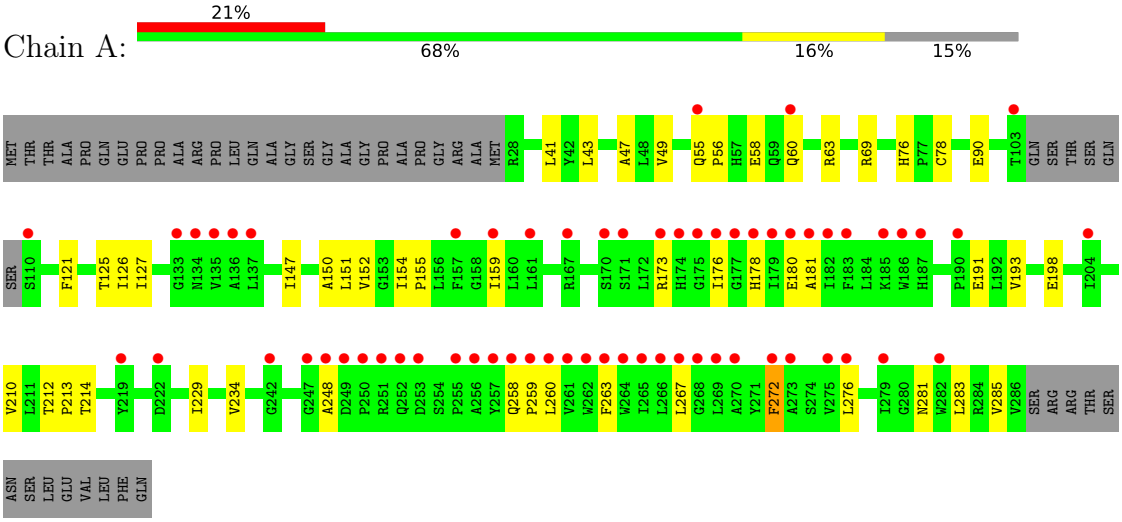
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	51	Total O 51 51	0	0
6	F	43	Total O 43 43	0	0
6	G	39	Total O 39 39	0	0

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.

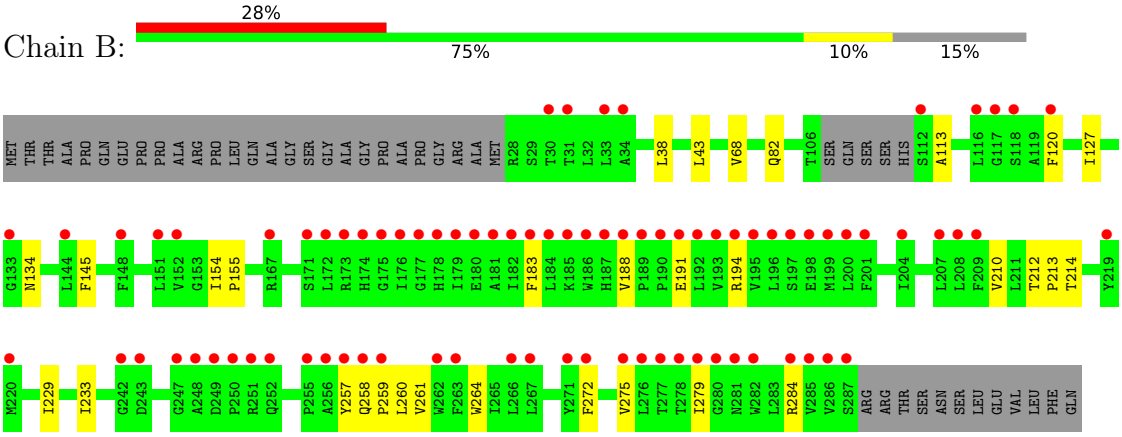
• Molecule 1: Isoform 2 of Potassium channel subfamily K member 4

Chain A:



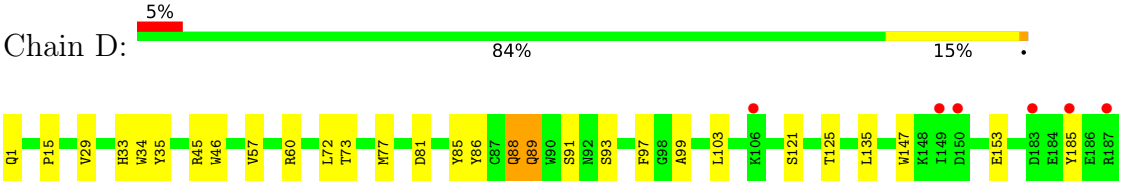
• Molecule 1: Isoform 2 of Potassium channel subfamily K member 4

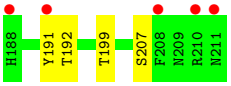
Chain B:



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

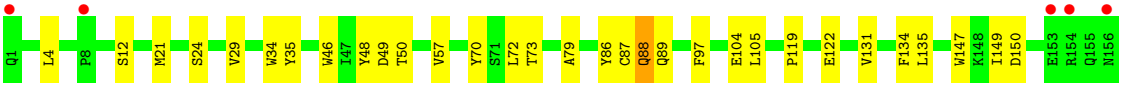
Chain D:

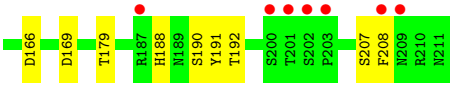




• Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN

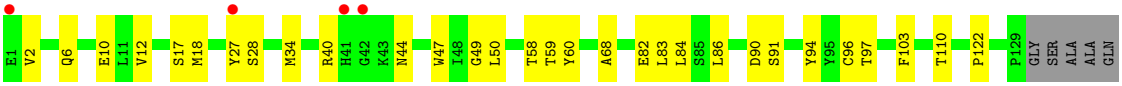
Chain F:

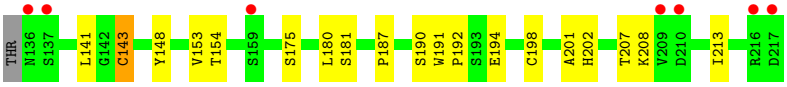




• Molecule 3: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT HEAVY CHAIN

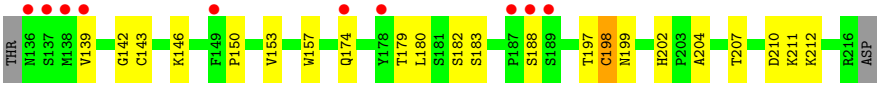
Chain E:





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

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.23Å 136.53Å 95.28Å 90.00° 94.54° 90.00°	Depositor
Resolution (Å)	47.54 – 2.77 47.49 – 2.78	Depositor EDS
% Data completeness (in resolution range)	68.6 (47.54-2.77) 68.6 (47.49-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (4.94%)	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 , 57.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.72	0/2017	0.80	0/2750
1	B	0.74	0/2035	0.79	0/2774
2	D	0.76	0/1655	0.90	0/2247
2	F	0.81	1/1655 (0.1%)	0.92	0/2247
3	E	0.74	0/1656	0.94	0/2260
3	G	0.74	0/1647	0.92	0/2249
All	All	0.75	1/10665 (0.0%)	0.87	0/14527

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	122	GLU	CD-OE1	5.21	1.31	1.25

There are no bond angle outliers.

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	48	0
1	B	1985	0	2007	26	0
2	D	1616	0	1542	27	0
2	F	1616	0	1542	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1614	0	1586	38	1
3	G	1605	0	1582	45	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
6	F	43	0	0	1	0
6	G	39	0	0	0	0
All	All	10651	0	10244	196	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 (196) 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: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:G:199:ASN:HD22	3:G:210:ASP:CG	1.93	0.71
3:E:10:GLU:OE2	6:E:301:HOH:O	2.09	0.70
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
3:G:199:ASN:ND2	3:G:210:ASP:CG	2.51	0.65
2:D:29:VAL:HG11	2:D:89:GLN:HG3	1.78	0.64
3:E:208:LYS:NZ	6:E:303:HOH:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:180:GLU:HG2	1:A:193:VAL:HG12	1.84	0.59
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
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
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
2:F:149:ILE:HG13	2:F:149:ILE:O	2.05	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
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
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:41:LEU:C	1:A:41:LEU:HD13	2.28	0.54
3:G:180:LEU:HD12	3:G:180:LEU:C	2.28	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: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
1:B:38:LEU:C	1:B:38:LEU:HD23	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:34:MET:HE2	3:E:96:CYS:HB2	1.90	0.52
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
2:D:35:TYR:CE1	2:D:45:ARG:HA	2.44	0.52
3:E:90:ASP:O	3:E:94:TYR:OH	2.22	0.52
3:E:180:LEU:C	3:E:180:LEU:HD12	2.30	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
3:E:50:LEU:C	3:E:50:LEU:HD12	2.29	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:G:197:THR:HG22	3:G:212:LYS:HA	1.91	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
1:A:283:LEU:C	1:A:283:LEU:HD13	2.33	0.48
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: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
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
2:D:72:LEU:C	2:D:72:LEU:HD23	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:ARG:NH1	2:D:81:ASP:OD1	2.49	0.46
3:E:191:TRP:C	6:E:316:HOH:O	2.53	0.46
1:A:58:GLU:OE2	1:B:113:ALA:N	2.48	0.46
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:G:34:MET:HE1	3:G:96:CYS:HB2	1.97	0.46
1:A:198:GLU:HA	1:A:198:GLU:OE1	2.17	0.45
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
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
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
3:G:50:LEU:C	3:G:50:LEU:HD12	2.38	0.43
1:B:275:VAL:O	1:B:279:ILE:HG22	2.18	0.43
1:A:260:LEU:C	1:A:260:LEU:HD23	2.39	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:72:LEU:HD23	2:F:72:LEU:C	2.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:121:SER:O	2:D:125:THR:HG23	2.21	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
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 (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%)	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 (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%)	204 (100%)	1 (0%)	88 95
1	B	209/243 (86%)	208 (100%)	1 (0%)	88 95
2	D	184/184 (100%)	181 (98%)	3 (2%)	62 86
2	F	184/184 (100%)	181 (98%)	3 (2%)	62 86
3	E	187/190 (98%)	184 (98%)	3 (2%)	62 86
3	G	186/190 (98%)	182 (98%)	4 (2%)	52 80
All	All	1155/1234 (94%)	1140 (99%)	15 (1%)	69 89

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	PHE
1	B	272	PHE
2	D	88	GLN
2	D	89	GLN
2	D	199	THR
3	E	18	MET
3	E	143	CYS
3	E	198	CYS
2	F	21	MET
2	F	88	GLN
2	F	89	GLN
3	G	18	MET
3	G	44	ASN
3	G	143	CYS
3	G	198	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	59	GLN
2	D	88	GLN
2	D	136	ASN
2	D	137	ASN
2	D	144	ASN
3	E	136	ASN
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 monosaccharides 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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	1.18	63 (24%)	0	0	46, 106, 174, 197	0
1	B	255/299 (85%)	1.96	83 (32%)	0	0	45, 107, 179, 199	0
2	D	211/211 (100%)	0.06	11 (5%)	27	22	38, 64, 104, 125	0
2	F	211/211 (100%)	0.15	12 (5%)	23	18	38, 64, 111, 127	0
3	E	211/217 (97%)	0.20	11 (5%)	27	22	34, 55, 85, 124	0
3	G	210/217 (96%)	0.24	16 (7%)	13	9	37, 60, 96, 156	0
All	All	1351/1454 (92%)	0.69	196 (14%)	2	1	34, 71, 164, 199	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	ALA	12.8
3	G	136	ASN	12.4
1	B	193	VAL	12.2
1	B	192	LEU	11.8
1	B	190	PRO	11.5
1	B	182	ILE	9.7
1	B	183	PHE	9.1
1	B	184	LEU	8.9
1	B	256	ALA	8.7
1	A	178	HIS	8.5
1	B	181	ALA	8.4
1	A	179	ILE	8.4
1	B	186	TRP	8.1
1	B	179	ILE	8.1
1	A	263	PHE	8.0
3	G	41	HIS	7.9
1	B	250	PRO	7.7
1	B	280	GLY	7.7
1	B	248	ALA	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	258	GLN	7.4
2	F	201	THR	7.3
1	B	282	TRP	7.2
1	B	194	ARG	7.2
1	B	251	ARG	7.1
1	B	189	PRO	7.1
1	B	195	VAL	7.0
1	B	257	TYR	7.0
1	B	197	SER	6.9
1	A	174	HIS	6.9
1	B	263	PHE	6.9
1	B	276	LEU	6.9
1	B	285	VAL	6.6
1	A	262	TRP	6.6
1	B	249	ASP	6.5
1	B	177	GLY	6.4
1	A	255	PRO	6.3
1	B	176	ILE	6.2
1	B	34	ALA	6.1
1	A	257	TYR	5.9
1	B	178	HIS	5.8
1	A	247	GLY	5.6
1	B	219	TYR	5.5
1	B	180	GLU	5.5
1	B	172	LEU	5.5
1	B	174	HIS	5.4
2	D	211	ASN	5.4
1	B	204	ILE	5.3
1	B	259	PRO	5.2
3	E	217	ASP	5.2
1	B	171	SER	5.2
3	G	137	SER	5.1
1	B	198	GLU	5.1
1	B	30	THR	5.1
1	A	270	ALA	5.1
1	B	187	HIS	5.1
1	B	188	VAL	5.1
1	B	185	LYS	5.0
1	B	199	MET	5.0
1	B	275	VAL	4.9
1	B	258	GLN	4.9
1	B	201	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	200	LEU	4.9
1	B	252	GLN	4.8
1	B	255	PRO	4.8
1	B	281	ASN	4.7
1	A	136	ALA	4.7
1	A	176	ILE	4.7
1	A	186	TRP	4.6
1	B	191	GLU	4.6
2	D	150	ASP	4.6
1	B	262	TRP	4.5
1	B	220	MET	4.5
1	A	183	PHE	4.5
1	B	196	LEU	4.5
2	F	202	SER	4.5
1	B	116	LEU	4.4
1	B	278	THR	4.4
1	A	261	VAL	4.4
1	A	171	SER	4.3
1	B	242	GLY	4.3
1	A	266	LEU	4.3
1	B	33	LEU	4.2
1	B	151	LEU	4.2
3	E	1	GLU	4.2
1	B	279	ILE	4.2
1	A	170	SER	4.2
1	B	267	LEU	4.1
1	B	148	PHE	3.9
1	A	103	THR	3.8
1	A	185	LYS	3.7
1	B	173	ARG	3.7
1	A	110	SER	3.6
1	A	253	ASP	3.6
1	B	247	GLY	3.6
1	A	282	TRP	3.6
1	A	272	PHE	3.6
1	A	167	ARG	3.5
3	G	40	ARG	3.5
1	B	144	LEU	3.5
1	B	118	SER	3.5
2	D	187	ARG	3.5
1	B	175	GLY	3.5
1	B	284	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	243	ASP	3.4
1	B	286	VAL	3.4
1	A	279	ILE	3.3
1	B	277	THR	3.3
1	B	209	PHE	3.3
1	A	204	ILE	3.3
3	G	138	MET	3.1
2	F	1	GLN	3.1
1	B	152	VAL	3.1
1	A	249	ASP	3.1
3	E	136	ASN	3.1
1	B	287	SER	3.1
2	F	187	ARG	3.0
1	A	177	GLY	3.0
1	A	180	GLU	3.0
3	E	216	ARG	3.0
1	B	207	LEU	3.0
1	A	190	PRO	3.0
2	D	188	HIS	3.0
1	A	135	VAL	3.0
1	B	208	LEU	3.0
1	A	222	ASP	2.9
2	F	156	ASN	2.9
1	A	256	ALA	2.9
1	A	182	ILE	2.9
1	B	31	THR	2.9
3	G	178	TYR	2.9
2	D	191	TYR	2.9
1	B	167	ARG	2.8
1	A	242	GLY	2.8
1	A	269	LEU	2.8
1	A	134	ASN	2.8
3	E	42	GLY	2.8
3	E	41	HIS	2.8
3	E	137	SER	2.8
1	B	271	TYR	2.8
1	A	137	LEU	2.8
1	A	133	GLY	2.7
1	A	187	HIS	2.7
1	A	264	TRP	2.7
3	G	42	GLY	2.7
1	A	157	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	267	LEU	2.7
1	B	266	LEU	2.6
3	G	188	SER	2.6
3	E	159	SER	2.6
1	A	275	VAL	2.5
1	A	252	GLN	2.5
1	B	117	GLY	2.5
3	G	189	SER	2.5
1	A	159	ILE	2.5
3	G	11	LEU	2.4
1	A	268	GLY	2.4
3	G	187	PRO	2.4
1	A	181	ALA	2.4
2	D	210	ARG	2.4
2	F	153	GLU	2.4
1	B	120	PHE	2.4
1	A	273	ALA	2.4
2	F	203	PRO	2.4
1	B	272	PHE	2.4
1	A	251	ARG	2.4
2	F	208	PHE	2.4
3	G	1	GLU	2.3
2	F	200	SER	2.3
1	A	265	ILE	2.3
2	D	208	PHE	2.3
1	A	60	GLN	2.2
1	A	276	LEU	2.2
2	D	185	TYR	2.2
1	A	55	GLN	2.2
3	G	174	GLN	2.2
1	A	260	LEU	2.2
2	D	183	ASP	2.2
3	G	16	ALA	2.2
1	B	112	SER	2.1
2	D	149	ILE	2.1
1	A	219	TYR	2.1
2	F	8	PRO	2.1
2	F	154	ARG	2.1
2	F	209	ASN	2.1
3	E	209	VAL	2.1
3	E	27	TYR	2.1
2	D	106	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	161	LEU	2.1
1	A	259	PRO	2.1
3	G	149	PHE	2.1
3	E	210	ASP	2.0
1	A	250	PRO	2.0
1	A	175	GLY	2.0
1	B	133	GLY	2.0
1	A	173	ARG	2.0
3	G	139	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

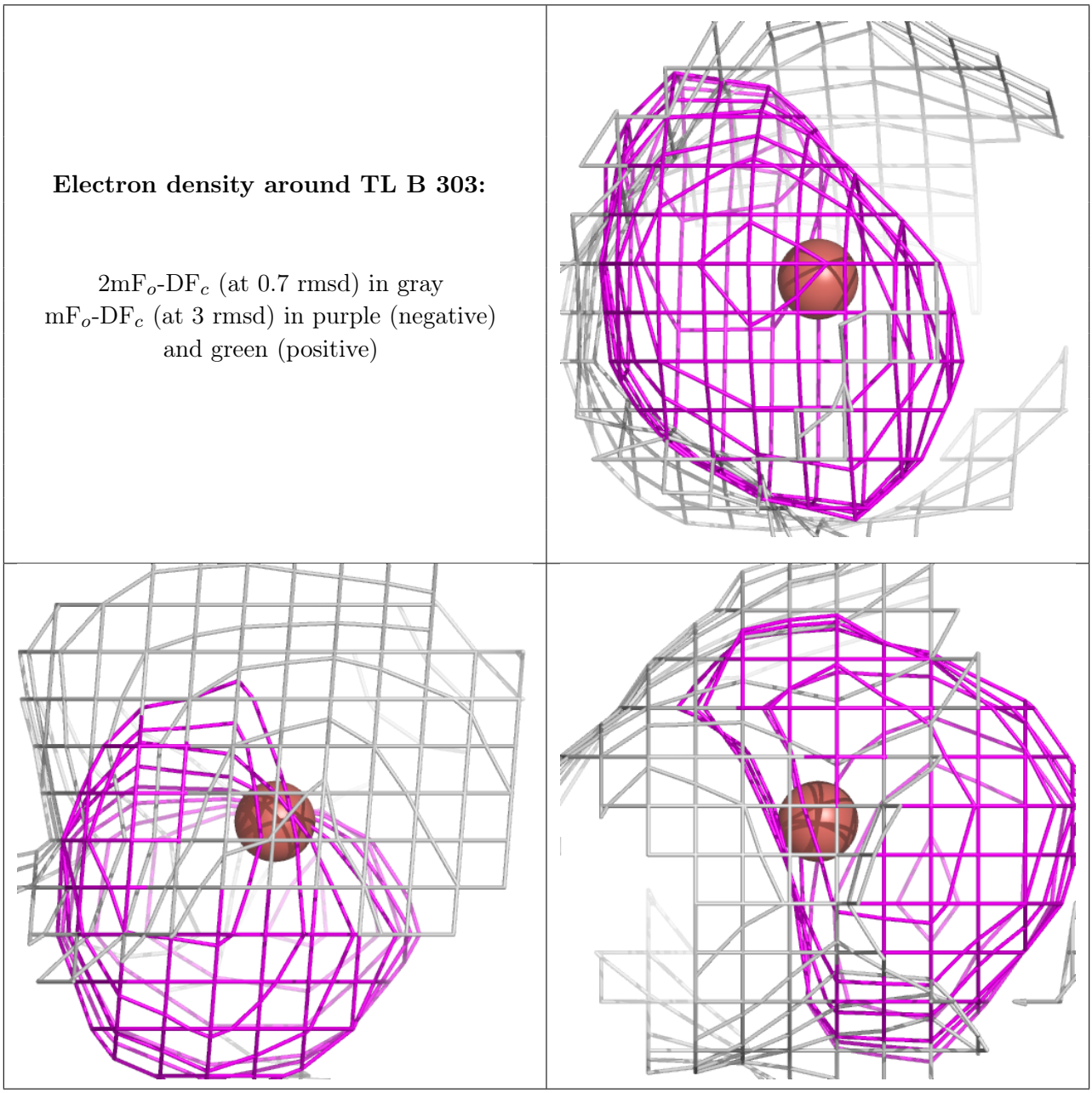
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TL	B	303	1/1	0.53	0.16	245,245,245,245	0
4	TL	A	306	1/1	0.60	0.21	220,220,220,220	0
5	CA	A	304	1/1	0.77	0.23	102,102,102,102	0
4	TL	B	302	1/1	0.85	0.08	183,183,183,183	0
4	TL	A	307	1/1	0.86	0.21	225,225,225,225	0
5	CA	G	301	1/1	0.98	0.10	63,63,63,63	0
4	TL	A	305	1/1	0.99	0.05	88,88,88,88	0
5	CA	A	303	1/1	0.99	0.05	107,107,107,107	0
4	TL	B	301	1/1	0.99	0.05	89,89,89,89	0
4	TL	A	302	1/1	0.99	0.05	88,88,88,88	0
4	TL	A	301	1/1	1.00	0.04	85,85,85,85	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.

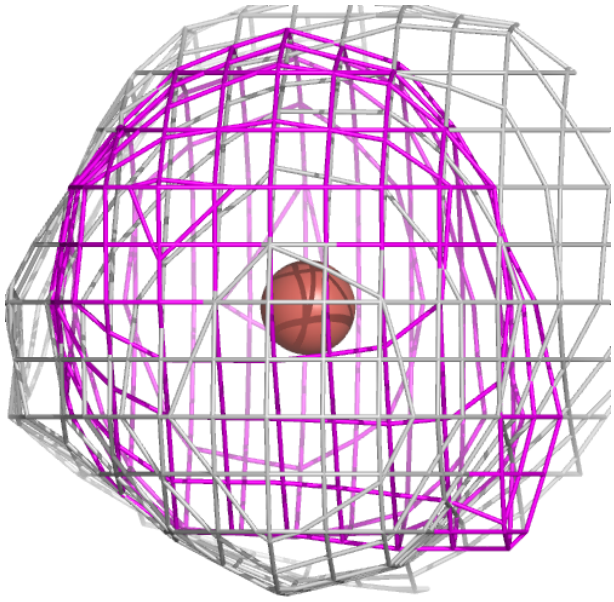
Electron density around TL B 303:

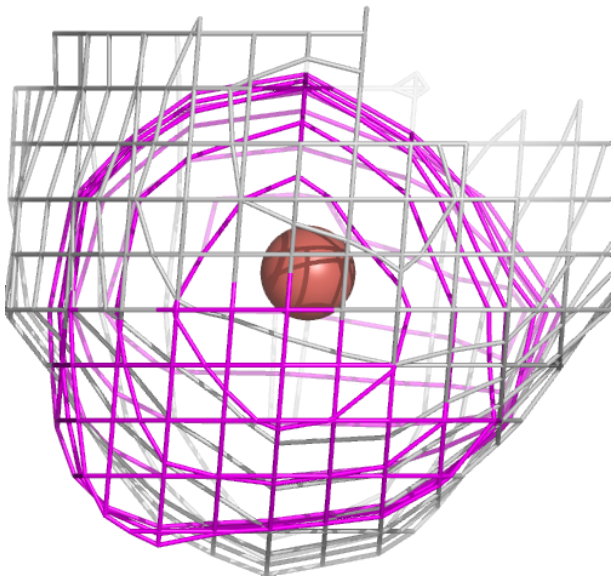
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

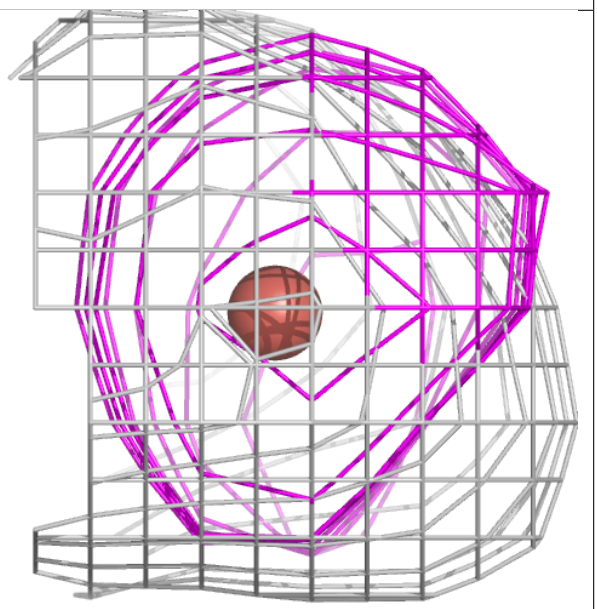


Electron density around TL A 306:

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

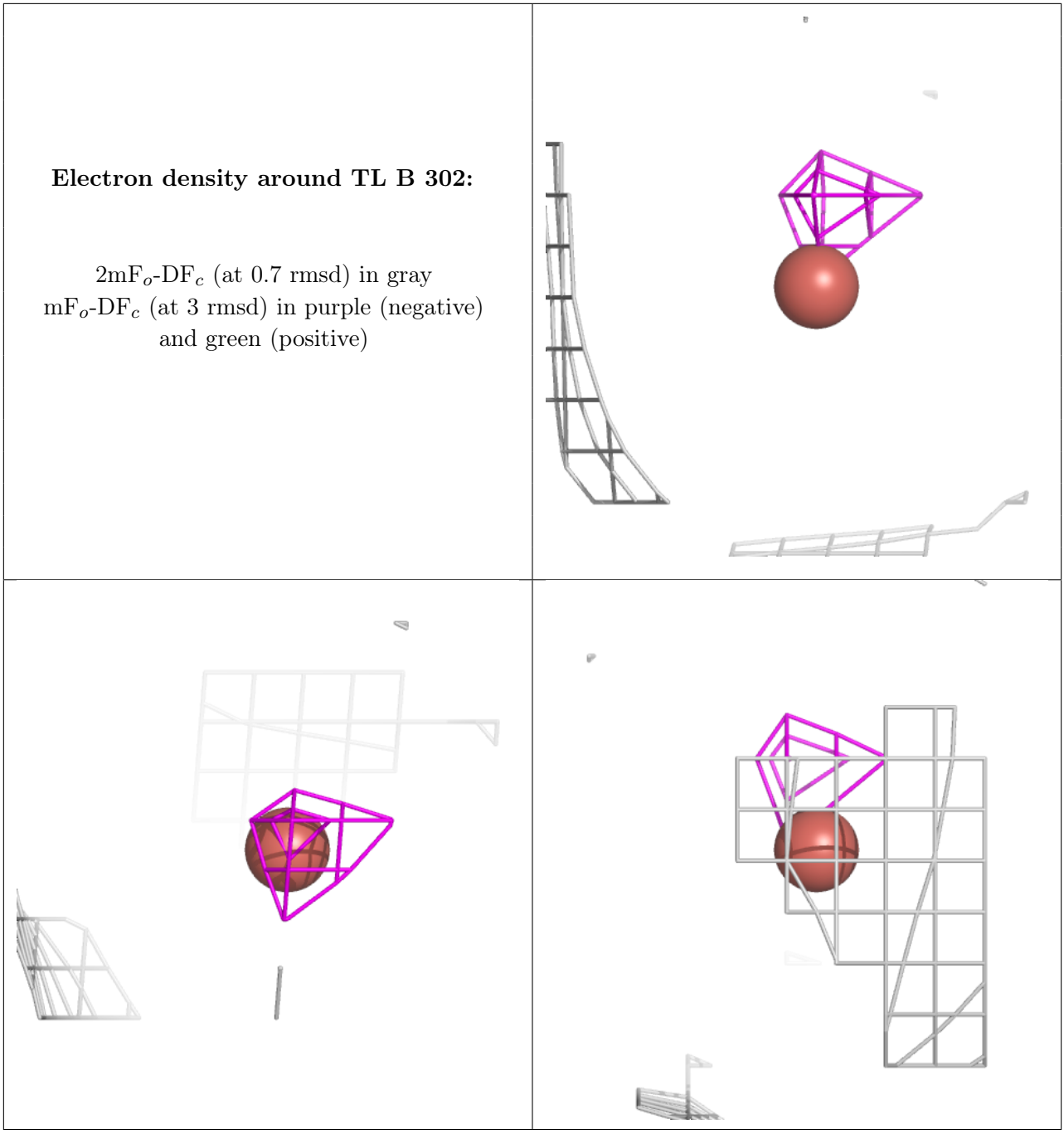






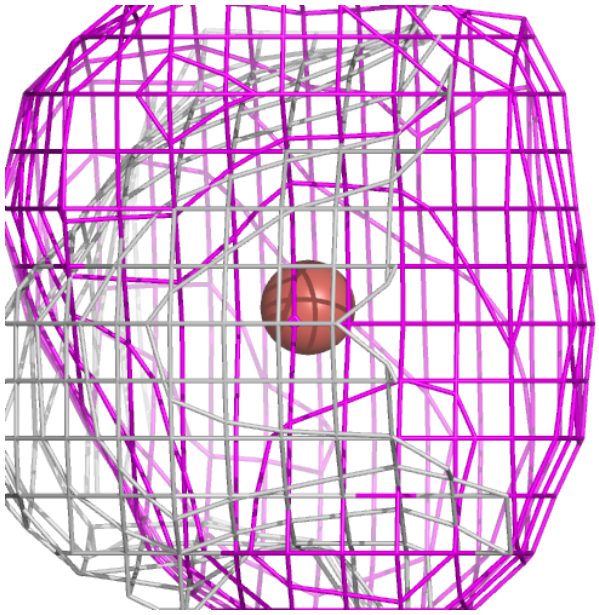
Electron density around TL B 302:

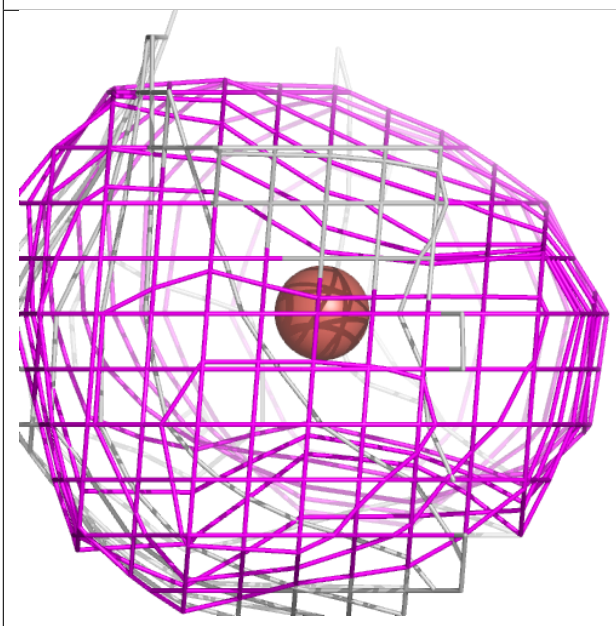
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

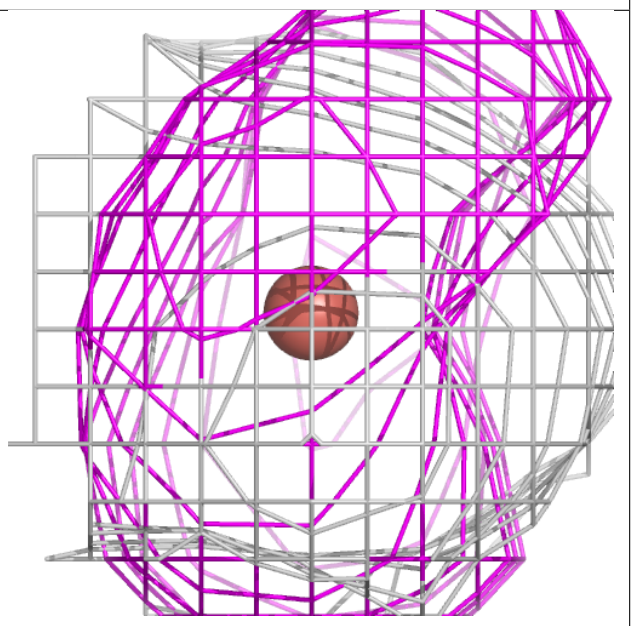


Electron density around TL A 307:

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

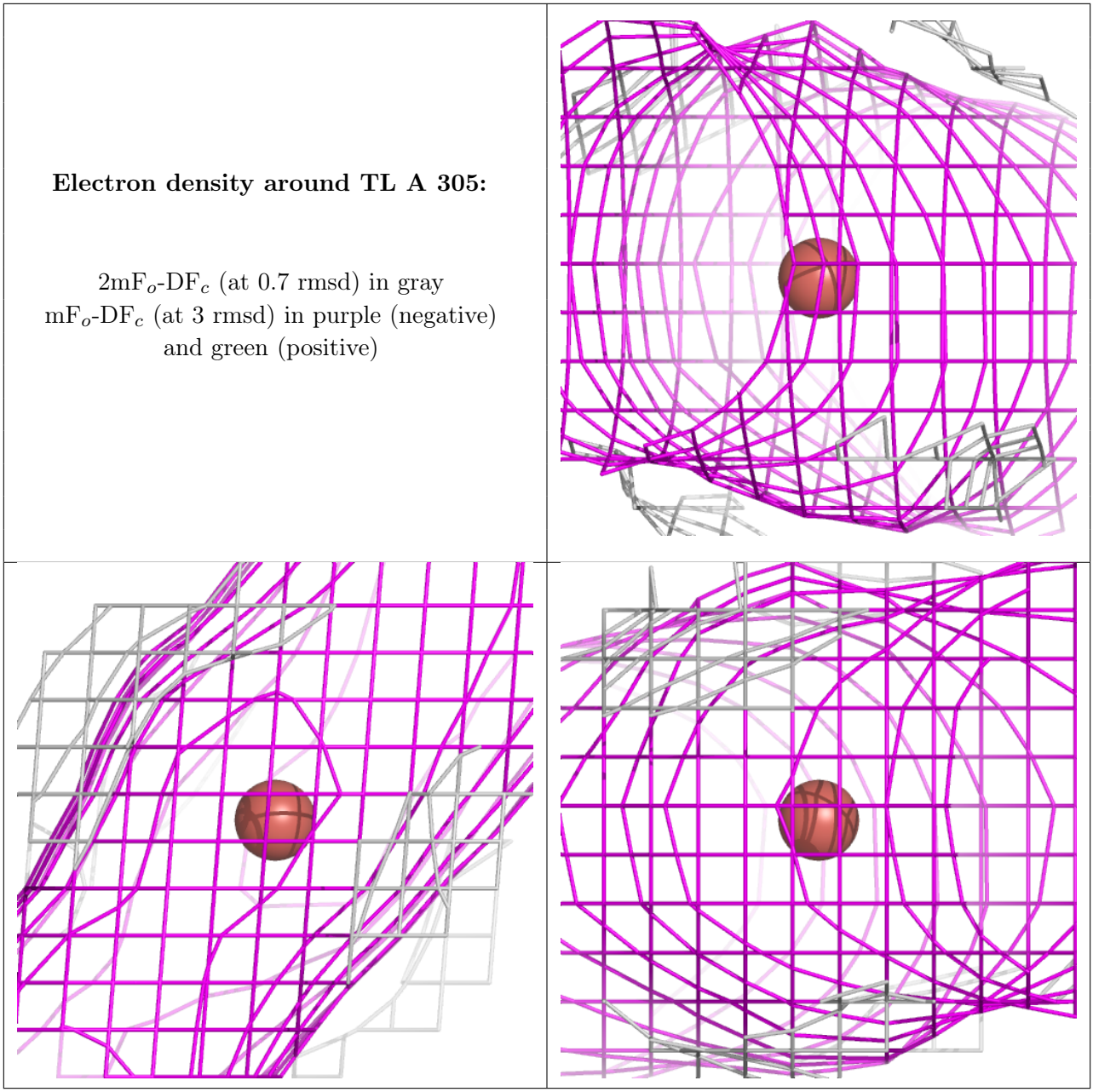






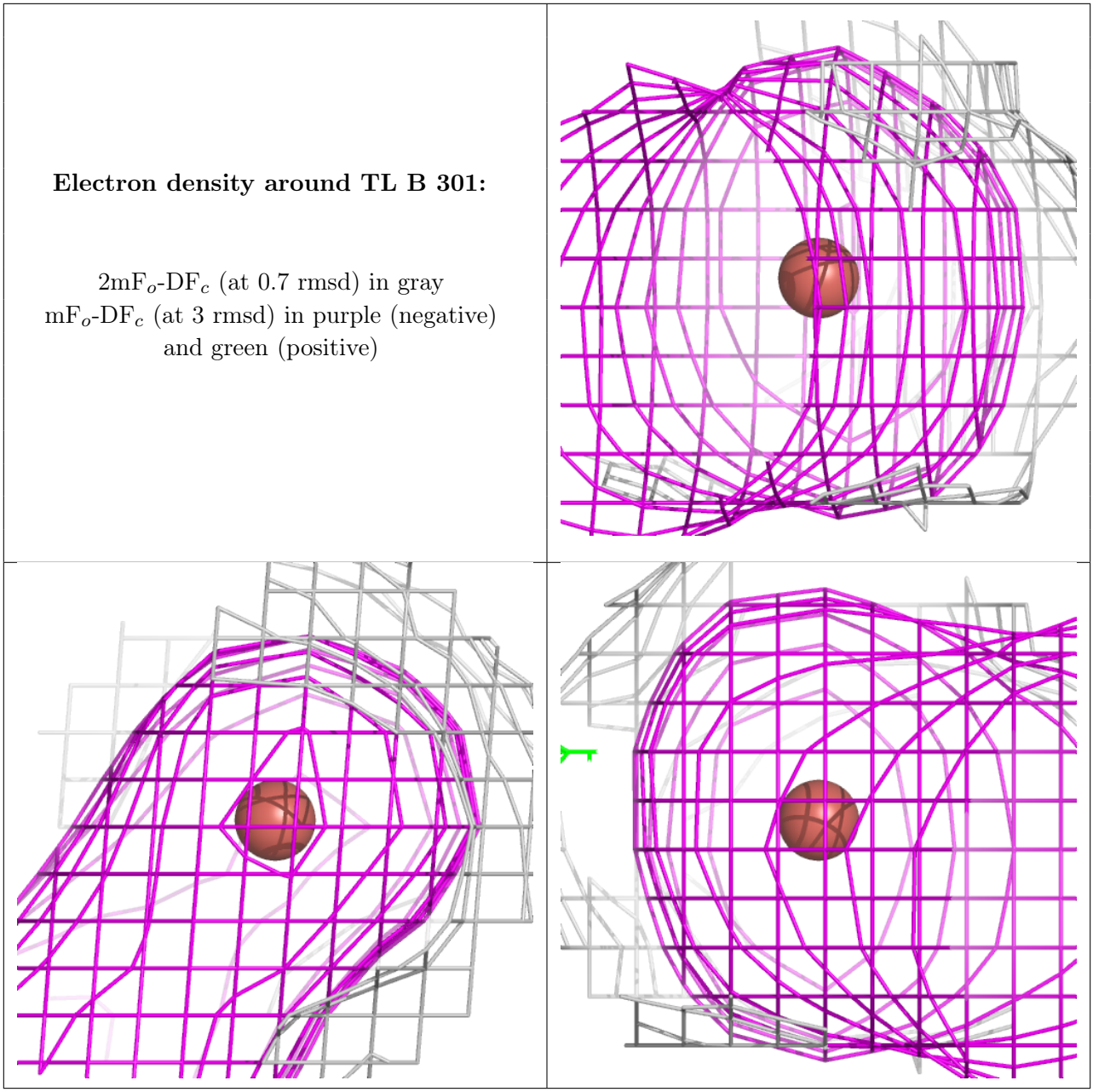
Electron density around TL A 305:

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



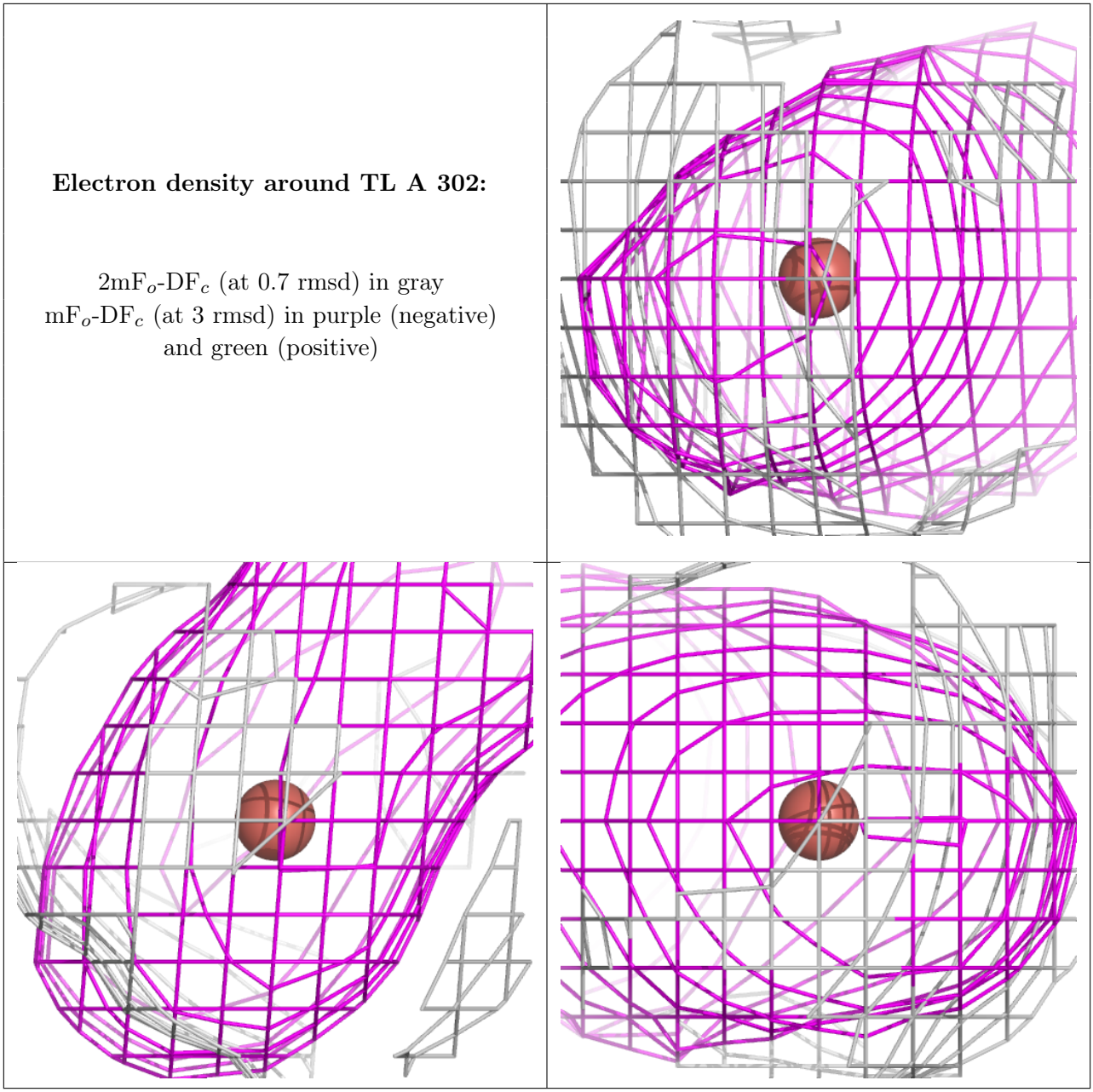
Electron density around TL B 301:

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



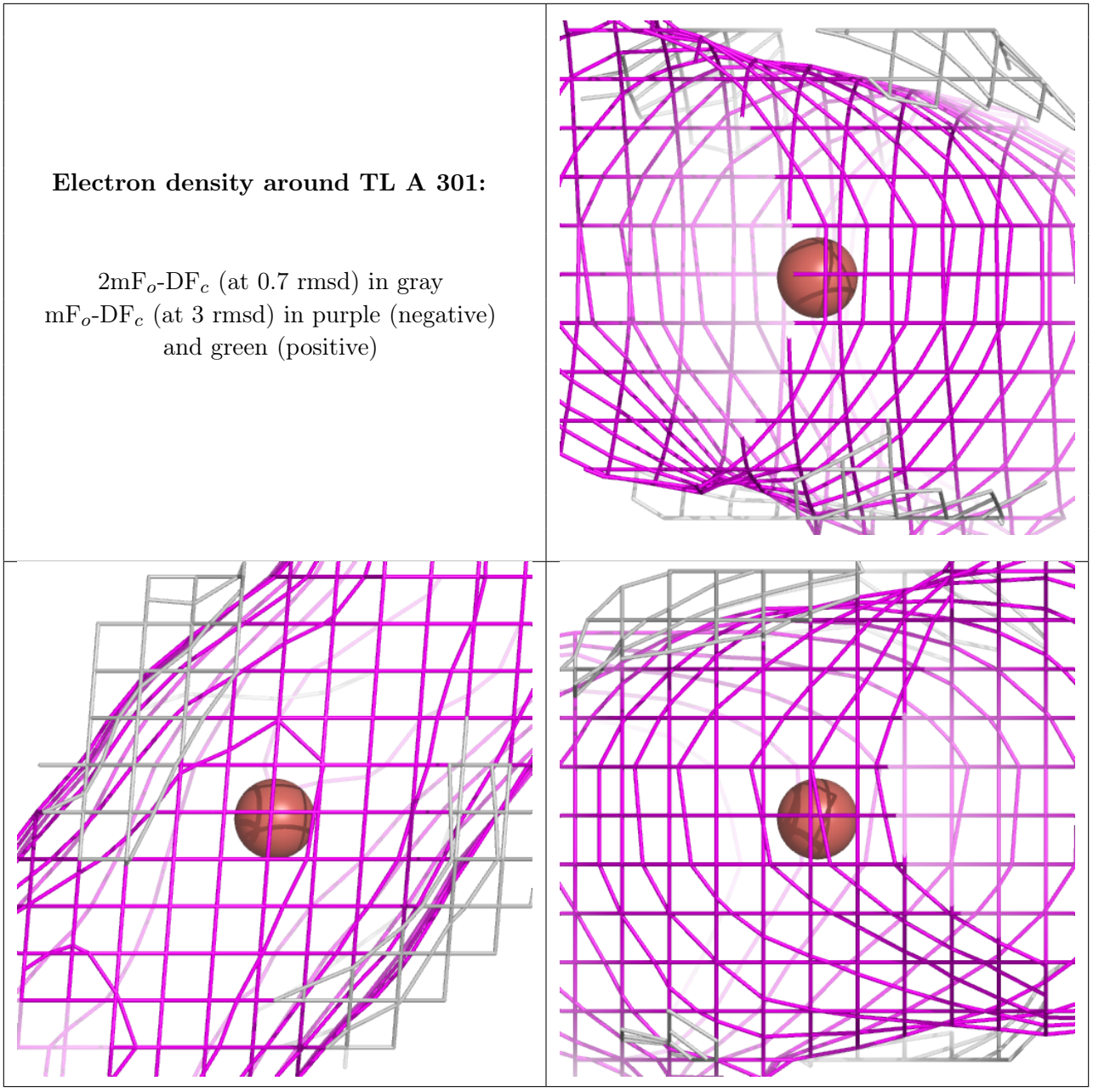
Electron density around TL A 302:

$2mF_o$-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 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.