



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2021 – 04:05 PM EDT

PDB ID : 7LJB
Title : Human TRAAK K⁺ channel mutant G158D in a K⁺ bound conductive conformation
Authors : Rietmeijer, R.A.; Brohawn, S.G.
Deposited on : 2021-01-28
Resolution : 2.97 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 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	:	2.23.1
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)	:	2.23.1

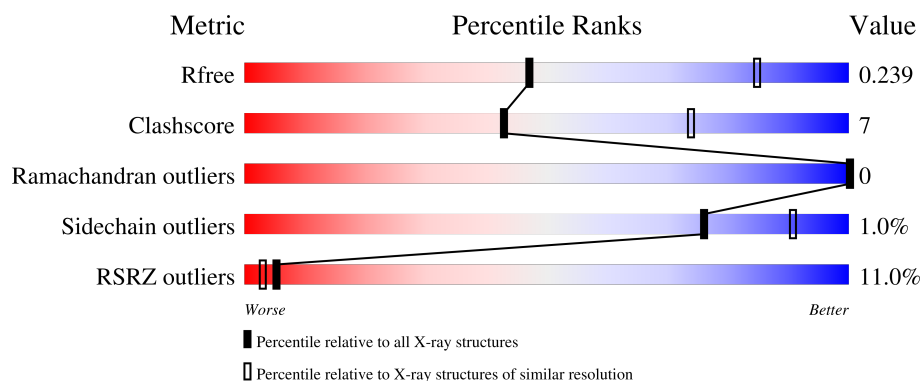
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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	<div> <div>18%</div> <div>74%</div> <div>10%</div> <div>15%</div> </div>
1	B	299	<div> <div>21%</div> <div>73%</div> <div>11%</div> <div>16%</div> </div>
2	D	211	<div> <div>3%</div> <div>85%</div> <div>14%</div> </div>
2	F	211	<div> <div>4%</div> <div>83%</div> <div>16%</div> </div>
3	E	217	<div> <div>5%</div> <div>81%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	217	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	K	A	306	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10586 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	251	Total	C	N	O	S	0	0	0
			1958	1293	317	342	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	158	ASP	GLY	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	158	ASP	GLY	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 (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	K	0	0
			4	4		
4	B	2	Total	K	0	0
			2	2		

- 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	36	Total	O	0	0
			36	36		
6	B	35	Total	O	0	0
			35	35		
6	D	38	Total	O	0	0
			38	38		

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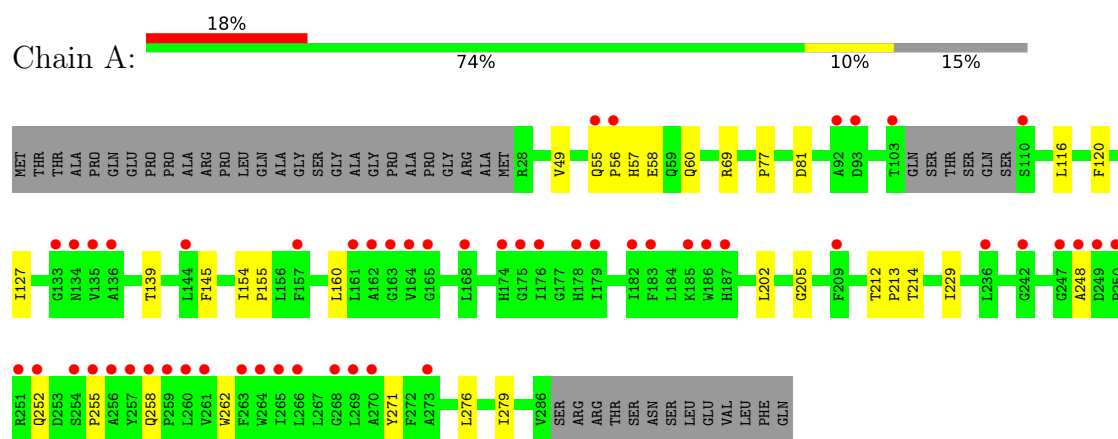
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	30	Total 30	O 30	0	0
6	F	34	Total 34	O 34	0	0
6	G	28	Total 28	O 28	0	0

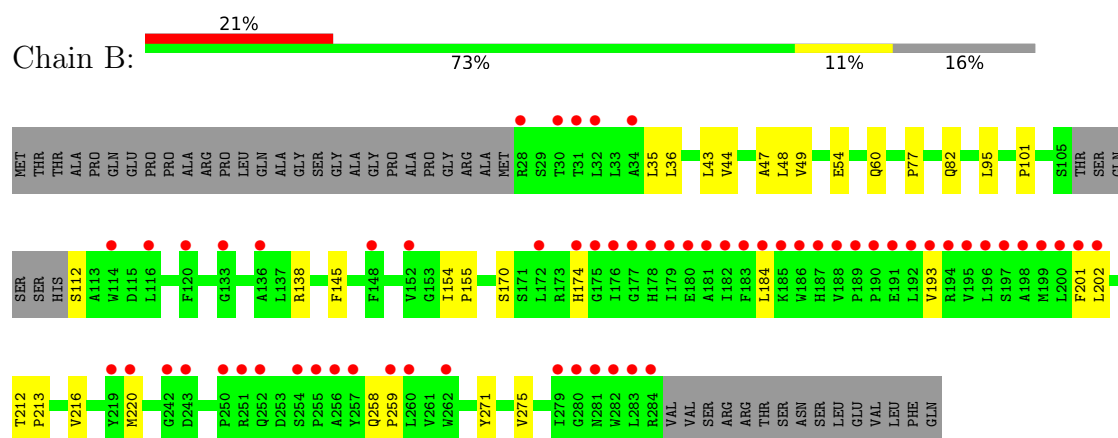
3 Residue-property plots [i](#)

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.

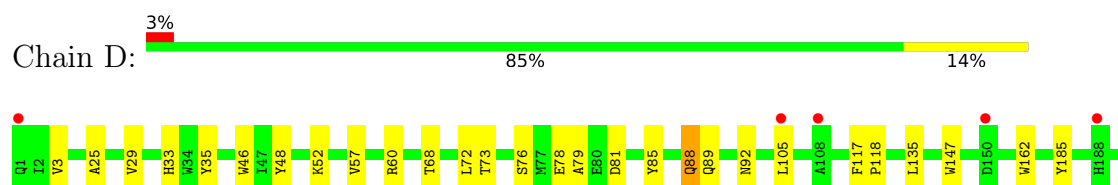
- Molecule 1: Isoform 2 of Potassium channel subfamily K member 4



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

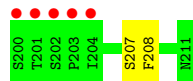
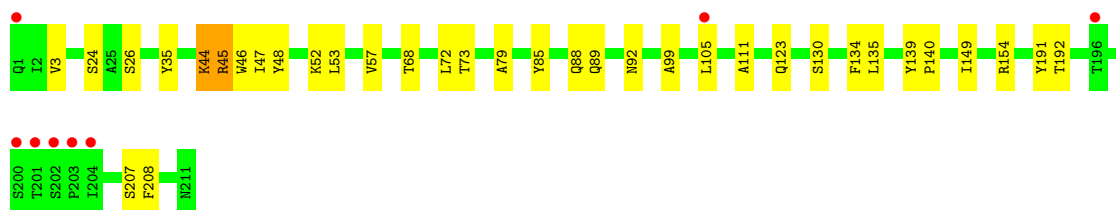
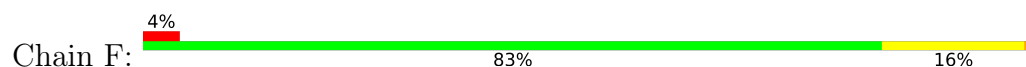


- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN

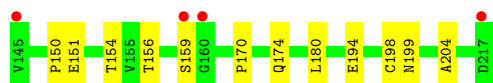
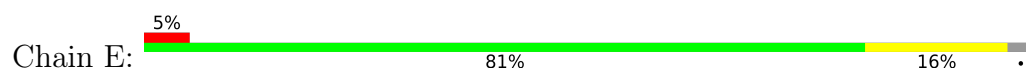




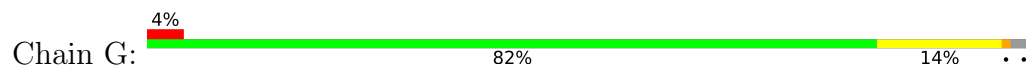
● Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



● 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	80.14Å 137.31Å 96.30Å 90.00° 94.72° 90.00°	Depositor
Resolution (Å)	48.03 – 2.97 47.99 – 2.97	Depositor EDS
% Data completeness (in resolution range)	74.0 (48.03-2.97) 74.1 (47.99-2.97)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.196 , 0.240 0.198 , 0.239	Depositor DCC
R_{free} test set	1575 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	91.9	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10586	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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, 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	0.72	0/2017	0.82	0/2751
1	B	0.73	0/2008	0.83	0/2737
2	D	0.72	0/1655	0.90	0/2247
2	F	0.73	0/1655	0.89	1/2247 (0.0%)
3	E	0.72	0/1656	0.92	0/2260
3	G	0.71	1/1647 (0.1%)	0.91	0/2249
All	All	0.72	1/10638 (0.0%)	0.87	1/14491 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	25	SER	CA-CB	-5.24	1.45	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	45	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1967	0	1986	29	0
1	B	1958	0	1978	27	0
2	D	1616	0	1542	21	0
2	F	1616	0	1542	29	0
3	E	1614	0	1586	27	1
3	G	1605	0	1582	28	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
5	A	2	0	0	0	0
5	G	1	0	0	0	1
6	A	36	0	0	0	0
6	B	35	0	0	0	0
6	D	38	0	0	7	0
6	E	30	0	0	1	0
6	F	34	0	0	1	0
6	G	28	0	0	2	0
All	All	10586	0	10216	138	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (138) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:SER:O	6:D:301:HOH:O	2.03	0.77
1:A:276:LEU:HA	1:A:279:ILE:HG22	1.68	0.76
1:A:77:PRO:HA	3:E:100:ASN:HD21	1.50	0.76
3:G:139:VAL:HG23	3:G:188:SER:HB3	1.70	0.73
1:B:77:PRO:HA	3:G:100:ASN:ND2	2.03	0.73
3:E:156:THR:OG1	3:E:199:ASN:HB2	1.90	0.72
1:B:77:PRO:HA	3:G:100:ASN:HD21	1.55	0.70
3:E:28:SER:HB2	3:G:28:SER:HB2	1.72	0.70
1:A:248:ALA:HB1	1:A:262:TRP:HE1	1.59	0.68
1:A:276:LEU:HA	1:A:279:ILE:CG2	2.25	0.67
2:F:35:TYR:HE2	2:F:88:GLN:HB2	1.60	0.66
3:G:34:MET:CE	3:G:96:CYS:HB2	2.25	0.66
2:F:111:ALA:O	6:F:301:HOH:O	2.13	0.66
3:E:18:MET:HG2	3:E:19:LYS:N	2.13	0.64
1:B:216:VAL:O	1:B:220:MET:HG2	1.97	0.64
2:F:99:ALA:HA	3:G:44:ASN:HB3	1.81	0.63
3:E:34:MET:CE	3:E:96:CYS:HB2	2.30	0.61
1:A:77:PRO:HA	3:E:100:ASN:ND2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:29:PHE:HB2	3:G:77:SER:HB2	1.83	0.60
2:F:79:ALA:HA	2:F:105:LEU:HD11	1.83	0.59
3:G:34:MET:HE1	3:G:96:CYS:HB2	1.84	0.59
1:A:69:ARG:NH1	1:A:81:ASP:OD1	2.35	0.58
3:G:25:SER:HA	6:G:421:HOH:O	2.03	0.58
1:A:116:LEU:HD21	1:B:48:LEU:HD23	1.85	0.58
1:B:212:THR:HB	1:B:213:PRO:HD3	1.85	0.58
3:E:29:PHE:HB2	3:E:77:SER:HB2	1.85	0.57
1:A:139:THR:OG1	1:B:54:GLU:OE2	2.15	0.57
1:A:205:GLY:HA3	1:A:271:TYR:CZ	2.40	0.57
1:A:212:THR:HB	1:A:213:PRO:HD3	1.86	0.57
3:E:44:ASN:N	3:E:44:ASN:OD1	2.38	0.57
2:F:134:PHE:CE2	3:G:183:SER:HB3	2.40	0.57
1:A:60:GLN:HB3	1:B:138:ARG:NH1	2.20	0.56
3:E:12:VAL:HG21	3:E:86:LEU:CD1	2.34	0.56
1:A:252:GLN:OE1	1:A:252:GLN:N	2.38	0.56
2:F:89:GLN:HE21	2:F:92:ASN:H	1.54	0.56
1:A:202:LEU:HA	1:A:271:TYR:OH	2.06	0.55
2:F:45:ARG:HD3	3:G:104:ASP:HA	1.88	0.55
1:B:202:LEU:HA	1:B:271:TYR:OH	2.07	0.54
1:A:127:ILE:CD1	1:B:43:LEU:HD21	2.38	0.54
1:A:55:GLN:N	1:A:56:PRO:HD2	2.23	0.54
2:F:89:GLN:NE2	2:F:92:ASN:H	2.06	0.54
2:F:134:PHE:CE2	3:G:183:SER:CB	2.91	0.54
3:G:195:THR:HA	6:G:406:HOH:O	2.08	0.53
1:B:201:PHE:HE1	1:B:275:VAL:HG22	1.73	0.53
2:D:3:VAL:HA	6:D:320:HOH:O	2.08	0.53
2:D:29:VAL:HG11	2:D:89:GLN:HG3	1.90	0.52
3:E:40:ARG:NH1	3:E:91:SER:O	2.43	0.52
2:D:35:TYR:O	2:D:85:TYR:HA	2.10	0.52
2:F:35:TYR:O	2:F:85:TYR:HA	2.09	0.52
6:D:331:HOH:O	3:E:44:ASN:HB3	2.10	0.51
2:D:25:ALA:O	2:D:68:THR:OG1	2.27	0.51
3:E:159:SER:H	3:E:199:ASN:ND2	2.09	0.50
2:F:123:GLN:HE22	2:F:130:SER:HB2	1.77	0.50
2:F:72:LEU:HD23	2:F:73:THR:N	2.26	0.49
3:G:12:VAL:HG21	3:G:86:LEU:CD1	2.42	0.49
2:D:79:ALA:HA	2:D:105:LEU:HD21	1.94	0.49
2:F:135:LEU:HD12	2:F:135:LEU:N	2.27	0.49
1:A:248:ALA:CB	1:A:262:TRP:HE1	2.26	0.49
3:E:34:MET:HE1	3:E:96:CYS:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:52:ASN:HB3	3:G:55:THR:OG1	2.13	0.49
2:F:46:TRP:O	2:F:57:VAL:HG21	2.13	0.48
3:G:195:THR:HG22	3:G:197:THR:HG23	1.95	0.48
1:A:276:LEU:HD13	1:A:279:ILE:HG21	1.94	0.48
2:D:135:LEU:N	2:D:135:LEU:HD12	2.28	0.48
2:F:149:ILE:HG22	2:F:191:TYR:CE1	2.48	0.48
1:A:252:GLN:HA	1:A:255:PRO:HG3	1.95	0.48
2:D:72:LEU:HD23	2:D:73:THR:N	2.29	0.48
3:E:174:GLN:NE2	6:E:303:HOH:O	2.46	0.48
1:A:127:ILE:HD13	1:B:43:LEU:HD21	1.94	0.48
6:D:331:HOH:O	3:E:44:ASN:CB	2.62	0.47
1:A:49:VAL:HG11	1:B:145:PHE:CE2	2.50	0.47
1:B:44:VAL:O	1:B:48:LEU:HG	2.15	0.47
2:D:35:TYR:HE2	2:D:88:GLN:CB	2.28	0.47
3:E:150:PRO:HD2	3:E:204:ALA:CB	2.45	0.47
3:G:12:VAL:HG21	3:G:86:LEU:HD12	1.95	0.47
1:B:95:LEU:HD21	1:B:101:PRO:HG3	1.97	0.47
2:F:72:LEU:HD23	2:F:72:LEU:C	2.36	0.46
2:F:149:ILE:HG13	2:F:149:ILE:O	2.15	0.46
2:D:46:TRP:O	2:D:57:VAL:HG21	2.15	0.46
1:A:258:GLN:OE1	1:A:258:GLN:HA	2.15	0.46
3:G:40:ARG:NH1	3:G:91:SER:O	2.45	0.46
3:G:18:MET:O	3:G:82:GLU:HA	2.15	0.45
2:D:78:GLU:OE1	6:D:302:HOH:O	2.21	0.45
2:D:162:TRP:O	3:E:170:PRO:HG2	2.16	0.45
3:E:12:VAL:HG21	3:E:86:LEU:HD12	1.98	0.45
6:D:317:HOH:O	3:E:43:LYS:HA	2.17	0.45
2:F:46:TRP:CD2	2:F:57:VAL:HG22	2.51	0.45
2:F:47:ILE:HG12	2:F:53:LEU:HD12	1.99	0.45
2:F:192:THR:HG22	2:F:207:SER:OG	2.17	0.45
2:D:60:ARG:HD2	2:D:81:ASP:OD2	2.17	0.45
3:E:52:ASN:HB3	3:E:55:THR:OG1	2.18	0.44
1:A:58:GLU:OE2	1:B:112:SER:HA	2.17	0.44
2:D:117:PHE:HA	2:D:118:PRO:HD3	1.86	0.44
1:B:154:ILE:N	1:B:155:PRO:HD2	2.33	0.44
3:E:51:ILE:HA	3:E:57:TYR:O	2.18	0.44
1:A:160:LEU:HD11	1:B:36:LEU:HA	2.00	0.44
2:F:35:TYR:HE2	2:F:88:GLN:CB	2.30	0.44
1:A:154:ILE:N	1:A:155:PRO:HD2	2.33	0.43
2:D:48:TYR:O	2:D:52:LYS:HB2	2.18	0.43
2:D:147:TRP:N	6:D:304:HOH:O	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3:VAL:HB	2:F:26:SER:HB3	1.99	0.43
2:D:89:GLN:NE2	2:D:92:ASN:H	2.15	0.43
3:G:51:ILE:HA	3:G:57:TYR:O	2.18	0.43
1:B:170:SER:O	1:B:174:HIS:HB2	2.18	0.43
2:F:35:TYR:CE2	2:F:88:GLN:HB2	2.48	0.43
2:D:60:ARG:NH1	2:D:81:ASP:OD1	2.52	0.43
2:F:139:TYR:CD1	2:F:140:PRO:HA	2.53	0.43
3:G:122:PRO:HB3	3:G:148:TYR:HB3	2.00	0.43
3:E:50:LEU:C	3:E:50:LEU:HD12	2.40	0.43
1:B:95:LEU:CD2	1:B:101:PRO:HG3	2.48	0.43
3:E:28:SER:CB	3:G:28:SER:HB2	2.43	0.43
2:F:123:GLN:HE22	2:F:130:SER:CB	2.32	0.43
2:F:24:SER:HA	2:F:68:THR:O	2.19	0.42
1:A:120:PHE:HA	1:B:47:ALA:HB2	2.01	0.42
1:B:258:GLN:HB3	1:B:259:PRO:HD3	2.00	0.42
2:D:192:THR:HG22	2:D:207:SER:OG	2.19	0.42
3:E:180:LEU:C	3:E:180:LEU:HD12	2.40	0.42
1:A:214:THR:HG21	1:A:229:ILE:HG12	2.02	0.42
1:A:276:LEU:CA	1:A:279:ILE:HG22	2.45	0.42
3:E:83:LEU:HB3	3:E:86:LEU:HD21	2.01	0.42
3:G:180:LEU:HD12	3:G:180:LEU:C	2.40	0.42
1:A:57:HIS:O	1:B:138:ARG:NH1	2.53	0.41
3:E:12:VAL:HG21	3:E:86:LEU:HD13	2.02	0.41
2:F:48:TYR:O	2:F:52:LYS:HB2	2.21	0.41
1:A:145:PHE:CZ	1:B:49:VAL:HG11	2.56	0.41
1:B:60:GLN:HA	1:B:60:GLN:OE1	2.20	0.41
3:G:150:PRO:HD2	3:G:204:ALA:CB	2.51	0.41
1:B:35:LEU:HD12	1:B:35:LEU:HA	1.87	0.41
1:B:82:GLN:OE1	3:G:50:LEU:HD21	2.21	0.41
2:F:44:LYS:HB2	2:F:44:LYS:HE3	1.76	0.41
3:G:50:LEU:C	3:G:50:LEU:HD12	2.41	0.41
2:D:33:HIS:HD2	2:D:88:GLN:HG3	1.86	0.40
3:G:29:PHE:CD2	3:G:77:SER:HA	2.56	0.40
2:D:185:TYR:HA	2:D:191:TYR:OH	2.21	0.40
3:E:51:ILE:HD13	3:E:72:VAL:HG13	2.02	0.40
2:F:191:TYR:HB2	2:F:208:PHE:CE2	2.56	0.40
1:B:184:LEU:HG	1:B:193:VAL:HG11	2.02	0.40
3:G:51:ILE:HD13	3:G:72:VAL:HG13	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:194:GLU:OE2	5:G:301:CA:CA[2_556]	1.65	0.55

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%)	243 (98%)	6 (2%)	0	100	100
1	B	247/299 (83%)	241 (98%)	6 (2%)	0	100	100
2	D	209/211 (99%)	197 (94%)	12 (6%)	0	100	100
2	F	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
3	E	207/217 (95%)	198 (96%)	9 (4%)	0	100	100
3	G	206/217 (95%)	196 (95%)	10 (5%)	0	100	100
All	All	1327/1454 (91%)	1277 (96%)	50 (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%)	205 (100%)	0	100	100
1	B	205/243 (84%)	205 (100%)	0	100	100
2	D	184/184 (100%)	183 (100%)	1 (0%)	88	95
2	F	184/184 (100%)	182 (99%)	2 (1%)	73	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	187/190 (98%)	181 (97%)	6 (3%)	39	72
3	G	186/190 (98%)	183 (98%)	3 (2%)	62	85
All	All	1151/1234 (93%)	1139 (99%)	12 (1%)	76	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	88	GLN
3	E	44	ASN
3	E	65	LYS
3	E	143	CYS
3	E	151	GLU
3	E	154	THR
3	E	198	CYS
2	F	44	LYS
2	F	154	ARG
3	G	18	MET
3	G	143	CYS
3	G	198	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	76	HIS
2	D	88	GLN
3	E	136	ASN
3	E	199	ASN
2	F	123	GLN
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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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%)	1.13	53 (20%) 1 0	66, 133, 202, 240	0
1	B	251/299 (83%)	1.22	62 (24%) 0 0	65, 133, 199, 230	0
2	D	211/211 (100%)	0.01	6 (2%) 53 34	59, 90, 119, 137	0
2	F	211/211 (100%)	0.04	8 (3%) 40 24	65, 94, 139, 163	0
3	E	211/217 (97%)	0.20	11 (5%) 27 16	60, 83, 112, 160	0
3	G	210/217 (96%)	0.12	8 (3%) 40 24	60, 87, 125, 174	0
All	All	1347/1454 (92%)	0.50	148 (10%) 5 3	59, 97, 183, 240	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	LEU	12.0
1	B	181	ALA	10.4
1	B	192	LEU	10.0
3	G	136	ASN	9.7
1	A	256	ALA	9.1
1	A	255	PRO	8.1
1	A	103	THR	7.8
2	F	201	THR	7.8
1	B	179	ILE	7.7
1	A	248	ALA	7.6
1	A	257	TYR	7.1
1	B	189	PRO	7.1
1	B	251	ARG	6.9
1	A	269	LEU	6.9
1	A	260	LEU	6.8
1	A	179	ILE	6.8
2	F	1	GLN	6.7
1	B	176	ILE	6.7
1	A	270	ALA	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	184	LEU	6.5
1	B	183	PHE	6.5
1	B	281	ASN	6.4
1	A	250	PRO	6.3
2	F	202	SER	6.1
1	A	264	TRP	6.0
3	E	41	HIS	6.0
1	B	148	PHE	5.9
1	B	190	PRO	5.9
1	A	259	PRO	5.8
1	A	178	HIS	5.8
1	B	188	VAL	5.5
1	A	165	GLY	5.4
1	B	178	HIS	5.4
1	B	193	VAL	5.3
1	A	247	GLY	5.3
1	B	180	GLU	5.3
1	A	162	ALA	5.1
1	A	182	ILE	5.0
1	B	34	ALA	5.0
1	B	187	HIS	4.9
1	A	161	LEU	4.8
1	B	194	ARG	4.8
1	B	279	ILE	4.8
2	F	203	PRO	4.7
1	A	186	TRP	4.7
1	B	191	GLU	4.6
3	G	41	HIS	4.5
3	G	137	SER	4.5
1	B	185	LYS	4.4
1	A	187	HIS	4.3
1	B	282	TRP	4.3
1	A	258	GLN	4.2
1	B	195	VAL	4.2
1	B	256	ALA	4.1
1	B	198	ALA	4.1
1	B	250	PRO	4.0
1	B	200	LEU	4.0
1	B	177	GLY	4.0
1	B	196	LEU	4.0
3	E	159	SER	3.9
1	B	255	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	174	HIS	3.9
1	A	254	SER	3.9
1	A	252	GLN	3.9
1	A	263	PHE	3.8
1	A	176	ILE	3.8
1	A	261	VAL	3.8
1	B	280	GLY	3.8
3	G	189	SER	3.7
1	A	133	GLY	3.6
1	B	182	ILE	3.6
1	A	249	ASP	3.6
1	A	134	ASN	3.6
1	A	251	ARG	3.5
1	B	186	TRP	3.5
1	B	199	MET	3.5
1	B	152	VAL	3.5
1	B	252	GLN	3.5
1	B	32	LEU	3.5
1	B	201	PHE	3.3
1	A	136	ALA	3.3
1	A	174	HIS	3.3
1	B	254	SER	3.3
1	B	197	SER	3.2
3	G	138	MET	3.2
2	D	211	ASN	3.2
3	E	1	GLU	3.2
3	E	112	LEU	3.1
1	B	28	ARG	3.1
1	A	183	PHE	3.0
1	B	242	GLY	3.0
2	D	1	GLN	3.0
2	D	105	LEU	2.9
1	B	284	ARG	2.9
3	E	217	ASP	2.9
3	E	26	GLY	2.9
1	B	220	MET	2.8
2	F	196	THR	2.8
3	G	62	GLN	2.8
1	B	283	LEU	2.8
1	A	273	ALA	2.8
1	A	268	GLY	2.7
1	B	202	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	31	THR	2.7
1	B	257	TYR	2.7
1	A	175	GLY	2.7
1	A	164	VAL	2.7
1	A	163	GLY	2.7
2	F	204	ILE	2.6
1	A	55	GLN	2.6
3	E	145	VAL	2.6
2	D	150	ASP	2.6
1	B	120	PHE	2.5
2	D	108	ALA	2.5
1	B	114	TRP	2.5
1	B	133	GLY	2.5
1	A	168	LEU	2.5
1	B	243	ASP	2.5
1	A	209	PHE	2.5
2	D	188	HIS	2.5
1	B	175	GLY	2.4
1	A	266	LEU	2.4
1	A	56	PRO	2.4
1	A	242	GLY	2.4
1	B	219	TYR	2.3
1	B	262	TRP	2.3
1	A	110	SER	2.3
1	A	265	ILE	2.3
3	G	174	GLN	2.3
3	G	188	SER	2.3
1	B	260	LEU	2.3
1	A	135	VAL	2.2
1	B	259	PRO	2.2
1	B	172	LEU	2.2
1	A	157	PHE	2.2
1	A	144	LEU	2.2
2	F	105	LEU	2.1
3	E	78	THR	2.1
2	F	200	SER	2.1
3	E	160	GLY	2.1
1	A	236	LEU	2.1
1	B	30	THR	2.1
1	A	92	ALA	2.1
3	E	27	TYR	2.1
3	E	124	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	136	ALA	2.0
1	A	185	LYS	2.0
1	A	93	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

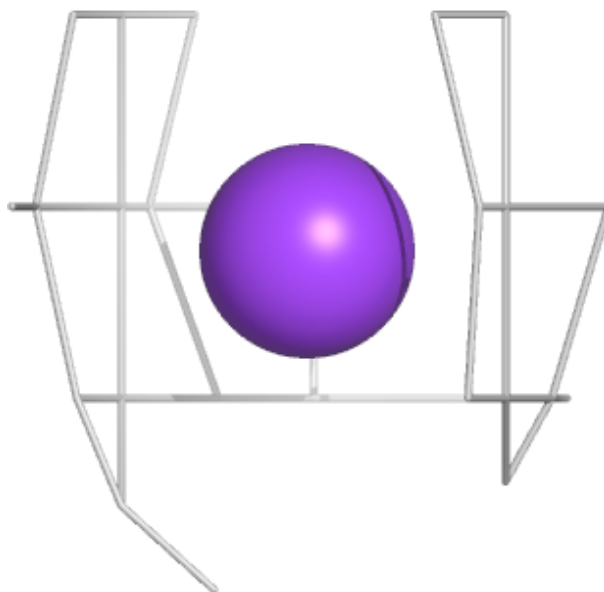
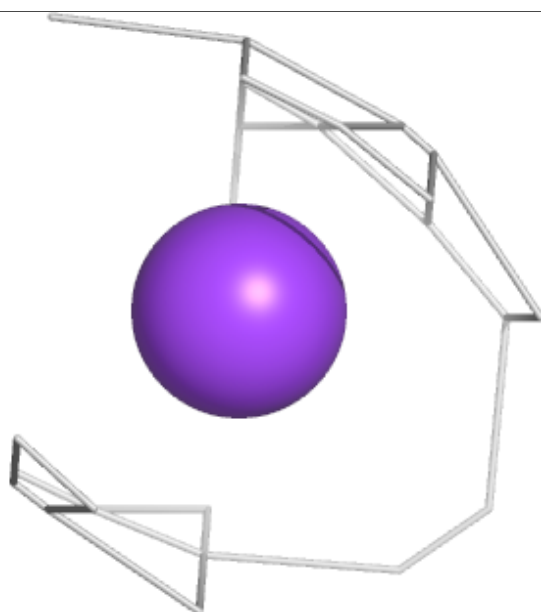
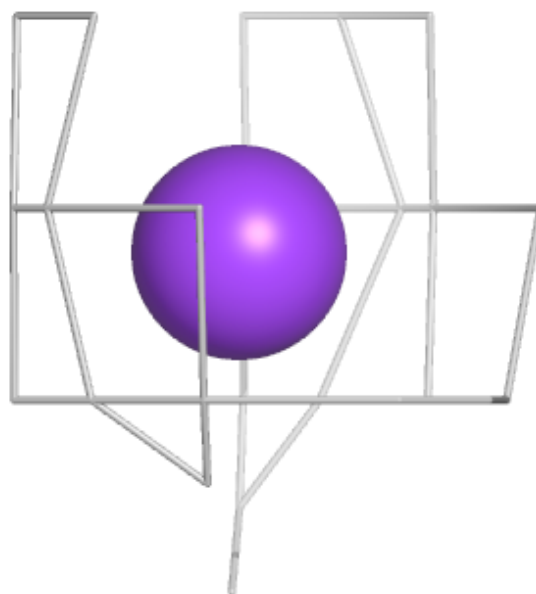
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K	A	306	1/1	0.77	0.49	113,113,113,113	0
4	K	A	302	1/1	0.89	0.17	111,111,111,111	0
4	K	A	303	1/1	0.93	0.44	99,99,99,99	0
4	K	B	302	1/1	0.95	0.11	103,103,103,103	0
5	CA	A	304	1/1	0.95	0.07	99,99,99,99	0
4	K	A	301	1/1	0.97	0.06	103,103,103,103	0
4	K	B	301	1/1	0.97	0.24	92,92,92,92	0
5	CA	A	305	1/1	0.97	0.08	113,113,113,113	0
5	CA	G	301	1/1	0.98	0.15	100,100,100,100	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.

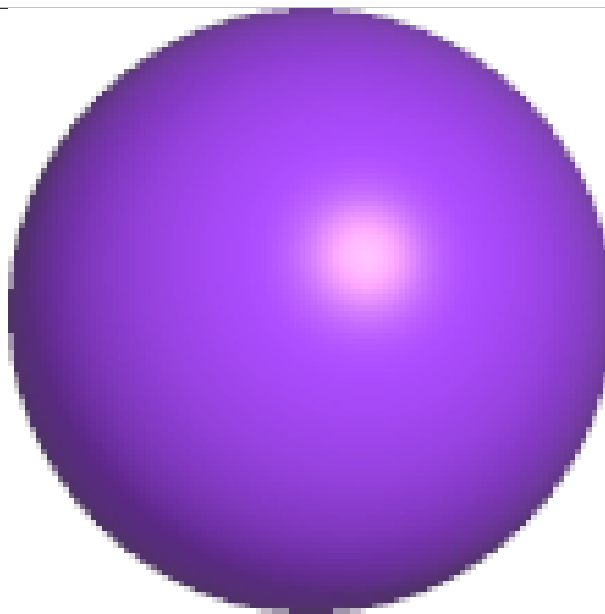
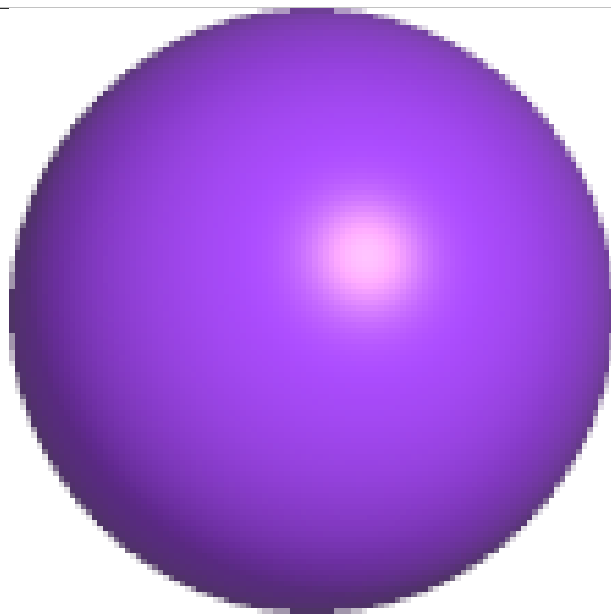
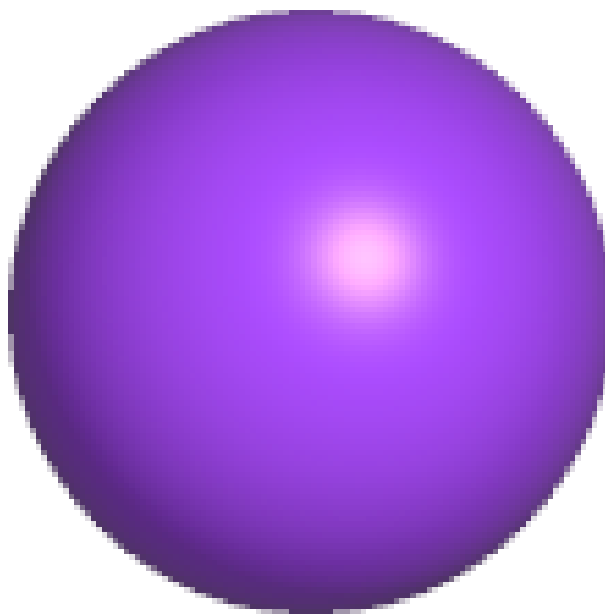
Electron density around K A 306:

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



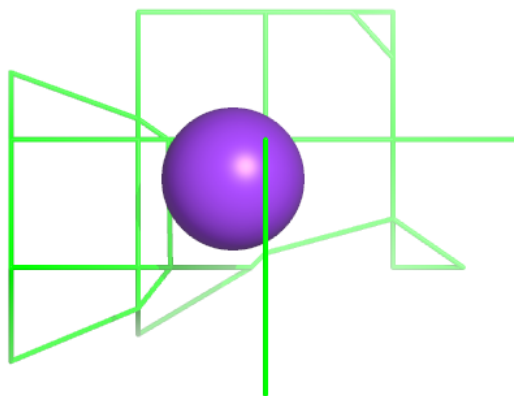
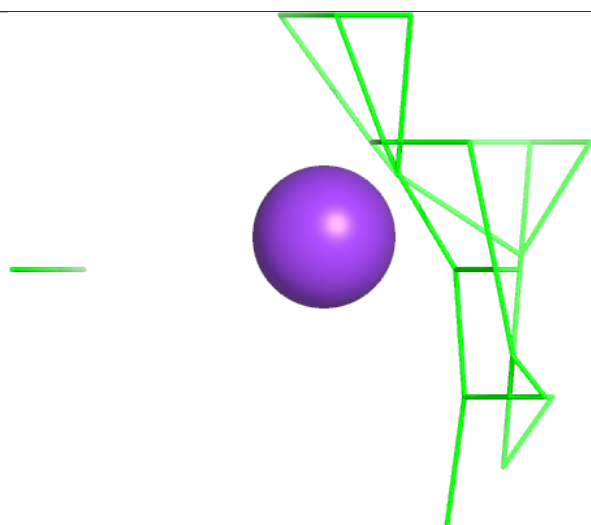
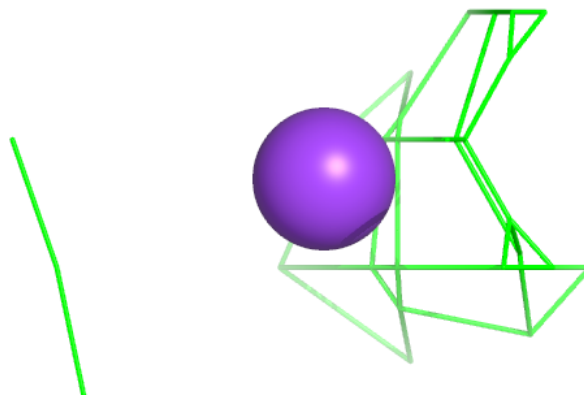
Electron density around K A 302:

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



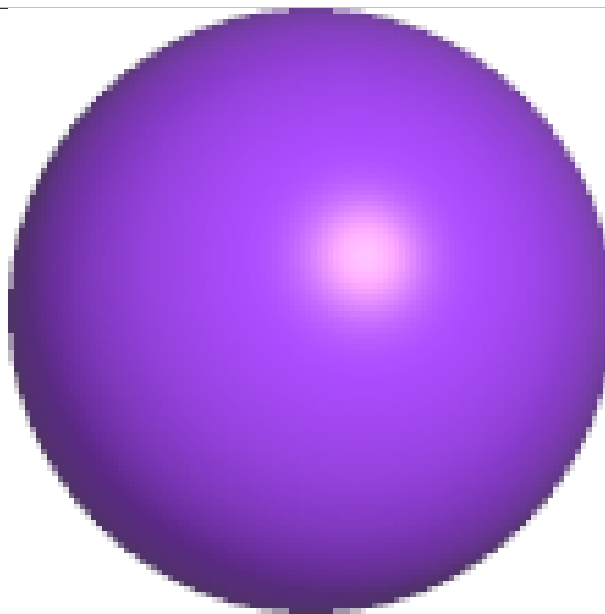
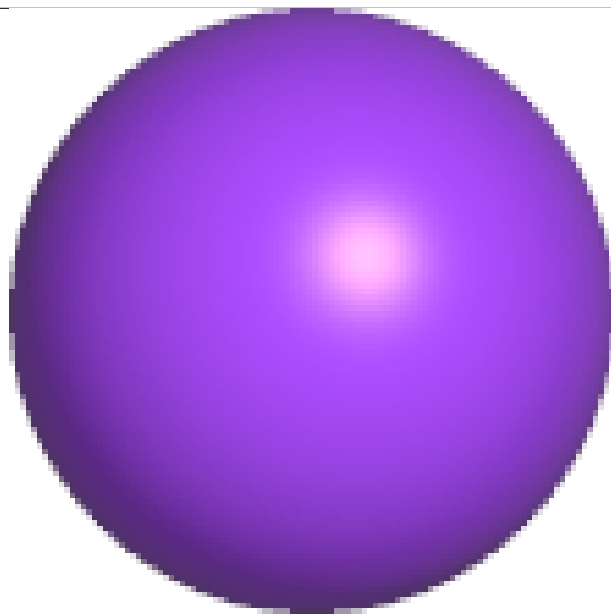
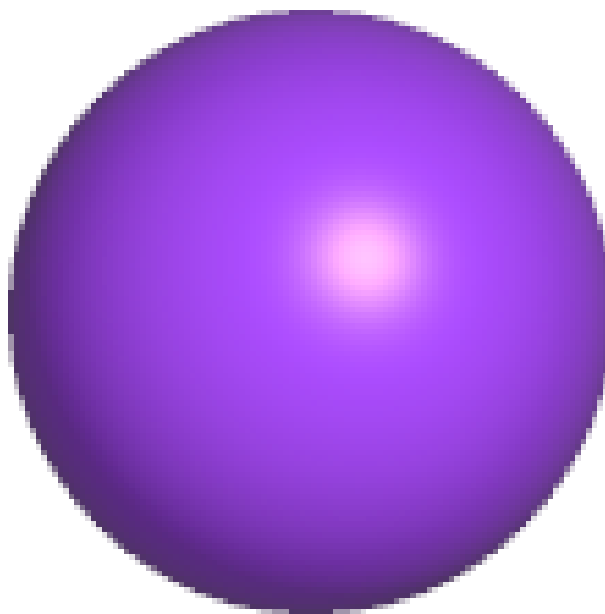
Electron density around K A 303:

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



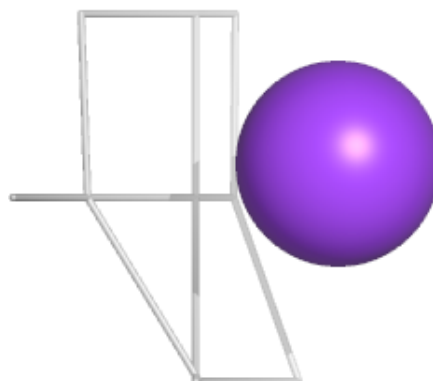
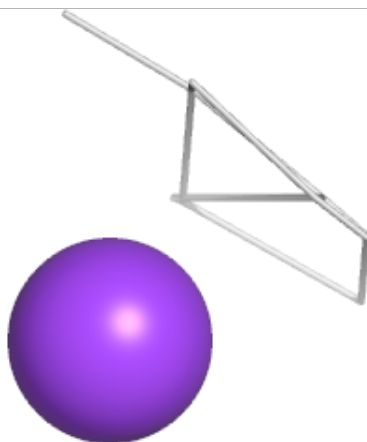
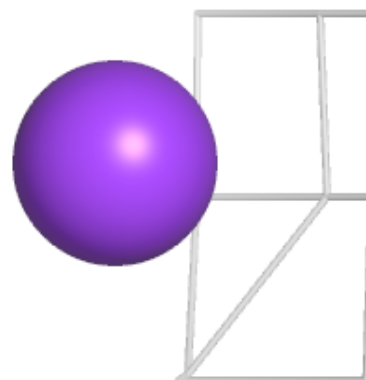
Electron density around K B 302:

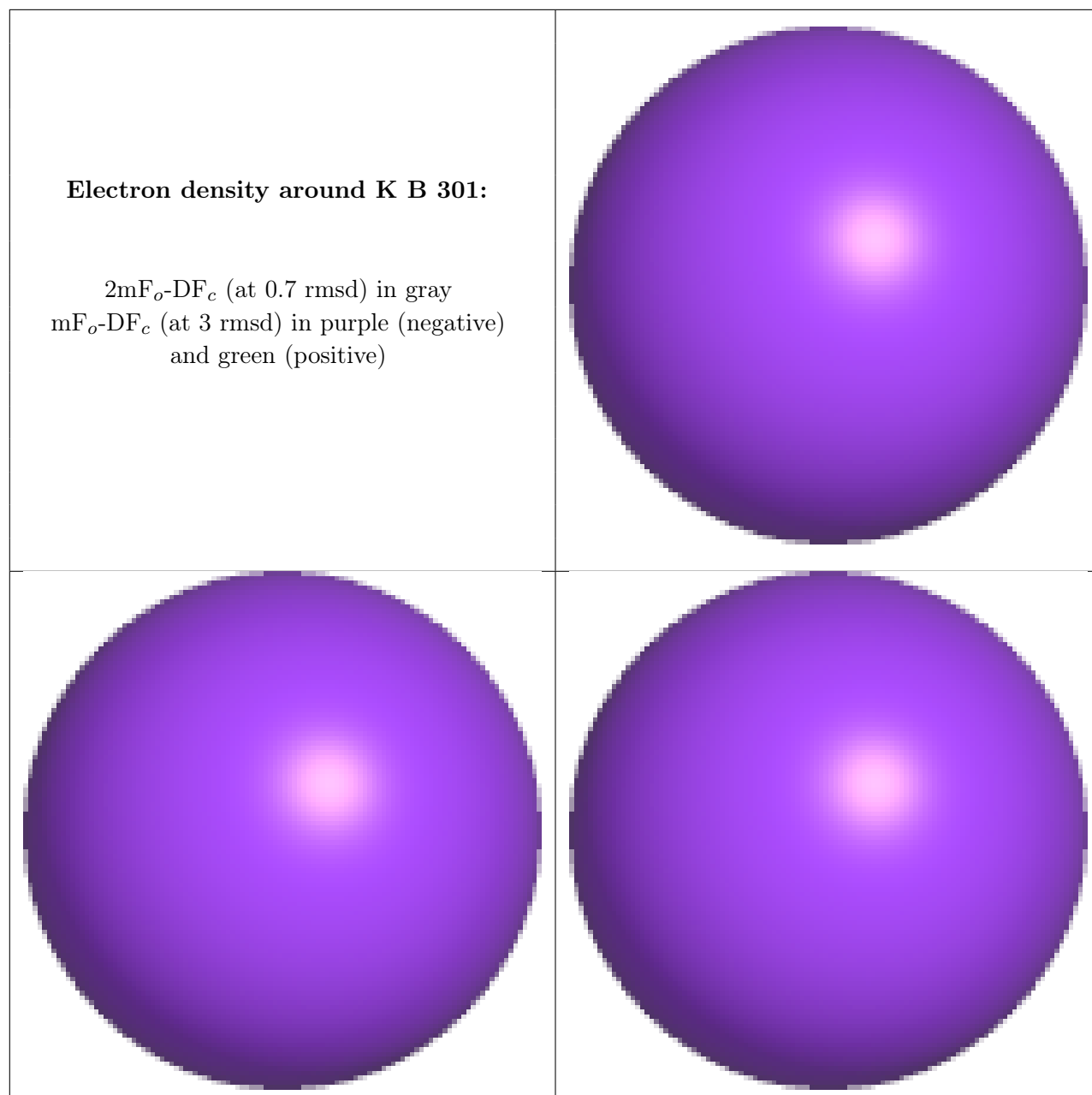
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around K A 301:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.