



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2021 – 04:04 PM EDT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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:

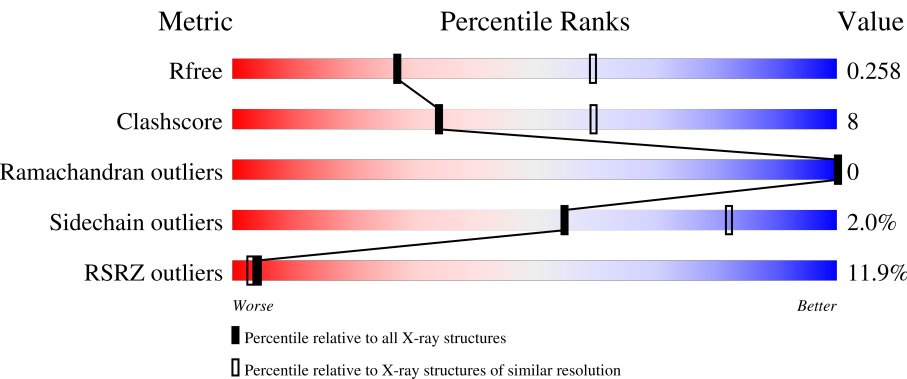
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	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  $\geq 3$ , 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><div></div><div>66%</div><div>19%</div><div>15%</div></div></div>
1	B	299	<div><div>26%</div><div><div></div><div>70%</div><div>15%</div><div>15%</div></div></div>
2	D	211	<div><div>2%</div><div><div></div><div>84%</div><div>15%</div><div>.</div></div></div>
2	F	211	<div><div>3%</div><div><div></div><div>87%</div><div>12%</div><div>.</div></div></div>
3	E	217	<div><div>2%</div><div><div></div><div>82%</div><div>14%</div><div>..</div></div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	G	217	<div><div></div><div>5%</div><div>79%</div><div>17%</div><div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10596 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Isoform 2 of Potassium channel subfamily K member 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1965	1301	318	340	6			
1	B	255	Total	C	N	O	S	0	0	0
			1982	1310	321	345	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	GLN	ASN	engineered mutation	UNP Q9NYG8-2
A	108	GLN	ASN	engineered mutation	UNP Q9NYG8-2
A	270	PRO	ALA	engineered mutation	UNP Q9NYG8-2
A	291	SER	-	expression tag	UNP Q9NYG8-2
A	292	ASN	-	expression tag	UNP Q9NYG8-2
A	293	SER	-	expression tag	UNP Q9NYG8-2
A	294	LEU	-	expression tag	UNP Q9NYG8-2
A	295	GLU	-	expression tag	UNP Q9NYG8-2
A	296	VAL	-	expression tag	UNP Q9NYG8-2
A	297	LEU	-	expression tag	UNP Q9NYG8-2
A	298	PHE	-	expression tag	UNP Q9NYG8-2
A	299	GLN	-	expression tag	UNP Q9NYG8-2
B	104	GLN	ASN	engineered mutation	UNP Q9NYG8-2
B	108	GLN	ASN	engineered mutation	UNP Q9NYG8-2
B	270	PRO	ALA	engineered mutation	UNP Q9NYG8-2
B	291	SER	-	expression tag	UNP Q9NYG8-2
B	292	ASN	-	expression tag	UNP Q9NYG8-2
B	293	SER	-	expression tag	UNP Q9NYG8-2
B	294	LEU	-	expression tag	UNP Q9NYG8-2
B	295	GLU	-	expression tag	UNP Q9NYG8-2
B	296	VAL	-	expression tag	UNP Q9NYG8-2
B	297	LEU	-	expression tag	UNP Q9NYG8-2
B	298	PHE	-	expression tag	UNP Q9NYG8-2
B	299	GLN	-	expression tag	UNP Q9NYG8-2

- Molecule 2 is a protein called ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	211	Total	C	N	O	S	0	0	0
			1616	1003	271	333	9			
2	F	211	Total	C	N	O	S	0	0	0
			1616	1003	271	333	9			

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	K	0	0
			5	5		
4	B	2	Total	K	0	0
			2	2		

- Molecule 5 is CALCIUM ION (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	33	Total	O	0	0
			33	33		
6	B	31	Total	O	0	0
			31	31		
6	D	24	Total	O	0	0
			24	24		

*Continued on next page...*

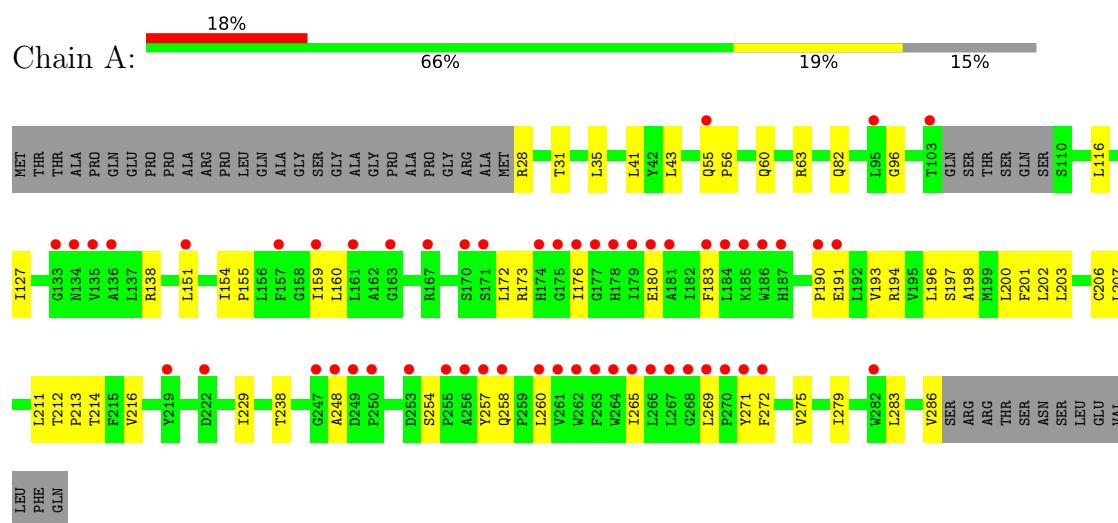
*Continued from previous page...*

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

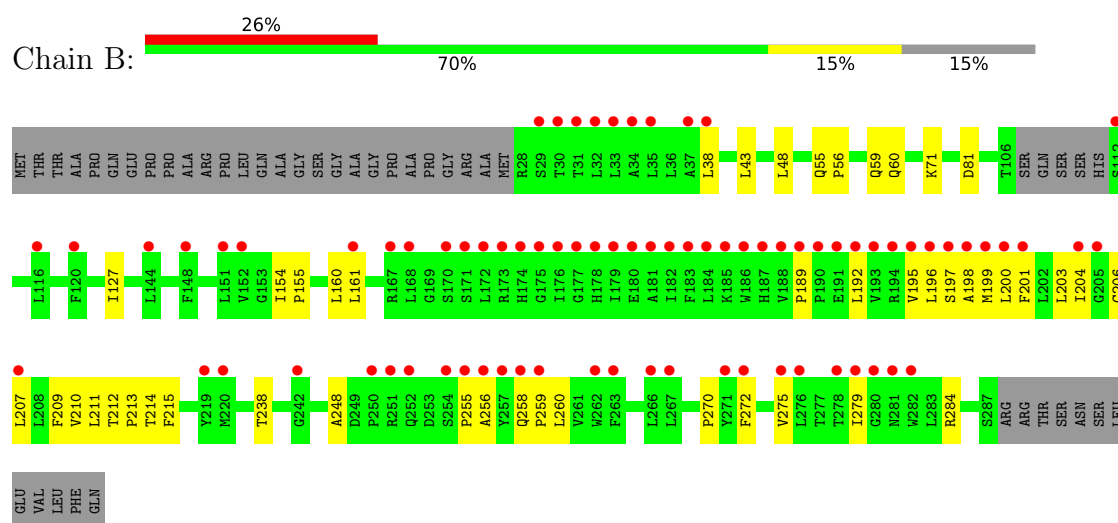
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

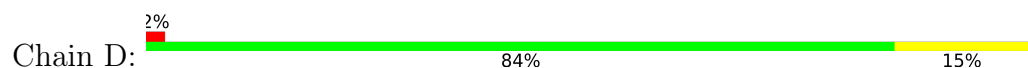
- Molecule 1: Isoform 2 of Potassium channel subfamily K member 4

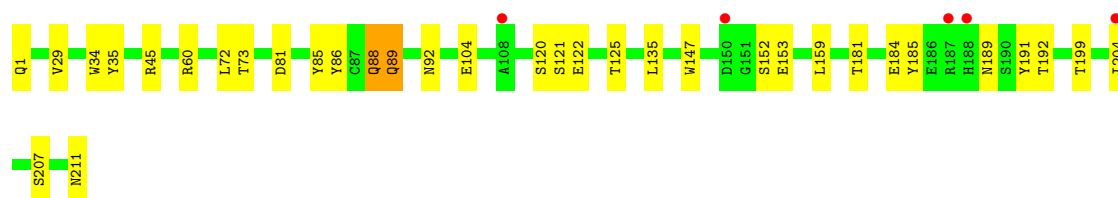


- Molecule 1: Isoform 2 of Potassium channel subfamily K member 4

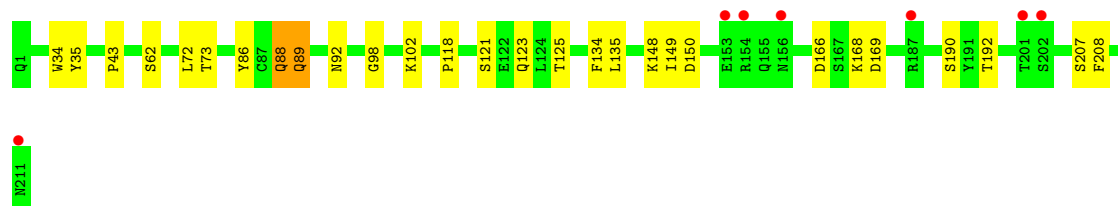
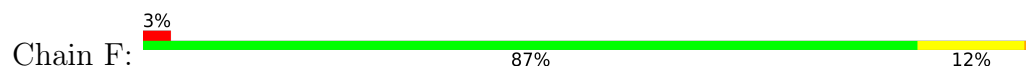


- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN

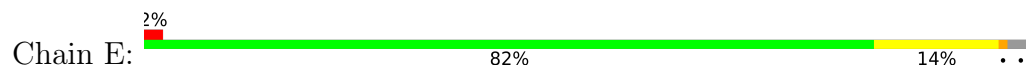




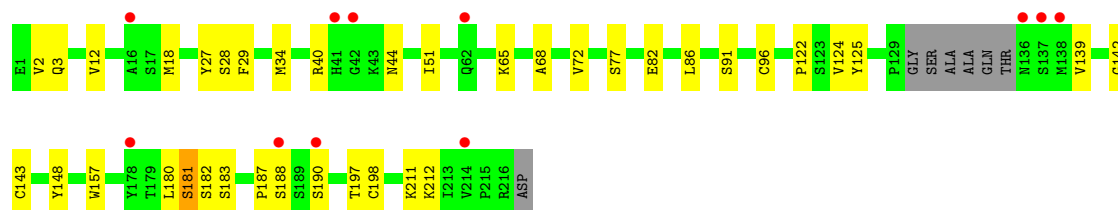
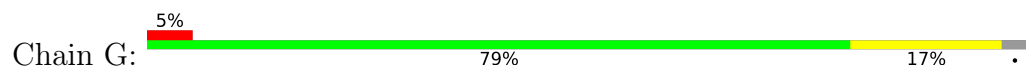
• Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.28Å 136.88Å 95.58Å 90.00° 94.24° 90.00°	Depositor
Resolution (Å)	47.66 – 2.78 47.66 – 2.78	Depositor EDS
% Data completeness (in resolution range)	63.2 (47.66-2.78) 63.3 (47.66-2.78)	Depositor EDS
$R_{merge}$	0.39	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.214 , 0.258 0.217 , 0.258	Depositor DCC
$R_{free}$ test set	1619 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.1	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	10596	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: K, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.69	0/2016	0.81	0/2750
1	B	0.73	0/2033	0.80	0/2773
2	D	0.72	0/1655	0.86	1/2247 (0.0%)
2	F	0.72	0/1655	0.89	0/2247
3	E	0.70	0/1656	0.89	1/2260 (0.0%)
3	G	0.70	0/1647	0.88	0/2249
All	All	0.71	0/10662	0.85	2/14526 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	45	ARG	NE-CZ-NH2	-6.86	116.87	120.30
3	E	143	CYS	CA-CB-SG	-5.47	104.16	114.00

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	1965	0	1986	46	1
1	B	1982	0	2005	40	0
2	D	1616	0	1542	20	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1616	0	1542	21	0
3	E	1614	0	1586	29	0
3	G	1605	0	1582	32	0
4	A	5	0	0	0	0
4	B	2	0	0	0	0
5	A	2	0	0	0	0
5	G	1	0	0	0	0
6	A	33	0	0	0	0
6	B	31	0	0	1	0
6	D	24	0	0	1	0
6	E	37	0	0	3	0
6	F	34	0	0	5	0
6	G	29	0	0	1	0
All	All	10596	0	10243	174	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 8.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ALA:O	1:A:201:PHE:HB3	1.80	0.82
2:F:35:TYR:HE1	2:F:88:GLN:HG2	1.45	0.81
2:D:35:TYR:HE2	2:D:88:GLN:HG2	1.47	0.79
1:B:195:VAL:O	1:B:199:MET:HG2	1.88	0.74
1:A:176:ILE:HD11	1:A:201:PHE:CD1	2.23	0.73
1:B:198:ALA:O	1:B:201:PHE:HB3	1.89	0.72
2:F:35:TYR:CE1	2:F:88:GLN:HG2	2.26	0.70
6:F:301:HOH:O	3:G:44:ASN:HA	1.90	0.70
2:D:181:THR:HG23	2:D:184:GLU:H	1.57	0.69
3:E:10:GLU:OE2	6:E:301:HOH:O	2.09	0.69
3:E:28:SER:HB2	3:G:28:SER:HB2	1.75	0.68
2:D:35:TYR:CE2	2:D:88:GLN:HG2	2.28	0.68
1:B:256:ALA:O	1:B:259:PRO:HD2	1.95	0.67
1:A:172:LEU:HD13	1:A:201:PHE:CE1	2.30	0.67
3:E:12:VAL:HG21	3:E:86:LEU:HD12	1.79	0.65
1:A:116:LEU:HD21	1:B:48:LEU:HD23	1.79	0.65
2:F:134:PHE:CE2	3:G:183:SER:HB3	2.31	0.65
3:E:10:GLU:C	3:E:11:LEU:HD12	2.17	0.65
1:A:172:LEU:HB3	1:A:201:PHE:HE1	1.62	0.65
3:G:12:VAL:HG21	3:G:86:LEU:HD12	1.78	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:PRO:HB2	1:B:192:LEU:HD13	1.78	0.64
1:B:200:LEU:C	1:B:200:LEU:HD13	2.19	0.63
3:E:83:LEU:HB3	3:E:86:LEU:HD21	1.80	0.63
1:A:214:THR:HG21	1:A:229:ILE:HG12	1.82	0.62
1:B:211:LEU:O	1:B:215:PHE:HD1	1.83	0.61
1:A:265:ILE:CG2	1:A:269:LEU:HD11	2.29	0.61
1:A:96:GLY:O	1:A:138:ARG:NH2	2.33	0.61
3:E:180:LEU:C	3:E:180:LEU:HD12	2.21	0.61
1:A:127:ILE:HD13	1:B:43:LEU:HD21	1.83	0.60
1:A:212:THR:HB	1:A:213:PRO:HD3	1.83	0.60
1:A:265:ILE:HG23	1:A:269:LEU:HD11	1.83	0.59
1:A:200:LEU:HD13	1:A:200:LEU:O	2.02	0.59
3:G:180:LEU:HD12	3:G:180:LEU:C	2.23	0.59
1:A:260:LEU:HD22	1:A:260:LEU:O	2.03	0.58
1:B:206:CYS:SG	1:B:211:LEU:CD2	2.91	0.58
3:E:12:VAL:HG21	3:E:86:LEU:CD1	2.34	0.58
1:A:127:ILE:CD1	1:B:43:LEU:HD21	2.33	0.57
1:B:212:THR:HB	1:B:213:PRO:HD3	1.86	0.57
2:F:166:ASP:HB3	2:F:169:ASP:OD2	2.05	0.57
1:B:256:ALA:C	1:B:259:PRO:HD2	2.25	0.57
2:D:60:ARG:NH1	2:D:81:ASP:OD1	2.38	0.56
3:E:34:MET:CE	3:E:96:CYS:HB2	2.36	0.56
1:A:214:THR:HG21	1:A:229:ILE:CG1	2.34	0.56
1:A:269:LEU:HD12	1:A:269:LEU:N	2.21	0.55
2:D:120:SER:HB2	2:D:122:GLU:OE1	2.05	0.55
3:E:34:MET:HE1	3:E:96:CYS:HB2	1.89	0.55
3:G:139:VAL:HG23	3:G:188:SER:HB3	1.89	0.55
3:G:34:MET:CE	3:G:96:CYS:HB2	2.37	0.55
1:A:200:LEU:HD13	1:A:200:LEU:C	2.28	0.54
1:A:202:LEU:HD12	1:A:203:LEU:N	2.22	0.54
3:G:139:VAL:HG23	3:G:188:SER:HA	1.89	0.54
3:G:51:ILE:HD13	3:G:72:VAL:HG13	1.90	0.54
1:A:248:ALA:HA	1:A:258:GLN:HB3	1.89	0.54
1:A:191:GLU:H	1:A:191:GLU:CD	2.10	0.54
2:F:149:ILE:HG13	2:F:149:ILE:O	2.08	0.54
1:A:172:LEU:CB	1:A:201:PHE:HE1	2.21	0.54
1:B:161:LEU:HD11	1:B:270:PRO:HD3	1.89	0.54
1:A:82:GLN:HG3	3:E:59:THR:HG21	1.90	0.53
3:E:11:LEU:CD1	3:E:11:LEU:N	2.71	0.53
3:G:139:VAL:CG2	3:G:188:SER:HB3	2.38	0.53
1:A:254:SER:HB3	1:A:257:TYR:CD2	2.44	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:51:ILE:HD13	3:E:72:VAL:HG13	1.91	0.53
1:A:41:LEU:C	1:A:41:LEU:HD13	2.28	0.53
3:G:34:MET:HE1	3:G:96:CYS:HB2	1.90	0.52
1:A:60:GLN:OE1	1:A:63:ARG:NH2	2.42	0.52
3:E:141:LEU:HD22	3:E:213:ILE:HG21	1.90	0.52
1:B:206:CYS:SG	1:B:211:LEU:HD21	2.50	0.52
3:G:28:SER:HA	6:G:410:HOH:O	2.09	0.51
3:G:29:PHE:CD1	3:G:77:SER:HA	2.45	0.51
1:A:159:ILE:HD12	1:B:284:ARG:HD3	1.93	0.51
2:F:72:LEU:HD23	2:F:73:THR:N	2.24	0.51
2:D:147:TRP:O	2:D:153:GLU:HA	2.10	0.51
2:D:29:VAL:HG11	2:D:89:GLN:HG3	1.91	0.51
1:B:198:ALA:HA	1:B:201:PHE:HB3	1.92	0.50
2:F:134:PHE:CE2	3:G:183:SER:CB	2.94	0.50
1:A:197:SER:O	1:A:201:PHE:N	2.43	0.50
3:E:151:GLU:HG3	3:E:178:TYR:CZ	2.47	0.50
1:A:213:PRO:HA	1:A:216:VAL:HB	1.94	0.50
2:F:192:THR:HG22	2:F:207:SER:OG	2.12	0.50
3:G:2:VAL:HG13	3:G:27:TYR:CD2	2.47	0.50
1:A:172:LEU:HB3	1:A:201:PHE:CE1	2.44	0.50
1:A:206:CYS:HB2	1:A:271:TYR:OH	2.11	0.50
2:D:192:THR:HG22	2:D:207:SER:OG	2.12	0.50
3:G:139:VAL:HG23	3:G:188:SER:CA	2.41	0.49
2:D:199:THR:HG22	2:D:199:THR:O	2.12	0.49
3:E:187:PRO:O	3:E:190:SER:HB2	2.11	0.49
1:B:59:GLN:HG2	6:B:405:HOH:O	2.13	0.49
2:F:98:GLY:O	6:F:301:HOH:O	2.20	0.49
2:D:72:LEU:HD23	2:D:73:THR:N	2.28	0.48
3:E:10:GLU:O	3:E:11:LEU:HD12	2.13	0.48
3:G:139:VAL:CG2	3:G:188:SER:HA	2.44	0.48
2:D:185:TYR:HA	2:D:191:TYR:OH	2.14	0.48
1:A:207:LEU:HD13	1:A:211:LEU:HD22	1.95	0.47
1:A:283:LEU:O	1:A:286:VAL:HB	2.13	0.47
2:D:159:LEU:HD21	3:E:174:GLN:NE2	2.29	0.47
1:A:160:LEU:C	1:A:160:LEU:HD23	2.33	0.47
3:E:68:ALA:HA	3:E:82:GLU:O	2.15	0.47
2:F:43:PRO:O	6:F:302:HOH:O	2.20	0.47
1:B:81:ASP:HB3	6:F:325:HOH:O	2.15	0.47
2:F:62:SER:HB3	6:F:317:HOH:O	2.14	0.47
1:A:154:ILE:N	1:A:155:PRO:HD2	2.29	0.47
1:A:82:GLN:HG2	6:D:307:HOH:O	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLN:HB3	1:B:259:PRO:HD3	1.96	0.47
2:F:135:LEU:HD12	2:F:135:LEU:N	2.30	0.47
1:B:154:ILE:N	1:B:155:PRO:HD2	2.29	0.46
3:G:68:ALA:HA	3:G:82:GLU:O	2.15	0.46
3:G:12:VAL:HG21	3:G:86:LEU:CD1	2.44	0.46
1:B:200:LEU:HD13	1:B:200:LEU:O	2.16	0.46
2:F:118:PRO:HB3	2:F:208:PHE:CZ	2.51	0.46
3:G:2:VAL:O	3:G:3:GLN:HG2	2.16	0.46
3:G:187:PRO:O	3:G:190:SER:HB2	2.16	0.45
1:A:269:LEU:N	1:A:269:LEU:CD1	2.79	0.45
3:E:29:PHE:CD2	3:E:77:SER:HA	2.52	0.45
3:E:41:HIS:HE1	3:E:43:LYS:HB2	1.80	0.45
3:E:173:LEU:HG	3:E:178:TYR:CE2	2.52	0.45
3:G:139:VAL:HG23	3:G:188:SER:CB	2.47	0.45
1:A:190:PRO:O	1:A:194:ARG:HG2	2.17	0.45
2:D:34:TRP:HA	2:D:86:TYR:O	2.17	0.45
3:E:40:ARG:HD3	6:E:320:HOH:O	2.17	0.45
1:B:55:GLN:N	1:B:56:PRO:CD	2.80	0.44
1:B:209:PHE:O	1:B:213:PRO:HG2	2.17	0.44
1:A:28:ARG:HA	1:A:31:THR:HB	1.99	0.44
3:G:142:GLY:HA2	3:G:182:SER:O	2.18	0.44
1:B:248:ALA:N	1:B:258:GLN:HE22	2.16	0.44
1:A:183:PHE:HB3	1:A:193:VAL:HG22	1.99	0.44
1:A:35:LEU:HD23	1:B:160:LEU:HA	2.00	0.44
3:G:122:PRO:HB3	3:G:148:TYR:HB3	2.00	0.44
1:A:180:GLU:HG2	1:A:193:VAL:HG12	2.00	0.43
1:A:254:SER:CB	1:A:257:TYR:CD2	3.01	0.43
3:G:197:THR:HG22	3:G:212:LYS:HA	2.01	0.43
1:B:55:GLN:O	1:B:59:GLN:HG3	2.18	0.43
1:B:60:GLN:HA	1:B:60:GLN:OE1	2.18	0.43
1:A:173:ARG:HA	1:A:176:ILE:HB	1.99	0.43
2:F:89:GLN:HE21	2:F:92:ASN:H	1.65	0.43
1:B:197:SER:O	1:B:201:PHE:N	2.47	0.43
2:F:134:PHE:CD2	3:G:183:SER:HB3	2.53	0.43
3:E:10:GLU:C	3:E:11:LEU:CD1	2.87	0.43
1:B:200:LEU:C	1:B:200:LEU:CD1	2.87	0.43
3:G:40:ARG:NH1	3:G:91:SER:O	2.52	0.43
2:F:34:TRP:HA	2:F:86:TYR:O	2.18	0.43
3:G:124:VAL:HG12	3:G:211:LYS:HG2	2.01	0.43
2:F:118:PRO:HB3	2:F:208:PHE:CE1	2.54	0.42
1:B:203:LEU:O	1:B:207:LEU:HG	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:LEU:HD11	1:B:204:ILE:CD1	2.49	0.42
2:D:89:GLN:HE21	2:D:92:ASN:H	1.66	0.42
3:E:142:GLY:HA2	3:E:182:SER:O	2.19	0.42
3:E:157:TRP:CZ3	3:E:198:CYS:HB3	2.54	0.42
1:A:275:VAL:O	1:A:279:ILE:HG12	2.18	0.42
1:B:260:LEU:C	1:B:260:LEU:HD23	2.39	0.42
3:E:143:CYS:O	3:E:181:SER:HA	2.20	0.42
1:A:43:LEU:HD21	1:B:127:ILE:CD1	2.50	0.42
1:A:55:GLN:N	1:A:56:PRO:CD	2.83	0.42
3:E:11:LEU:HD12	3:E:11:LEU:N	2.32	0.42
1:B:196:LEU:HA	1:B:199:MET:HB2	2.03	0.41
2:F:150:ASP:HA	2:F:190:SER:OG	2.20	0.41
3:G:157:TRP:CZ3	3:G:198:CYS:HB3	2.55	0.41
1:B:255:PRO:O	1:B:259:PRO:HD3	2.21	0.41
2:D:35:TYR:O	2:D:85:TYR:HA	2.21	0.41
2:D:121:SER:O	2:D:125:THR:HG23	2.21	0.41
1:B:275:VAL:O	1:B:279:ILE:HG22	2.20	0.41
2:D:189:ASN:ND2	2:D:211:ASN:OD1	2.38	0.41
2:F:121:SER:O	2:F:125:THR:HG23	2.20	0.41
2:D:135:LEU:N	2:D:135:LEU:HD12	2.35	0.41
1:B:255:PRO:O	1:B:259:PRO:CD	2.69	0.41
2:F:148:LYS:HB2	2:F:192:THR:OG1	2.21	0.41
3:G:139:VAL:CG2	3:G:188:SER:CB	2.98	0.41
3:E:11:LEU:HD11	6:E:315:HOH:O	2.20	0.41
2:F:123:GLN:HG3	3:G:125:TYR:CE2	2.56	0.40
3:G:143:CYS:O	3:G:181:SER:HA	2.21	0.40
2:D:159:LEU:HD11	3:E:174:GLN:CD	2.42	0.40
1:B:38:LEU:HD23	1:B:38:LEU:C	2.41	0.40
1:B:210:VAL:O	1:B:214:THR:HG23	2.21	0.40
1:B:197:SER:O	1:B:200:LEU:HB3	2.21	0.40
2:D:192:THR:HG22	2:D:207:SER:CB	2.52	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLU:OE2	2:D:153:GLU:N[2_645]	2.17	0.03

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

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

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/243 (84%)	201 (98%)	4 (2%)	55	82
1	B	208/243 (86%)	205 (99%)	3 (1%)	67	87
2	D	184/184 (100%)	178 (97%)	6 (3%)	38	69
2	F	184/184 (100%)	180 (98%)	4 (2%)	52	80
3	E	187/190 (98%)	184 (98%)	3 (2%)	62	86
3	G	186/190 (98%)	183 (98%)	3 (2%)	62	86
All	All	1154/1234 (94%)	1131 (98%)	23 (2%)	55	82



All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	LEU
1	A	196	LEU
1	A	238	THR
1	A	272	PHE
1	B	71	LYS
1	B	238	THR
1	B	272	PHE
2	D	1	GLN
2	D	88	GLN
2	D	89	GLN
2	D	104	GLU
2	D	152	SER
2	D	204	ILE
3	E	11	LEU
3	E	18	MET
3	E	181	SER
2	F	88	GLN
2	F	89	GLN
2	F	102	LYS
2	F	168	LYS
3	G	18	MET
3	G	65	LYS
3	G	181	SER

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	258	GLN
2	D	136	ASN
2	D	144	ASN
3	E	44	ASN
3	E	167	HIS
3	E	174	GLN
2	F	92	ASN
3	G	174	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	253/299 (84%)	1.14	55 (21%) 0 0	42, 108, 168, 188	0
1	B	255/299 (85%)	1.86	79 (30%) 0 0	40, 100, 179, 223	0
2	D	211/211 (100%)	0.05	5 (2%) 59 54	32, 57, 94, 114	0
2	F	211/211 (100%)	0.14	7 (3%) 46 41	33, 58, 102, 125	0
3	E	211/217 (97%)	0.10	4 (1%) 66 63	30, 50, 77, 112	0
3	G	210/217 (96%)	0.22	11 (5%) 27 22	33, 53, 82, 129	0
All	All	1351/1454 (92%)	0.64	161 (11%) 4 3	30, 64, 154, 223	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	LEU	15.1
1	B	190	PRO	12.6
3	G	136	ASN	11.9
1	A	174	HIS	11.0
1	B	189	PRO	10.9
1	B	251	ARG	10.8
1	B	181	ALA	10.3
1	B	193	VAL	10.2
1	A	179	ILE	9.6
1	A	248	ALA	9.5
1	A	256	ALA	8.7
1	B	188	VAL	8.6
1	B	179	ILE	8.6
1	B	257	TYR	8.2
1	B	252	GLN	8.0
1	B	219	TYR	7.9
1	B	186	TRP	7.6
3	G	41	HIS	7.2
1	B	182	ILE	6.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	257	TYR	6.9
1	B	180	GLU	6.8
1	A	255	PRO	6.8
3	G	137	SER	6.6
1	B	183	PHE	6.5
1	B	187	HIS	6.4
1	A	178	HIS	6.4
1	B	178	HIS	6.3
1	B	255	PRO	6.3
1	B	176	ILE	6.3
1	B	30	THR	6.1
1	B	31	THR	6.1
1	B	197	SER	6.0
1	B	250	PRO	6.0
1	A	183	PHE	6.0
1	B	173	ARG	6.0
1	B	259	PRO	5.9
1	B	34	ALA	5.8
1	B	116	LEU	5.8
1	B	177	GLY	5.6
1	B	184	LEU	5.5
1	B	276	LEU	5.5
1	B	191	GLU	5.5
1	B	220	MET	5.5
1	A	170	SER	5.4
1	B	263	PHE	5.2
1	B	185	LYS	5.2
3	E	136	ASN	5.1
1	B	171	SER	5.1
1	A	180	GLU	5.0
1	B	256	ALA	4.9
1	B	174	HIS	4.9
1	B	32	LEU	4.8
1	A	263	PHE	4.8
1	A	270	PRO	4.7
1	B	194	ARG	4.5
1	A	175	GLY	4.5
1	A	262	TRP	4.5
2	F	156	ASN	4.5
1	B	278	THR	4.5
2	F	201	THR	4.5
1	B	198	ALA	4.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	196	LEU	4.4
1	B	201	PHE	4.3
1	B	275	VAL	4.2
1	B	195	VAL	4.1
1	B	281	ASN	4.1
1	B	199	MET	3.9
1	A	258	GLN	3.9
3	E	137	SER	3.9
1	B	175	GLY	3.9
1	A	247	GLY	3.9
2	D	187	ARG	3.8
1	B	266	LEU	3.8
1	A	269	LEU	3.8
1	A	190	PRO	3.8
1	A	266	LEU	3.7
1	A	176	ILE	3.7
1	B	33	LEU	3.7
1	A	187	HIS	3.5
1	B	168	LEU	3.5
1	A	161	LEU	3.5
2	F	202	SER	3.5
1	B	38	LEU	3.5
1	A	249	ASP	3.4
1	B	200	LEU	3.4
1	B	172	LEU	3.4
1	B	148	PHE	3.4
3	G	188	SER	3.4
1	B	167	ARG	3.3
1	A	186	TRP	3.3
1	A	135	VAL	3.3
2	D	150	ASP	3.3
1	A	260	LEU	3.3
1	B	35	LEU	3.3
1	B	271	TYR	3.2
1	A	261	VAL	3.1
1	B	262	TRP	3.1
1	A	134	ASN	3.1
1	A	253	ASP	3.1
1	B	151	LEU	3.0
2	D	108	ALA	3.0
1	A	136	ALA	3.0
1	B	254	SER	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	242	GLY	3.0
1	B	258	GLN	3.0
1	B	204	ILE	3.0
1	B	280	GLY	2.9
1	A	159	ILE	2.9
1	A	151	LEU	2.9
3	G	62	GLN	2.9
3	E	1	GLU	2.9
1	A	250	PRO	2.9
1	A	267	LEU	2.8
1	A	55	GLN	2.8
2	F	187	ARG	2.8
1	B	37	ALA	2.8
3	G	138	MET	2.8
1	B	112	SER	2.8
3	G	42	GLY	2.8
2	F	154	ARG	2.8
1	B	152	VAL	2.7
1	B	205	GLY	2.7
1	A	191	GLU	2.7
1	B	282	TRP	2.7
1	B	272	PHE	2.6
1	A	163	GLY	2.6
1	B	279	ILE	2.6
1	A	133	GLY	2.6
2	D	188	HIS	2.6
1	A	282	TRP	2.5
1	A	181	ALA	2.5
1	A	219	TYR	2.5
1	A	265	ILE	2.5
1	B	144	LEU	2.5
1	A	272	PHE	2.5
1	B	120	PHE	2.4
2	D	204	ILE	2.4
2	F	153	GLU	2.4
1	A	177	GLY	2.3
1	A	157	PHE	2.3
1	A	264	TRP	2.3
2	F	211	ASN	2.3
1	A	271	TYR	2.3
3	G	214	VAL	2.3
3	G	16	ALA	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	222	ASP	2.3
1	B	29	SER	2.2
1	A	268	GLY	2.2
3	E	216	ARG	2.2
1	B	170	SER	2.2
1	B	207	LEU	2.2
1	A	185	LYS	2.2
1	B	267	LEU	2.2
1	A	95	LEU	2.2
1	A	103	THR	2.1
1	A	171	SER	2.1
3	G	190	SER	2.1
3	G	178	TYR	2.1
1	A	184	LEU	2.0
1	B	161	LEU	2.0
1	A	167	ARG	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<sup>th</sup> 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.

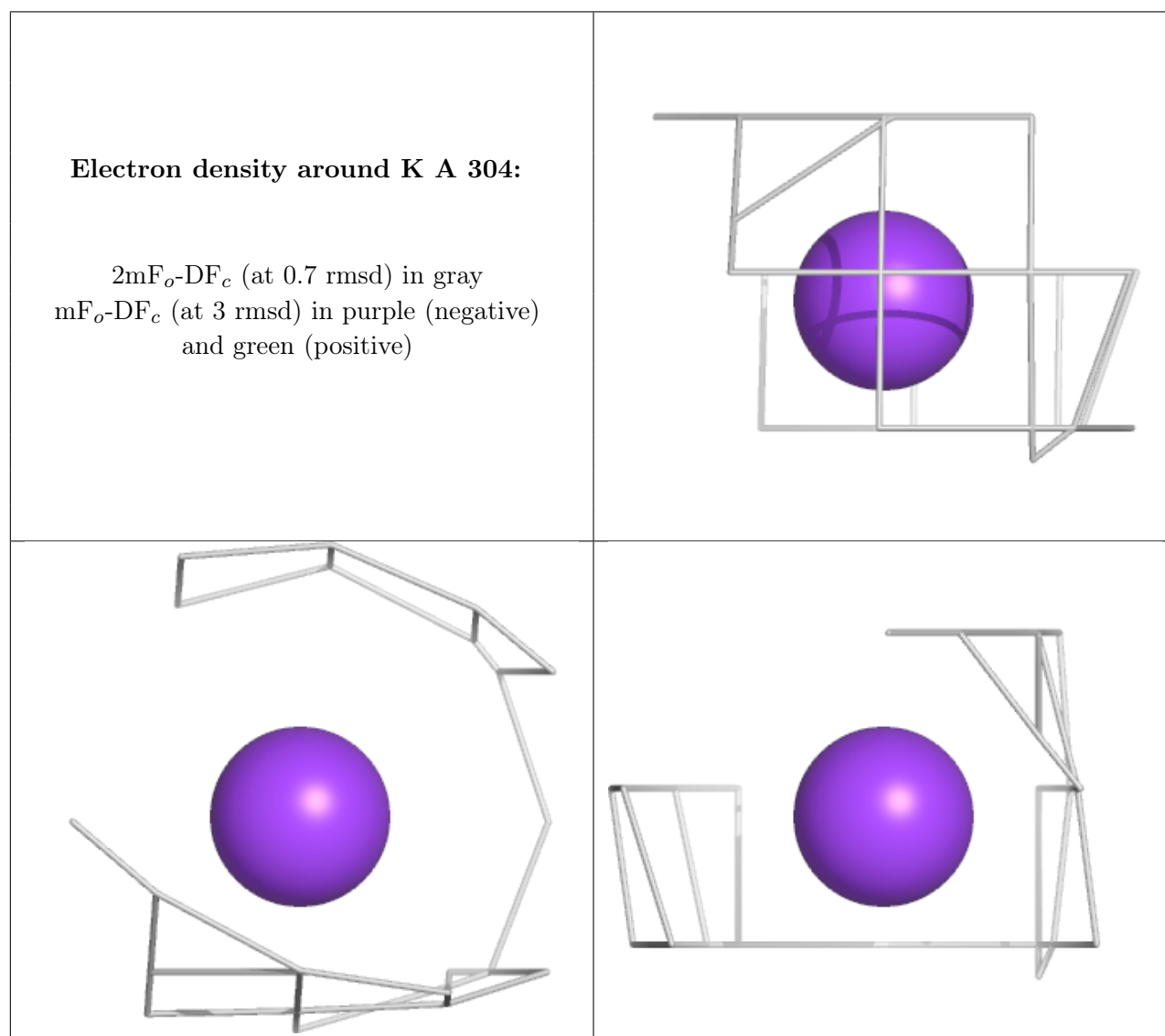
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	K	A	304	1/1	0.67	0.24	88,88,88,88	0
5	CA	A	305	1/1	0.72	0.07	120,120,120,120	0
5	CA	A	306	1/1	0.81	0.23	118,118,118,118	0
4	K	B	302	1/1	0.88	0.51	86,86,86,86	0
4	K	B	301	1/1	0.94	0.32	70,70,70,70	0
4	K	A	303	1/1	0.98	0.23	36,36,36,36	0
4	K	A	302	1/1	0.99	0.22	27,27,27,27	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	K	A	307	1/1	0.99	0.25	37,37,37,37	0
4	K	A	301	1/1	0.99	0.25	29,29,29,29	0
5	CA	G	301	1/1	0.99	0.08	50,50,50,50	0

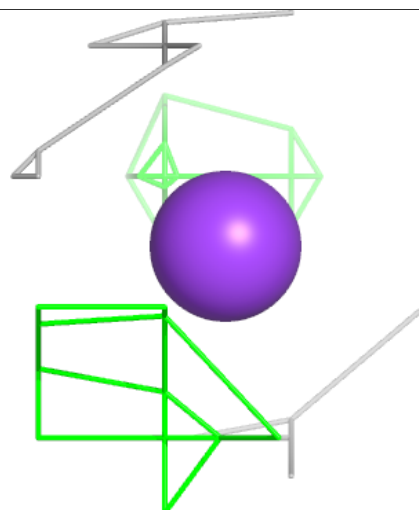
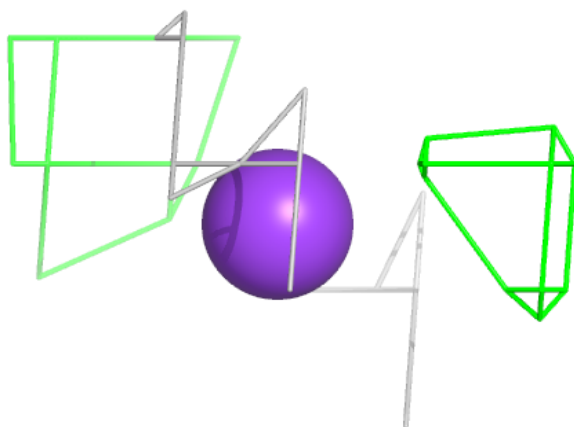
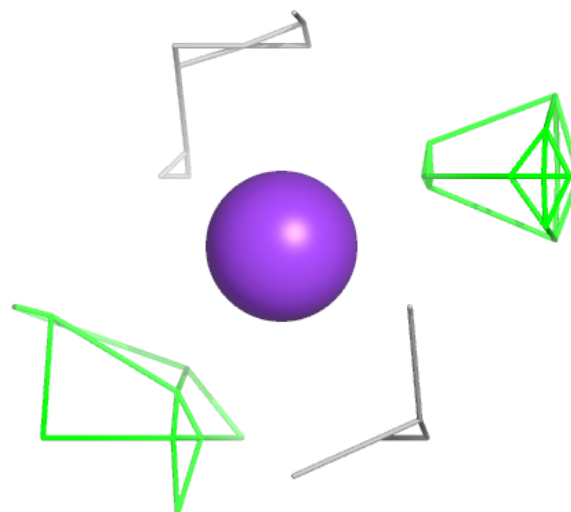
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





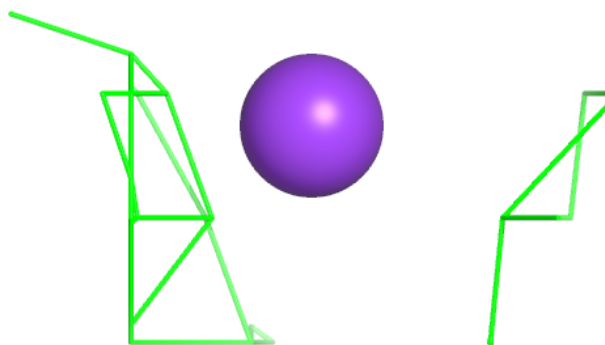
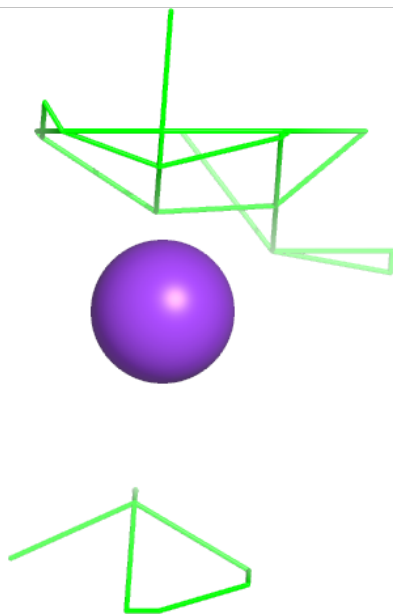
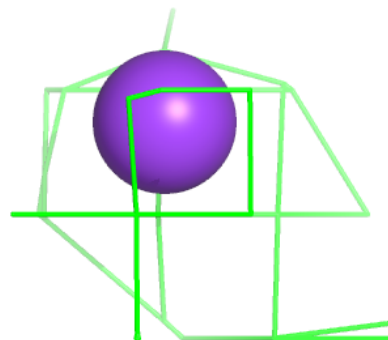
**Electron density around K B 302:**

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



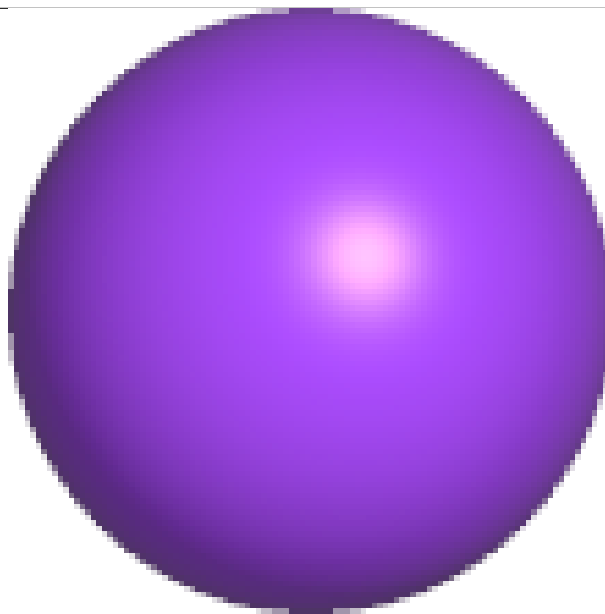
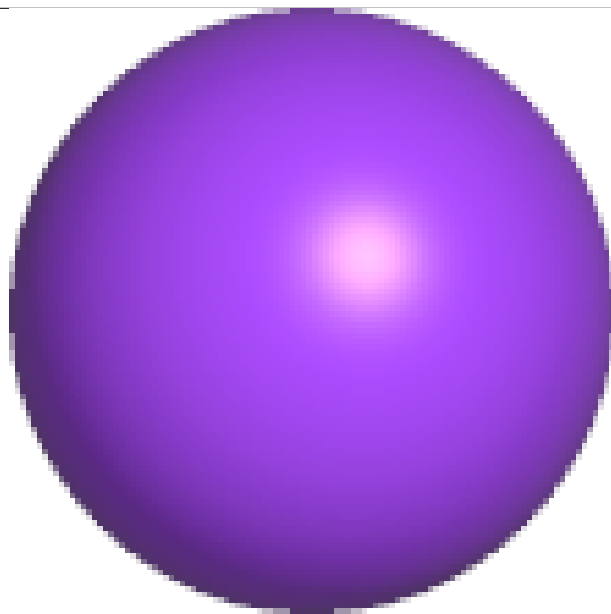
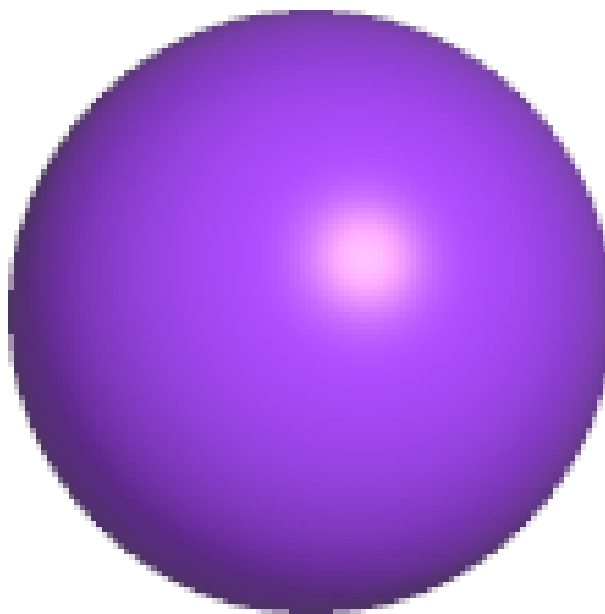
**Electron density around K B 301:**

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



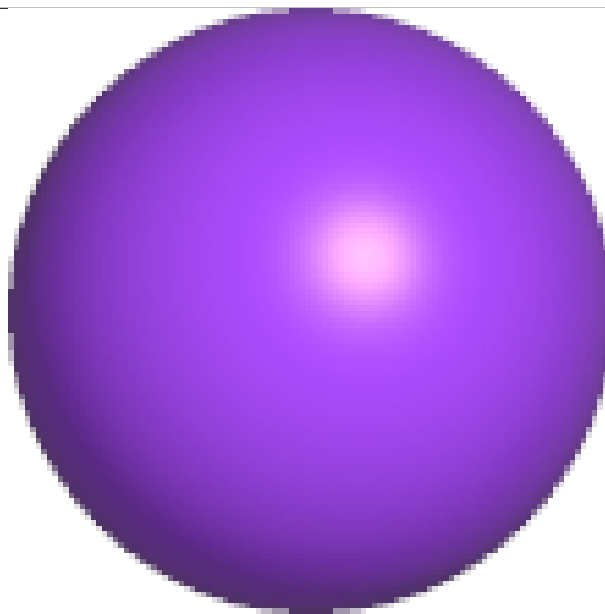
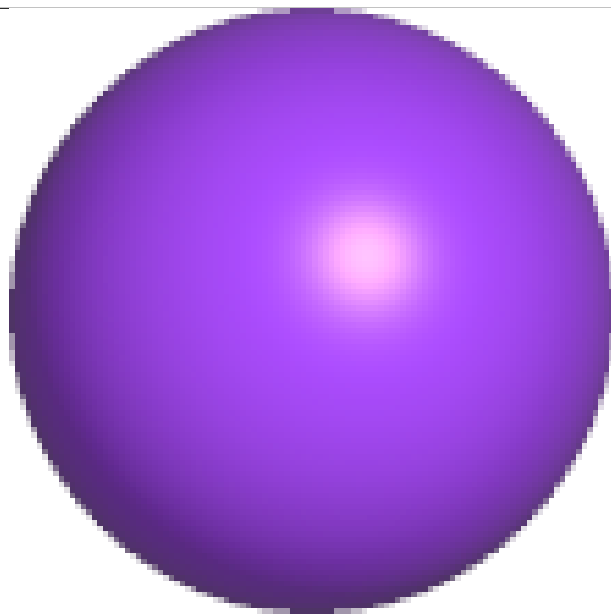
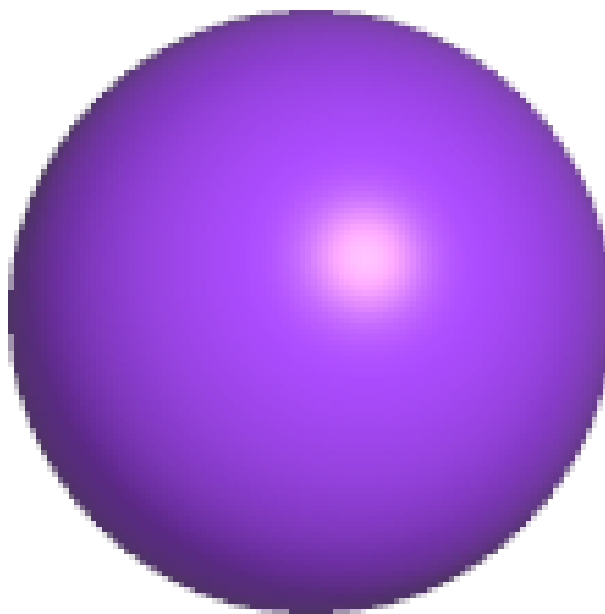
**Electron density around K A 303:**

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



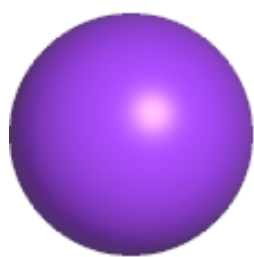
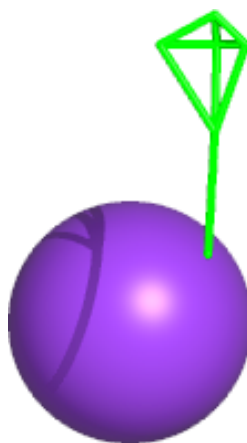
**Electron density around K A 302:**

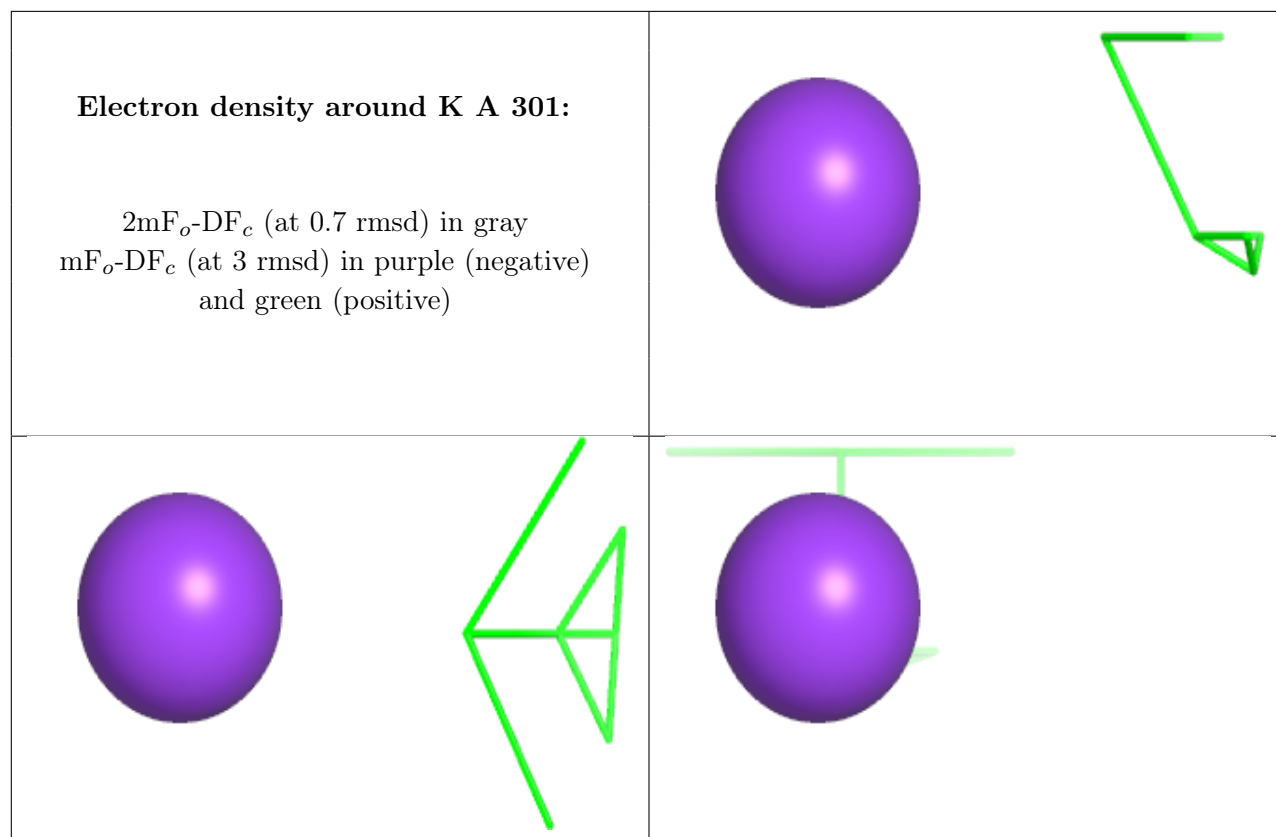
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around K 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.