Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 01:44 PM EDT

PDB ID	:	7KD9
Title	:	Crystal Structure of Gallic Acid Decarboxylase from Arxula adeninivorans
Authors	:	Zeug, M.; Markovic, N.; Iancu, C.V.; Tripp, J.; Oreb, M.; Choe, J.
Deposited on	:	2020-10-08
Resolution	:	1.94 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 (i) 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 (1)) were used in the production of this report:

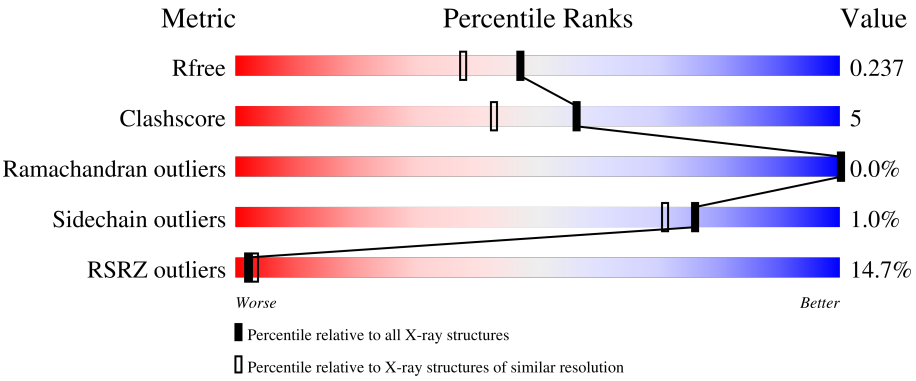
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	231	10% 93% 6%
1	B	231	11% 87% 10%
1	C	231	6% 89% 10%
1	D	231	7% 92% 6%
1	E	231	30% 78% 16% 5%

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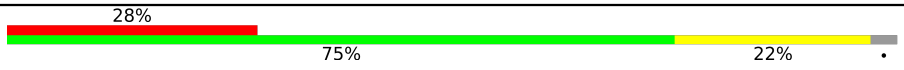
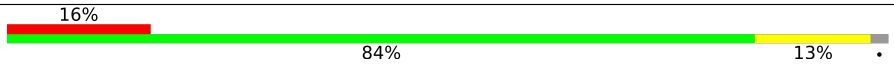
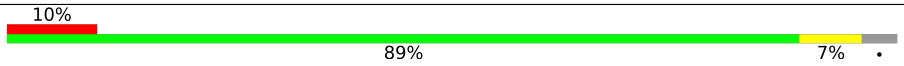
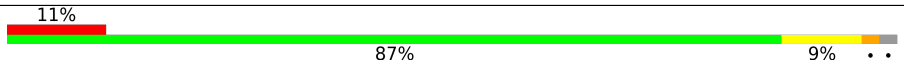
Mol	Chain	Length	Quality of chain
1	F	231	
1	G	231	
1	H	231	
1	I	231	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17583 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 Gallate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1919	1244	309	353	13			
1	B	225	Total	C	N	O	S	0	0	0
			1865	1208	302	343	12			
1	C	227	Total	C	N	O	S	0	0	0
			1891	1228	305	346	12			
1	D	226	Total	C	N	O	S	0	0	0
			1879	1219	304	344	12			
1	E	219	Total	C	N	O	S	0	0	0
			1809	1171	292	334	12			
1	F	225	Total	C	N	O	S	0	0	0
			1865	1208	302	343	12			
1	G	226	Total	C	N	O	S	0	0	0
			1879	1219	304	344	12			
1	H	222	Total	C	N	O	S	0	0	0
			1835	1187	298	338	12			
1	I	226	Total	C	N	O	S	0	0	0
			1877	1217	303	345	12			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		
2	G	1	Total	K	0	0
			1	1		

- Molecule 3 is water.

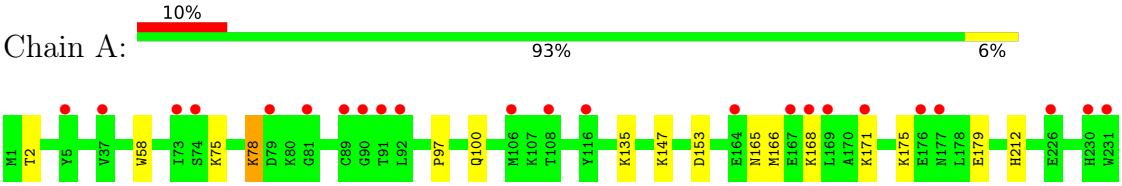
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	107	Total O 107 107	0	0
3	B	81	Total O 81 81	0	0
3	C	97	Total O 97 97	0	0
3	D	116	Total O 116 116	0	0
3	E	45	Total O 45 45	0	0
3	F	50	Total O 50 50	0	0
3	G	75	Total O 75 75	0	0
3	H	104	Total O 104 104	0	0
3	I	86	Total O 86 86	0	0

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.

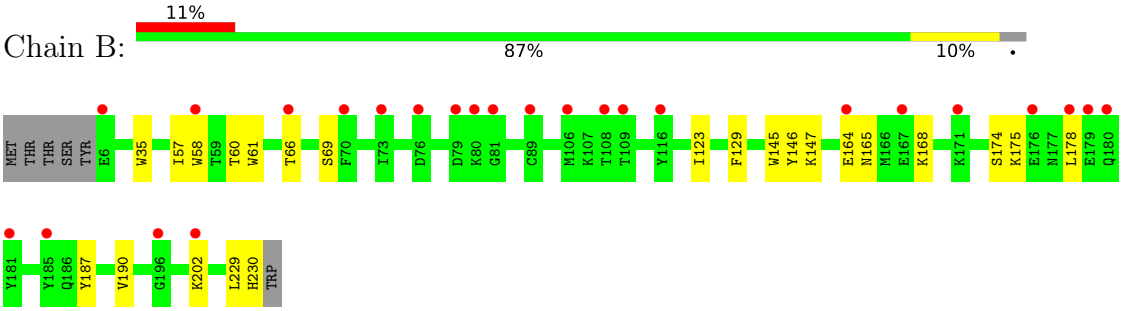
• Molecule 1: Gallate decarboxylase

Chain A:



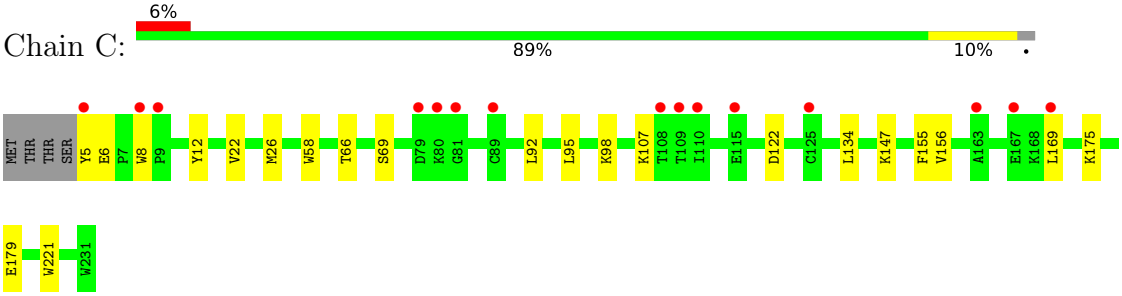
• Molecule 1: Gallate decarboxylase

Chain B:



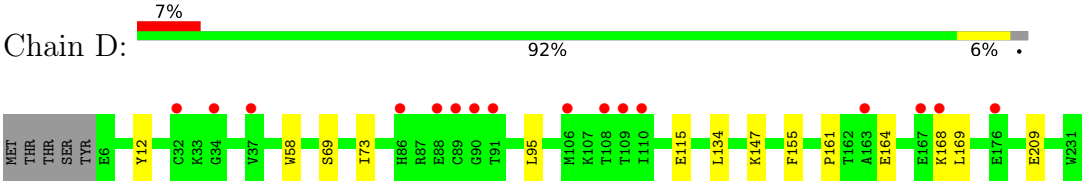
• Molecule 1: Gallate decarboxylase

Chain C:



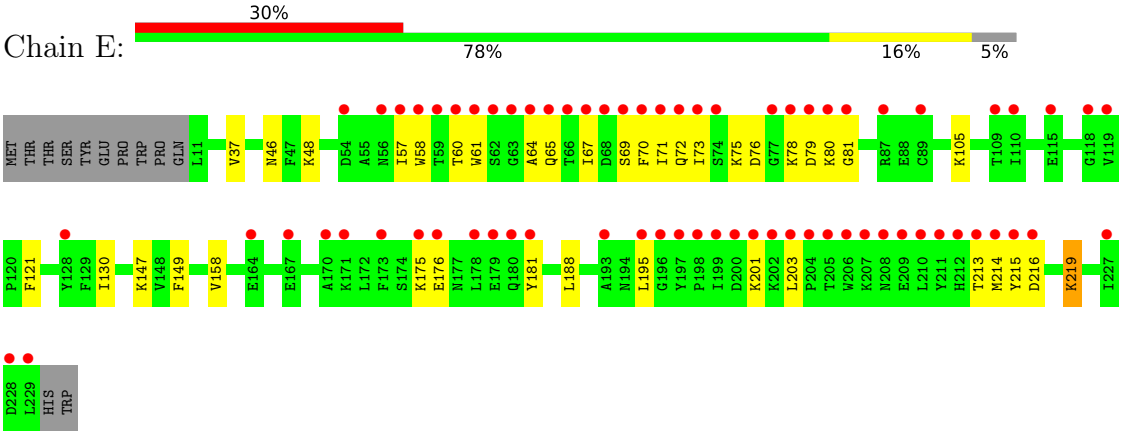
• Molecule 1: Gallate decarboxylase

Chain D:



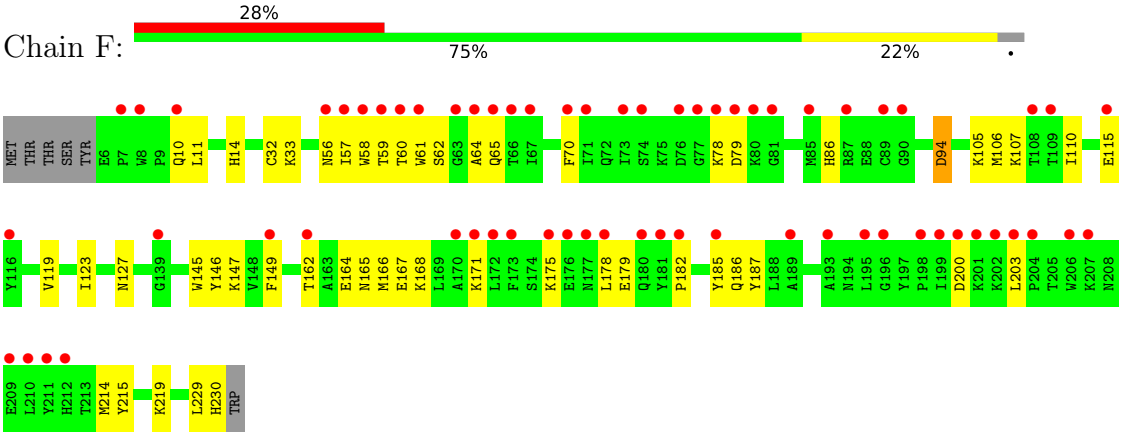
• Molecule 1: Gallate decarboxylase

Chain E:



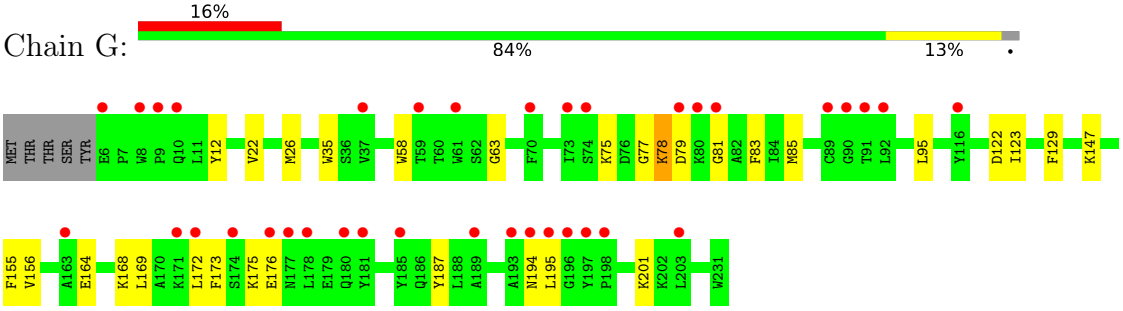
• Molecule 1: Gallate decarboxylase

Chain F:



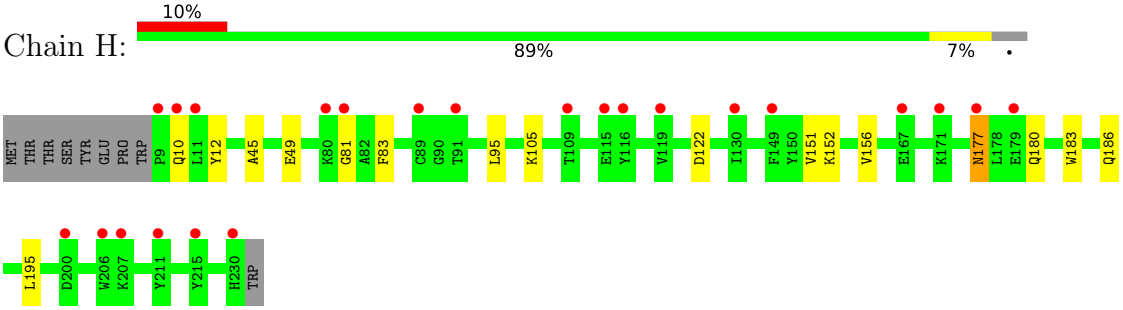
• Molecule 1: Gallate decarboxylase

Chain G:



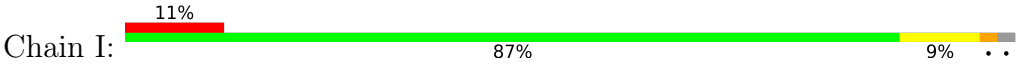
• Molecule 1: Gallate decarboxylase

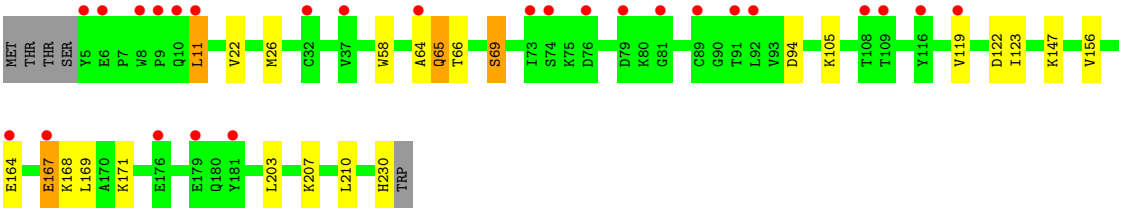
Chain H:



• Molecule 1: Gallate decarboxylase

Chain I:


11%
87%
9%


MET
THR
THR
SER
Y5
E6
P7
W8
P9
Q10
L11
V22
M26
C32
V37
W58
A64
Q65
T66
S69
I73
S74
K75
D76
D79
K80
G81
C89
G90
T91
L92
V93
D94
K105
T108
T109
Y116
V119
D122
I123
K147
V156

E164
E167
K168
L169
A170
K171
E176
E179
Q180
Y181
L203
K207
L210
H230
TRP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	91.63Å 265.30Å 93.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.61 – 1.94 46.61 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.61-1.94) 99.6 (46.61-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.191 , 0.237 0.191 , 0.237	Depositor DCC
R_{free} test set	8294 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17583	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: 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	0.44	0/1979	0.57	0/2682
1	B	0.42	0/1922	0.58	0/2603
1	C	0.40	0/1951	0.55	0/2644
1	D	0.44	0/1938	0.58	0/2626
1	E	0.36	0/1861	0.55	0/2517
1	F	0.39	0/1922	0.56	0/2603
1	G	0.43	0/1938	0.58	0/2626
1	H	0.42	0/1889	0.59	0/2555
1	I	0.40	0/1935	0.56	0/2621
All	All	0.41	0/17335	0.57	0/23477

There are no bond length outliers.

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	1919	0	1840	12	0
1	B	1865	0	1790	13	0
1	C	1891	0	1809	14	0
1	D	1879	0	1800	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1809	0	1745	30	0
1	F	1865	0	1790	41	0
1	G	1879	0	1800	24	0
1	H	1835	0	1768	10	0
1	I	1877	0	1799	18	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	G	1	0	0	0	0
3	A	107	0	0	2	0
3	B	81	0	0	0	0
3	C	97	0	0	0	0
3	D	116	0	0	0	0
3	E	45	0	0	0	0
3	F	50	0	0	0	0
3	G	75	0	0	0	0
3	H	104	0	0	1	0
3	I	86	0	0	1	0
All	All	17583	0	16141	164	0

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 5.

All (164) 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:E:71:ILE:O	1:E:75:LYS:HB2	1.32	1.26
1:E:213:THR:O	1:E:216:ASP:HB2	1.73	0.88
1:E:76:ASP:HB3	1:E:79:ASP:HB2	1.56	0.87
1:G:75:LYS:O	1:G:78:LYS:HB2	1.85	0.75
1:F:57:ILE:HB	1:F:146:TYR:HE1	1.52	0.74
1:F:33:LYS:HA	1:F:106:MET:HE1	1.67	0.74
1:E:70:PHE:HA	1:E:73:ILE:HD12	1.77	0.67
1:C:6:GLU:OE1	1:C:8:TRP:C	2.34	0.66
1:F:175:LYS:HD2	1:F:175:LYS:H	1.60	0.66
1:E:71:ILE:O	1:E:75:LYS:CB	2.27	0.65
1:I:65:GLN:NE2	1:I:69:SER:OG	2.30	0.65
1:F:60:THR:HG23	1:F:61:TRP:H	1.63	0.64
1:G:164:GLU:O	1:G:168:LYS:HG2	1.96	0.64
1:F:175:LYS:O	1:F:179:GLU:HG2	1.98	0.64
1:D:164:GLU:O	1:D:168:LYS:HG3	1.99	0.62
1:E:78:LYS:HA	1:E:81:GLY:HA2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:PHE:HA	1:E:158:VAL:HG23	1.84	0.60
1:G:81:GLY:HA3	1:G:195:LEU:HD11	1.85	0.59
1:F:167:GLU:O	1:F:171:LYS:HD3	2.02	0.59
1:I:207:LYS:NZ	3:I:303:HOH:O	2.36	0.59
1:A:175:LYS:HE2	1:A:179:GLU:OE2	2.04	0.58
1:F:178:LEU:HB3	1:F:186:GLN:OE1	2.04	0.57
1:A:166:MET:HG2	1:D:161:PRO:O	2.05	0.57
1:E:76:ASP:HB3	1:E:79:ASP:CB	2.31	0.57
1:I:65:GLN:HE21	1:I:65:GLN:HA	1.70	0.56
1:E:60:THR:HA	1:E:203:LEU:HD11	1.88	0.55
1:F:32:CYS:C	1:F:106:MET:HE3	2.26	0.55
1:E:78:LYS:HD2	1:E:81:GLY:HA2	1.87	0.55
1:A:97:PRO:HA	1:A:100:GLN:OE1	2.07	0.55
1:G:122:ASP:HB2	1:G:156:VAL:HB	1.88	0.55
1:B:123:ILE:HD12	1:B:187:TYR:HB3	1.88	0.55
1:D:58:TRP:CG	1:D:147:LYS:HE3	2.43	0.54
1:E:80:LYS:HE3	1:E:195:LEU:HG	1.89	0.54
1:F:182:PRO:HD2	1:F:185:TYR:OH	2.08	0.54
1:F:57:ILE:HB	1:F:146:TYR:CE1	2.38	0.53
1:F:162:THR:HB	1:F:165:ASN:HD22	1.73	0.53
1:D:69:SER:O	1:D:73:ILE:HG12	2.08	0.53
1:F:32:CYS:HB3	1:F:106:MET:HE3	1.91	0.53
1:I:58:TRP:CG	1:I:147:LYS:HE3	2.44	0.53
1:F:149:PHE:CZ	1:F:214:MET:HE3	2.44	0.52
1:B:66:THR:N	1:B:69:SER:OG	2.43	0.52
1:F:57:ILE:HG13	1:F:65:GLN:O	2.10	0.52
1:F:162:THR:HG22	1:F:164:GLU:H	1.75	0.52
1:G:85:MET:SD	1:H:151:VAL:HG11	2.50	0.52
1:G:172:LEU:HD12	1:G:173:PHE:CE2	2.45	0.51
1:F:10:GLN:NE2	1:F:11:LEU:O	2.44	0.51
1:B:164:GLU:O	1:B:168:LYS:HG3	2.09	0.51
1:D:209:GLU:H	1:D:209:GLU:CD	2.13	0.51
1:E:71:ILE:HD12	1:E:72:GLN:HG2	1.91	0.51
1:G:175:LYS:HD3	1:G:175:LYS:H	1.75	0.51
1:G:123:ILE:HD12	1:G:187:TYR:HB3	1.93	0.51
1:E:58:TRP:NE1	1:E:64:ALA:HB2	2.26	0.50
1:E:65:GLN:HB3	1:E:69:SER:OG	2.12	0.50
1:A:58:TRP:CD2	1:A:147:LYS:HE3	2.46	0.50
1:F:185:TYR:CZ	1:F:203:LEU:HD12	2.46	0.50
1:F:59:THR:HB	1:F:62:SER:OG	2.12	0.49
1:C:58:TRP:CD2	1:C:147:LYS:HE3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:122:ASP:HB2	1:I:156:VAL:HB	1.94	0.49
1:A:165:ASN:HA	1:A:168:LYS:HG2	1.94	0.49
1:F:162:THR:O	1:F:166:MET:HG3	2.13	0.49
1:F:115:GLU:HA	1:F:119:VAL:O	2.12	0.49
1:H:81:GLY:O	1:H:195:LEU:HD21	2.11	0.49
1:B:178:LEU:HD23	1:B:190:VAL:HG21	1.95	0.48
1:A:175:LYS:HE2	1:A:179:GLU:CD	2.33	0.48
1:E:213:THR:O	1:E:216:ASP:CB	2.56	0.48
1:E:175:LYS:HZ3	1:E:176:GLU:CD	2.17	0.48
1:G:79:ASP:O	1:G:81:GLY:N	2.45	0.48
1:E:149:PHE:HE1	1:E:214:MET:SD	2.37	0.48
1:A:100:GLN:HE21	1:A:135:LYS:HD2	1.79	0.48
1:F:58:TRP:NE1	1:F:64:ALA:HB2	2.29	0.47
1:B:57:ILE:HG23	1:B:146:TYR:CD1	2.49	0.47
1:G:58:TRP:CG	1:G:147:LYS:HE3	2.50	0.47
1:G:155:PHE:CZ	1:G:169:LEU:HD13	2.49	0.47
1:C:58:TRP:CG	1:C:147:LYS:HE3	2.50	0.47
1:D:58:TRP:HB2	1:D:147:LYS:HG3	1.97	0.47
1:G:85:MET:HE2	1:H:152:LYS:HE2	1.95	0.47
1:A:78:LYS:HE3	3:A:485:HOH:O	2.15	0.47
1:G:22:VAL:O	1:G:26:MET:HG2	2.14	0.47
1:H:122:ASP:HB2	1:H:156:VAL:HB	1.96	0.47
1:G:77:GLY:O	1:G:79:ASP:N	2.48	0.47
1:D:58:TRP:CD2	1:D:147:LYS:HE3	2.51	0.46
1:F:79:ASP:OD2	1:F:79:ASP:N	2.38	0.46
1:H:49:GLU:OE2	1:I:11:LEU:HD22	2.16	0.46
1:E:181:TYR:HA	1:E:201:LYS:HE3	1.98	0.46
1:G:58:TRP:HA	1:G:63:GLY:O	2.16	0.46
1:I:164:GLU:O	1:I:168:LYS:HB2	2.16	0.46
1:F:147:LYS:HE3	1:F:229:LEU:HB3	1.97	0.46
1:A:168:LYS:O	1:A:171:LYS:HG2	2.16	0.45
1:F:166:MET:HE3	1:F:166:MET:HB3	1.89	0.45
1:D:12:TYR:HB3	1:D:95:LEU:O	2.16	0.45
1:F:58:TRP:CD2	1:F:147:LYS:HE2	2.51	0.45
1:F:86:HIS:CD2	1:F:110:ILE:HG12	2.51	0.45
1:G:172:LEU:HD21	1:G:194:ASN:ND2	2.32	0.45
1:F:57:ILE:HD13	1:F:70:PHE:CD1	2.51	0.45
1:A:75:LYS:HD3	3:A:455:HOH:O	2.17	0.45
1:E:37:VAL:HA	1:F:107:LYS:HD2	1.99	0.45
1:F:164:GLU:O	1:F:168:LYS:HG3	2.16	0.45
1:F:56:ASN:HD22	1:F:230:HIS:CE1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:TYR:HB3	1:G:95:LEU:O	2.18	0.44
1:C:98:LYS:HE3	1:C:98:LYS:HB2	1.57	0.44
1:F:60:THR:HG23	1:F:61:TRP:N	2.31	0.44
1:F:94:ASP:OD2	1:F:105:LYS:NZ	2.50	0.44
1:E:219:LYS:HD2	1:E:219:LYS:N	2.33	0.44
1:E:48:LYS:HA	1:E:67:ILE:HD11	2.00	0.44
1:E:149:PHE:CE2	1:E:215:TYR:HE2	2.36	0.43
1:I:94:ASP:OD2	1:I:105:LYS:NZ	2.40	0.43
1:C:92:LEU:HD23	1:C:92:LEU:HA	1.77	0.43
1:D:164:GLU:HG2	1:D:168:LYS:HE3	2.01	0.43
1:B:60:THR:OG1	1:B:61:TRP:N	2.51	0.43
1:G:155:PHE:HZ	1:G:169:LEU:HD13	1.83	0.43
1:F:215:TYR:O	1:F:219:LYS:HD2	2.17	0.43
1:C:66:THR:CG2	1:C:69:SER:H	2.31	0.43
1:E:57:ILE:HD12	1:E:57:ILE:C	2.39	0.43
1:D:155:PHE:CZ	1:D:169:LEU:HD13	2.54	0.43
1:E:58:TRP:CG	1:E:147:LYS:HE2	2.54	0.43
1:G:35:TRP:CD1	1:G:129:PHE:HE2	2.36	0.43
1:C:155:PHE:CZ	1:C:169:LEU:HD13	2.54	0.43
1:G:172:LEU:HD21	1:G:194:ASN:HD21	1.84	0.43
1:I:122:ASP:O	1:I:123:ILE:HD13	2.18	0.43
1:I:167:GLU:O	1:I:171:LYS:HD2	2.19	0.42
1:B:58:TRP:HZ2	1:B:230:HIS:HA	1.84	0.42
1:B:165:ASN:HA	1:B:168:LYS:HD3	2.01	0.42
1:C:134:LEU:HD23	1:C:221:TRP:CH2	2.55	0.42
1:H:177:ASN:ND2	1:H:180:GLN:OE1	2.52	0.42
1:A:175:LYS:HG2	1:A:179:GLU:HG3	2.02	0.42
1:G:58:TRP:CD2	1:G:147:LYS:HE3	2.55	0.42
1:I:58:TRP:NE1	1:I:64:ALA:HB2	2.34	0.42
1:B:174:SER:O	1:B:178:LEU:HG	2.20	0.42
1:C:175:LYS:HE2	1:C:179:GLU:OE2	2.19	0.42
1:H:105:LYS:HD3	3:H:386:HOH:O	2.19	0.42
1:F:33:LYS:CA	1:F:106:MET:HE1	2.43	0.41
1:F:57:ILE:CB	1:F:146:TYR:HE1	2.28	0.41
1:F:123:ILE:HD12	1:F:187:TYR:HB3	2.02	0.41
1:I:22:VAL:O	1:I:26:MET:HG2	2.19	0.41
1:H:12:TYR:HB3	1:H:95:LEU:O	2.20	0.41
1:I:66:THR:OG1	1:I:69:SER:HB3	2.20	0.41
1:C:122:ASP:HB2	1:C:156:VAL:HB	2.01	0.41
1:F:200:ASP:HB3	1:F:203:LEU:HD21	2.02	0.41
1:I:58:TRP:HZ2	1:I:230:HIS:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LYS:O	1:B:178:LEU:N	2.53	0.41
1:E:46:ASN:HD22	1:F:14:HIS:CE1	2.38	0.41
1:G:176:GLU:CD	1:G:176:GLU:H	2.24	0.41
1:E:72:GLN:HA	1:E:75:LYS:HB3	2.02	0.41
1:H:183:TRP:O	1:H:186:GLN:HG2	2.20	0.41
1:B:58:TRP:CD2	1:B:147:LYS:HE3	2.56	0.41
1:E:72:GLN:HA	1:E:75:LYS:CB	2.51	0.41
1:E:188:LEU:HD12	1:E:188:LEU:HA	1.94	0.41
1:G:172:LEU:HD12	1:G:173:PHE:CZ	2.56	0.41
1:A:2:THR:O	1:A:212:HIS:HD2	2.03	0.41
1:B:35:TRP:CD1	1:B:129:PHE:HE2	2.38	0.41
1:C:22:VAL:O	1:C:26:MET:HG2	2.21	0.41
1:E:60:THR:OG1	1:E:61:TRP:N	2.53	0.41
1:G:75:LYS:HD3	1:G:75:LYS:C	2.41	0.41
1:F:145:TRP:HB3	1:F:229:LEU:HD12	2.03	0.41
1:C:12:TYR:HB3	1:C:95:LEU:O	2.21	0.40
1:I:210:LEU:HD23	1:I:210:LEU:HA	1.89	0.40
1:H:45:ALA:HB1	1:I:11:LEU:HD11	2.03	0.40
1:C:107:LYS:HE2	1:F:86:HIS:O	2.21	0.40
1:C:6:GLU:OE1	1:C:8:TRP:O	2.39	0.40
1:B:145:TRP:HB3	1:B:229:LEU:HD12	2.04	0.40
1:E:105:LYS:HG2	1:E:130:ILE:HD13	2.03	0.40
1:F:110:ILE:HG13	1:F:127:ASN:HD21	1.87	0.40
1:I:119:VAL:HG11	1:I:169:LEU:HD11	2.04	0.40
1:I:203:LEU:HD23	1:I:203:LEU:HA	1.96	0.40

There are no symmetry-related clashes.

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	229/231 (99%)	222 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	223/231 (96%)	211 (95%)	12 (5%)	0	100	100
1	C	225/231 (97%)	217 (96%)	8 (4%)	0	100	100
1	D	224/231 (97%)	217 (97%)	7 (3%)	0	100	100
1	E	217/231 (94%)	205 (94%)	12 (6%)	0	100	100
1	F	223/231 (96%)	215 (96%)	8 (4%)	0	100	100
1	G	224/231 (97%)	213 (95%)	10 (4%)	1 (0%)	34	24
1	H	220/231 (95%)	210 (96%)	10 (4%)	0	100	100
1	I	224/231 (97%)	213 (95%)	11 (5%)	0	100	100
All	All	2009/2079 (97%)	1923 (96%)	85 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	78	LYS

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	204/204 (100%)	202 (99%)	2 (1%)	76	71
1	B	198/204 (97%)	197 (100%)	1 (0%)	88	88
1	C	200/204 (98%)	199 (100%)	1 (0%)	88	88
1	D	199/204 (98%)	197 (99%)	2 (1%)	76	71
1	E	192/204 (94%)	191 (100%)	1 (0%)	88	88
1	F	198/204 (97%)	196 (99%)	2 (1%)	76	71
1	G	199/204 (98%)	197 (99%)	2 (1%)	76	71
1	H	195/204 (96%)	192 (98%)	3 (2%)	65	56
1	I	199/204 (98%)	195 (98%)	4 (2%)	55	42
All	All	1784/1836 (97%)	1766 (99%)	18 (1%)	76	71

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LYS
1	A	153	ASP
1	B	202	LYS
1	C	5	TYR
1	D	115	GLU
1	D	134	LEU
1	E	219	LYS
1	F	78	LYS
1	F	94	ASP
1	G	83	PHE
1	G	201	LYS
1	H	10	GLN
1	H	83	PHE
1	H	177	ASN
1	I	11	LEU
1	I	65	GLN
1	I	69	SER
1	I	167	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	212	HIS
1	B	72	GLN
1	C	186	GLN
1	E	46	ASN
1	E	186	GLN
1	F	10	GLN
1	F	46	ASN
1	F	56	ASN
1	F	177	ASN
1	F	192	GLN
1	G	177	ASN
1	G	192	GLN
1	H	10	GLN
1	I	19	ASN
1	I	65	GLN
1	I	138	ASN
1	I	180	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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	231/231 (100%)	0.58	23 (9%) 7 10	21, 40, 81, 105	0
1	B	225/231 (97%)	0.71	25 (11%) 5 8	23, 43, 86, 129	0
1	C	227/231 (98%)	0.42	15 (6%) 18 24	29, 41, 78, 132	0
1	D	226/231 (97%)	0.40	16 (7%) 16 22	21, 36, 75, 92	0
1	E	219/231 (94%)	1.58	70 (31%) 0 0	25, 57, 141, 164	0
1	F	225/231 (97%)	1.28	64 (28%) 0 0	27, 56, 116, 152	0
1	G	226/231 (97%)	0.86	36 (15%) 1 2	22, 43, 85, 133	0
1	H	222/231 (96%)	0.61	23 (10%) 6 9	22, 39, 76, 133	0
1	I	226/231 (97%)	0.69	26 (11%) 4 7	20, 43, 82, 133	0
All	All	2027/2079 (97%)	0.79	298 (14%) 2 3	20, 43, 100, 164	0

All (298) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	73	ILE	15.2
1	C	5	TYR	12.3
1	G	81	GLY	10.8
1	I	5	TYR	10.0
1	F	73	ILE	9.7
1	E	70	PHE	9.3
1	G	80	LYS	9.2
1	E	64	ALA	8.5
1	E	206	TRP	8.3
1	E	60	THR	7.7
1	E	215	TYR	7.6
1	E	80	LYS	7.2
1	E	59	THR	7.0
1	G	9	PRO	6.8
1	A	81	GLY	6.6

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Mol	Chain	Res	Type	RSRZ
1	E	199	ILE	6.6
1	F	58	TRP	6.5
1	E	58	TRP	6.4
1	E	56	ASN	6.4
1	E	57	ILE	6.4
1	E	61	TRP	6.3
1	H	9	PRO	6.3
1	H	81	GLY	6.2
1	E	200	ASP	6.1
1	E	211	TYR	6.1
1	F	79	ASP	6.0
1	E	209	GLU	5.9
1	F	202	LYS	5.9
1	F	89	CYS	5.8
1	I	9	PRO	5.8
1	E	212	HIS	5.4
1	F	61	TRP	5.3
1	A	231	TRP	5.3
1	E	201	LYS	5.3
1	F	80	LYS	5.3
1	F	203	LEU	5.3
1	E	78	LYS	5.2
1	F	59	THR	5.2
1	F	70	PHE	5.1
1	A	89	CYS	5.1
1	F	57	ILE	5.1
1	G	89	CYS	5.1
1	F	81	GLY	5.0
1	F	178	LEU	4.9
1	E	68	ASP	4.7
1	F	189	ALA	4.7
1	E	63	GLY	4.7
1	G	198	PRO	4.6
1	F	64	ALA	4.6
1	E	197	TYR	4.6
1	F	176	GLU	4.5
1	B	180	GLN	4.5
1	E	210	LEU	4.4
1	G	171	LYS	4.4
1	G	8	TRP	4.3
1	E	74	SER	4.3
1	B	89	CYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	175	LYS	4.3
1	E	228	ASP	4.3
1	H	230	HIS	4.2
1	E	208	ASN	4.1
1	E	213	THR	4.1
1	E	203	LEU	4.1
1	F	78	LYS	4.1
1	F	181	TYR	4.0
1	E	67	ILE	4.0
1	E	176	GLU	4.0
1	A	73	ILE	3.9
1	H	80	LYS	3.9
1	E	79	ASP	3.8
1	B	58	TRP	3.8
1	F	8	TRP	3.7
1	E	202	LYS	3.7
1	F	56	ASN	3.7
1	E	66	THR	3.7
1	E	198	PRO	3.7
1	F	185	TYR	3.7
1	B	66	THR	3.7
1	F	173	PHE	3.7
1	G	177	ASN	3.6
1	H	207	LYS	3.6
1	H	89	CYS	3.6
1	G	197	TYR	3.6
1	F	177	ASN	3.6
1	C	109	THR	3.5
1	I	73	ILE	3.5
1	I	6	GLU	3.5
1	F	116	TYR	3.5
1	I	119	VAL	3.5
1	F	193	ALA	3.4
1	G	176	GLU	3.4
1	F	74	SER	3.4
1	D	167	GLU	3.4
1	E	180	GLN	3.4
1	G	79	ASP	3.4
1	I	167	GLU	3.4
1	E	128	TYR	3.4
1	F	196	GLY	3.4
1	I	8	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	193	ALA	3.4
1	A	92	LEU	3.4
1	H	11	LEU	3.4
1	H	206	TRP	3.3
1	G	178	LEU	3.3
1	F	180	GLN	3.3
1	F	172	LEU	3.3
1	G	195	LEU	3.3
1	E	205	THR	3.3
1	H	149	PHE	3.2
1	B	164	GLU	3.2
1	H	200	ASP	3.2
1	E	171	LYS	3.2
1	C	81	GLY	3.2
1	E	216	ASP	3.2
1	B	79	ASP	3.2
1	D	108	THR	3.2
1	E	115	GLU	3.1
1	D	89	CYS	3.1
1	F	76	ASP	3.1
1	E	214	MET	3.1
1	C	79	ASP	3.1
1	A	90	GLY	3.1
1	B	196	GLY	3.1
1	I	81	GLY	3.1
1	H	177	ASN	3.1
1	G	6	GLU	3.1
1	E	65	GLN	3.1
1	F	198	PRO	3.1
1	G	10	GLN	3.0
1	F	182	PRO	3.0
1	C	8	TRP	3.0
1	B	109	THR	3.0
1	F	60	THR	3.0
1	F	66	THR	3.0
1	H	167	GLU	3.0
1	B	81	GLY	3.0
1	F	201	LYS	3.0
1	E	54	ASP	3.0
1	F	149	PHE	3.0
1	F	206	TRP	3.0
1	C	89	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	167	GLU	2.9
1	A	91	THR	2.9
1	F	199	ILE	2.9
1	D	37	VAL	2.9
1	E	229	LEU	2.9
1	G	180	GLN	2.9
1	E	71	ILE	2.9
1	F	171	LYS	2.9
1	D	109	THR	2.9
1	I	89	CYS	2.9
1	D	110	ILE	2.9
1	G	73	ILE	2.9
1	F	63	GLY	2.9
1	G	163	ALA	2.9
1	G	172	LEU	2.9
1	E	167	GLU	2.9
1	F	71	ILE	2.9
1	G	194	ASN	2.9
1	E	207	LYS	2.9
1	F	210	LEU	2.9
1	F	200	ASP	2.9
1	E	175	LYS	2.9
1	E	179	GLU	2.8
1	A	230	HIS	2.8
1	G	116	TYR	2.8
1	E	227	ILE	2.8
1	I	79	ASP	2.8
1	A	74	SER	2.8
1	B	70	PHE	2.8
1	E	72	GLN	2.8
1	F	108	THR	2.7
1	F	87	ARG	2.7
1	G	74	SER	2.7
1	B	73	ILE	2.7
1	H	130	ILE	2.7
1	A	177	ASN	2.7
1	H	91	THR	2.7
1	C	163	ALA	2.6
1	E	178	LEU	2.6
1	E	204	PRO	2.6
1	E	195	LEU	2.6
1	C	115	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	109	THR	2.6
1	A	171	LYS	2.6
1	F	7	PRO	2.6
1	A	116	TYR	2.6
1	B	185	TYR	2.6
1	H	215	TYR	2.6
1	H	179	GLU	2.6
1	D	91	THR	2.6
1	F	209	GLU	2.5
1	B	80	LYS	2.5
1	I	91	THR	2.5
1	C	125	CYS	2.5
1	C	9	PRO	2.5
1	C	108	THR	2.5
1	B	202	LYS	2.5
1	I	11	LEU	2.5
1	E	62	SER	2.5
1	E	87	ARG	2.5
1	F	212	HIS	2.5
1	A	5	TYR	2.5
1	B	108	THR	2.5
1	E	89	CYS	2.5
1	F	170	ALA	2.4
1	C	110	ILE	2.4
1	B	76	ASP	2.4
1	G	59	THR	2.4
1	I	32	CYS	2.4
1	G	193	ALA	2.4
1	A	37	VAL	2.4
1	E	164	GLU	2.4
1	H	211	TYR	2.4
1	E	119	VAL	2.4
1	F	90	GLY	2.4
1	B	178	LEU	2.4
1	B	6	GLU	2.4
1	G	189	ALA	2.4
1	H	119	VAL	2.4
1	B	171	LYS	2.4
1	I	164	GLU	2.4
1	G	174	SER	2.4
1	I	176	GLU	2.3
1	F	195	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	34	GLY	2.3
1	G	181	TYR	2.3
1	G	196	GLY	2.3
1	I	10	GLN	2.3
1	B	106	MET	2.3
1	H	109	THR	2.3
1	I	76	ASP	2.3
1	G	185	TYR	2.3
1	G	70	PHE	2.3
1	I	64	ALA	2.3
1	G	203	LEU	2.3
1	B	116	TYR	2.3
1	C	80	LYS	2.3
1	E	181	TYR	2.2
1	E	173	PHE	2.2
1	F	85	MET	2.2
1	A	176	GLU	2.2
1	E	170	ALA	2.2
1	E	110	ILE	2.2
1	G	61	TRP	2.2
1	E	196	GLY	2.2
1	G	90	GLY	2.2
1	A	167	GLU	2.2
1	I	181	TYR	2.2
1	F	162	THR	2.2
1	A	226	GLU	2.2
1	E	77	GLY	2.2
1	H	10	GLN	2.2
1	B	181	TYR	2.2
1	F	109	THR	2.2
1	A	168	LYS	2.2
1	D	32	CYS	2.2
1	E	69	SER	2.2
1	D	106	MET	2.2
1	I	109	THR	2.2
1	I	116	TYR	2.2
1	D	90	GLY	2.1
1	F	207	LYS	2.1
1	B	167	GLU	2.1
1	A	79	ASP	2.1
1	G	91	THR	2.1
1	D	168	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	171	LYS	2.1
1	G	37	VAL	2.1
1	A	106	MET	2.1
1	E	81	GLY	2.1
1	F	77	GLY	2.1
1	D	176	GLU	2.1
1	F	67	ILE	2.1
1	F	115	GLU	2.1
1	G	92	LEU	2.1
1	I	74	SER	2.1
1	H	116	TYR	2.1
1	B	179	GLU	2.1
1	A	169	LEU	2.1
1	A	164	GLU	2.1
1	I	179	GLU	2.1
1	I	37	VAL	2.1
1	B	176	GLU	2.1
1	C	169	LEU	2.1
1	D	88	GLU	2.0
1	F	10	GLN	2.0
1	D	86	HIS	2.0
1	D	163	ALA	2.0
1	F	139	GLY	2.0
1	H	115	GLU	2.0
1	F	65	GLN	2.0
1	F	211	TYR	2.0
1	E	118	GLY	2.0
1	F	204	PRO	2.0
1	I	92	LEU	2.0
1	A	108	THR	2.0
1	I	108	THR	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)

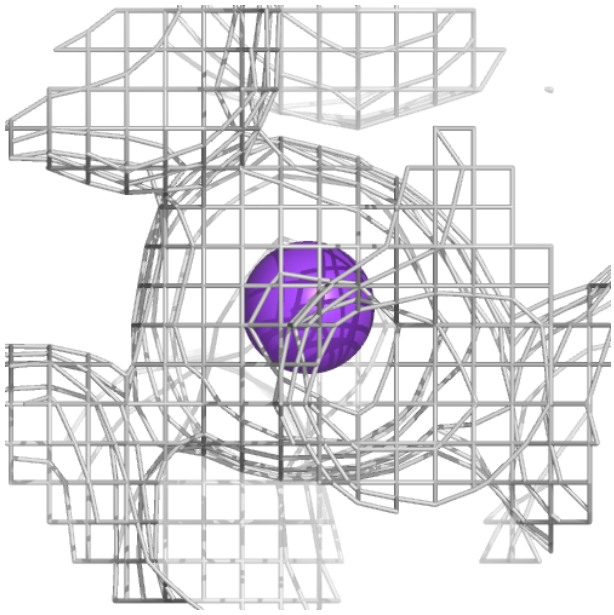
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

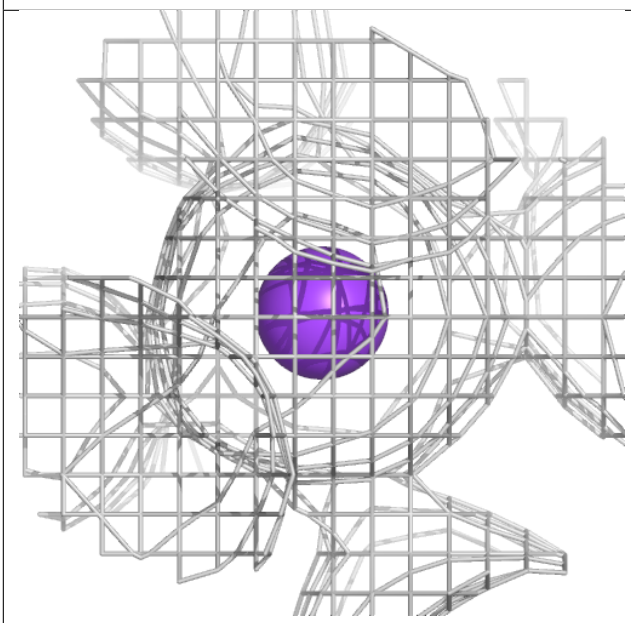
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	K	A	301	1/1	1.00	0.20	26,26,26,26	0
2	K	C	301	1/1	1.00	0.15	29,29,29,29	0
2	K	G	301	1/1	1.00	0.22	25,25,25,25	0

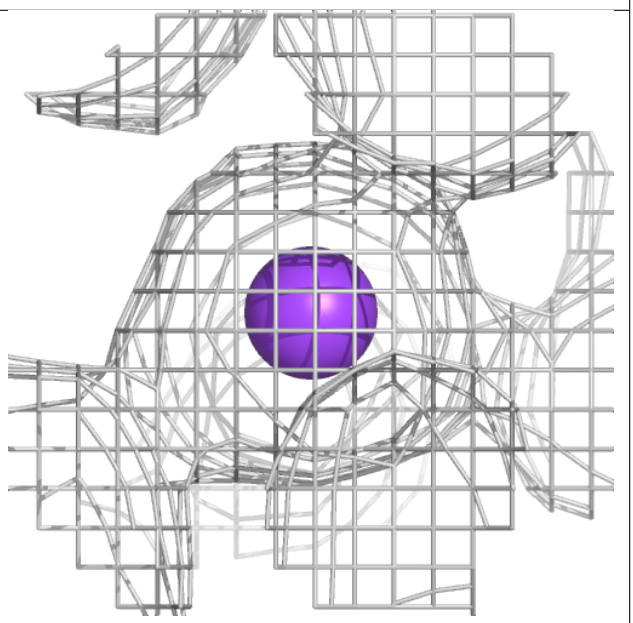
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around K A 301:

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

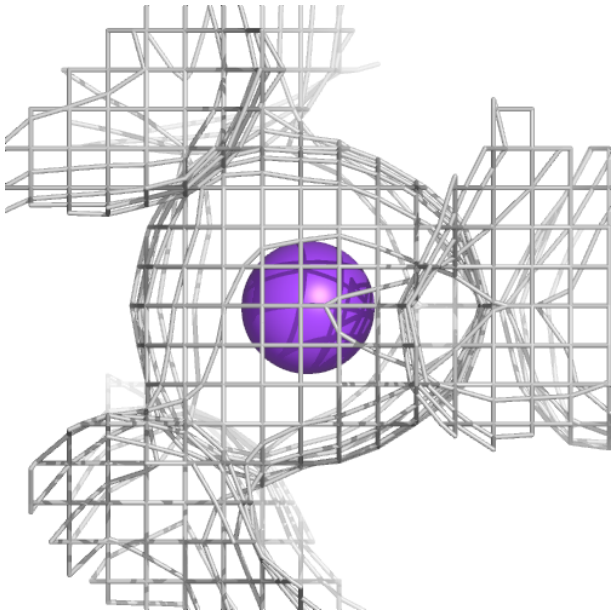


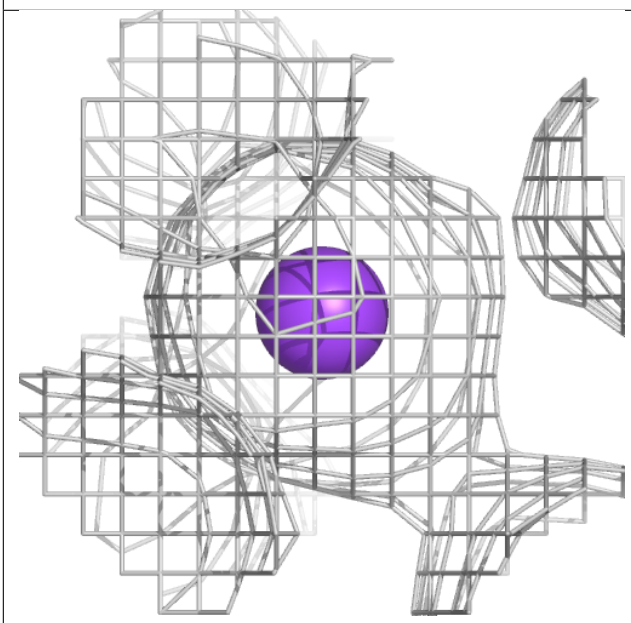


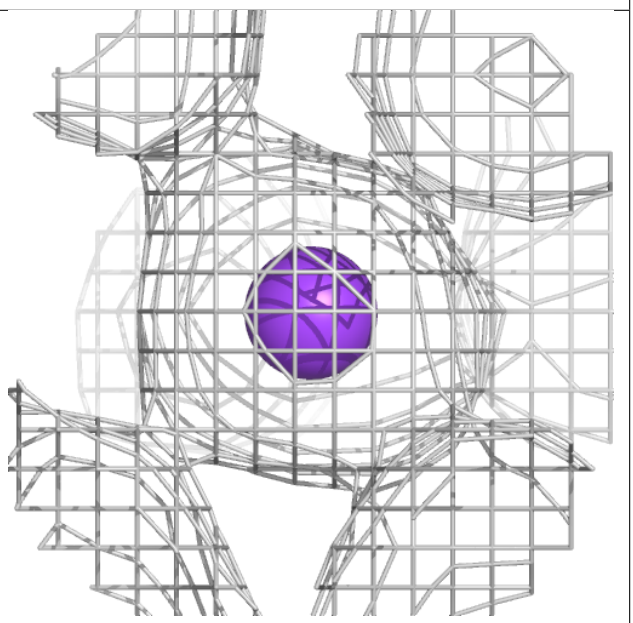


Electron density around K C 301:

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

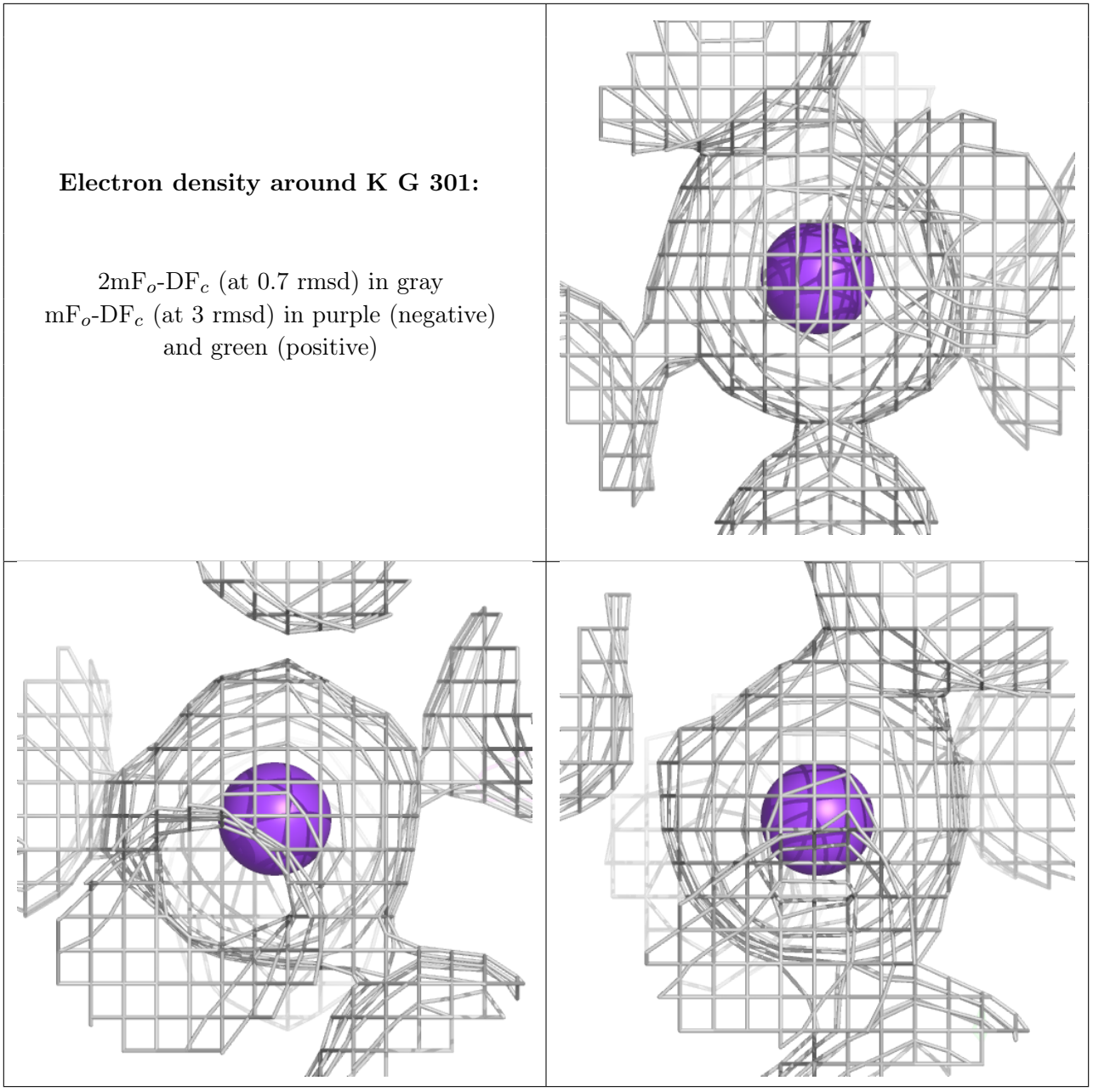






Electron density around K G 301:

$2mF_o$-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.