



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:47 AM UTC

PDB ID : 7KD9 / pdb_00007kd9
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

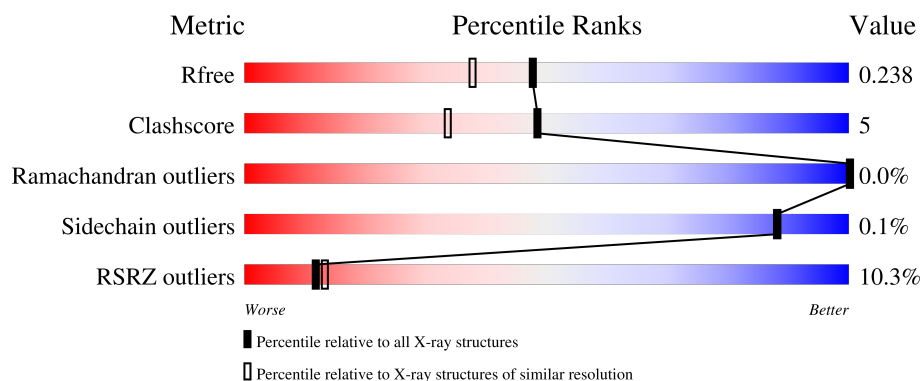
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	231	3% 94% 6%
1	B	231	9% 88% 10% .
1	C	231	3% 88% 10% .
1	D	231	% 90% 8% .
1	E	231	18% 77% 18% 5%

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Mol	Chain	Length	Quality of chain
1	F	231	22% 75% 23%
1	G	231	20% 84% 13%
1	H	231	8% 87% 9%
1	I	231	6% 86% 12%

2 Entry composition

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 (CCD ID: 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 107	O 107	0	0
3	B	81	Total 81	O 81	0	0
3	C	97	Total 97	O 97	0	0
3	D	116	Total 116	O 116	0	0
3	E	45	Total 45	O 45	0	0
3	F	50	Total 50	O 50	0	0
3	G	75	Total 75	O 75	0	0
3	H	104	Total 104	O 104	0	0
3	I	86	Total 86	O 86	0	0

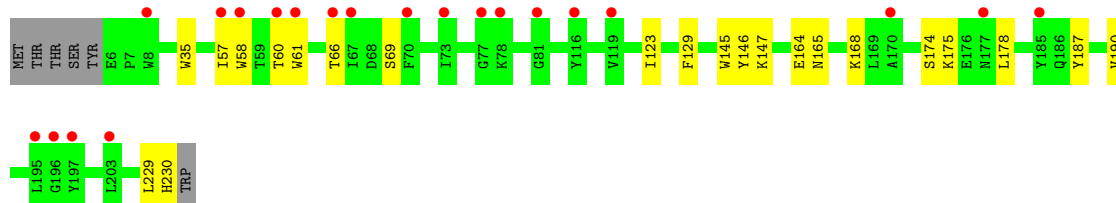
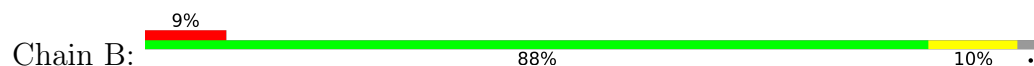
3 Residue-property plots

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.

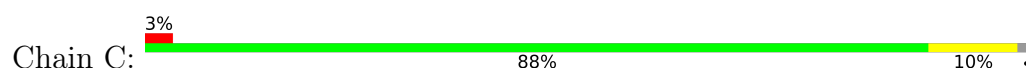
- Molecule 1: Gallate decarboxylase



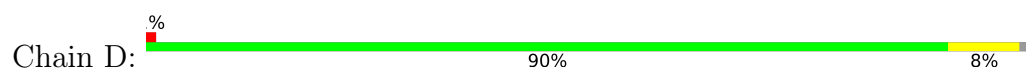
- Molecule 1: Gallate decarboxylase



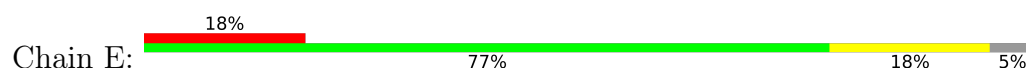
- Molecule 1: Gallate decarboxylase

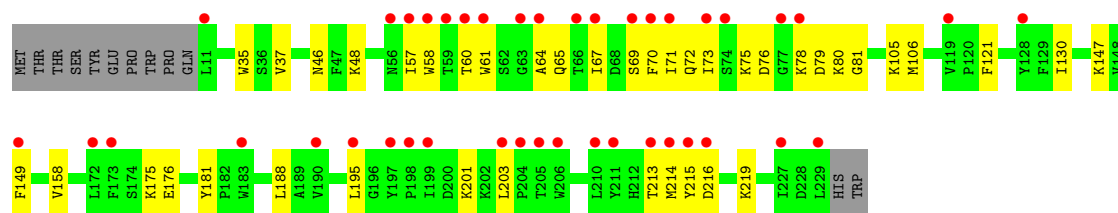


- Molecule 1: Gallate decarboxylase

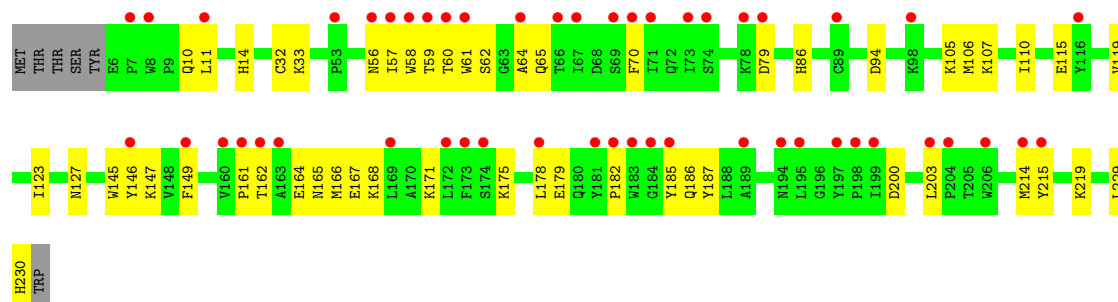
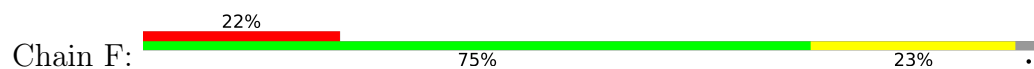


- Molecule 1: Gallate decarboxylase

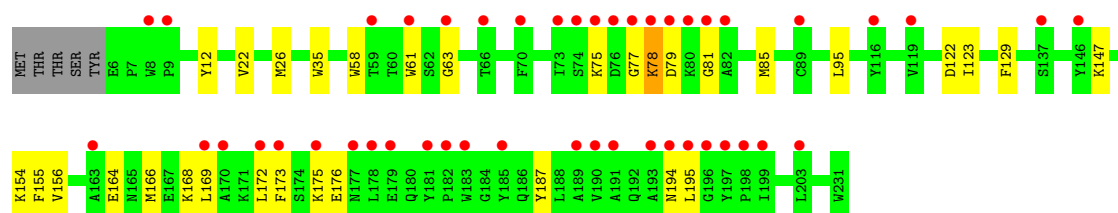
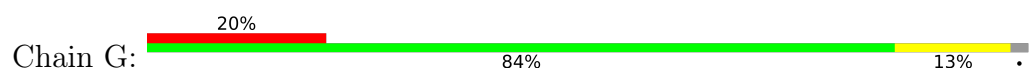




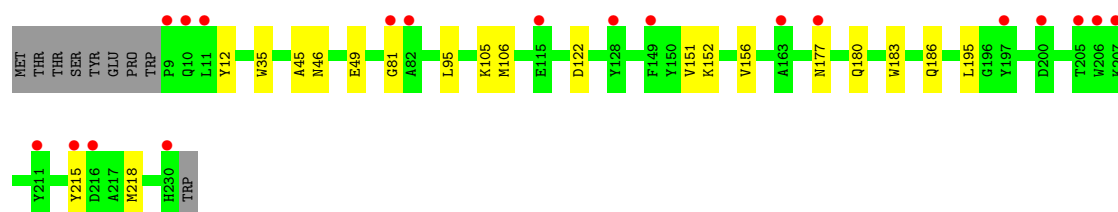
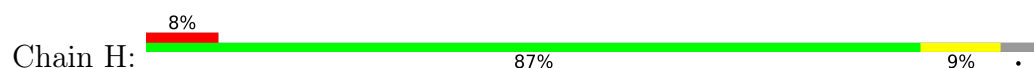
• Molecule 1: Gallate decarboxylase



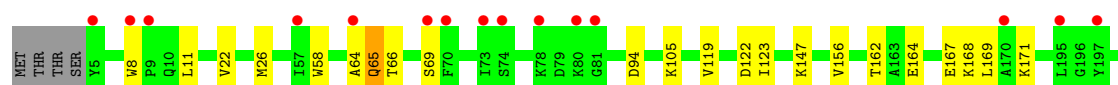
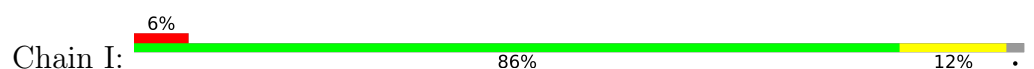
• Molecule 1: Gallate decarboxylase



• Molecule 1: Gallate decarboxylase



• Molecule 1: Gallate decarboxylase





4 Data and refinement statistics

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) 99.7 (46.61-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.191 , 0.237 0.192 , 0.238	Depositor DCC
R_{free} test set	8294 reflections (4.89%)	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 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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:
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	0.38	0/1979	0.57	0/2682
1	B	0.34	0/1922	0.57	0/2603
1	C	0.32	0/1951	0.51	0/2644
1	D	0.37	0/1938	0.58	0/2626
1	E	0.30	0/1861	0.54	0/2517
1	F	0.32	0/1922	0.53	0/2603
1	G	0.35	0/1938	0.58	0/2626
1	H	0.35	0/1889	0.57	0/2555
1	I	0.32	0/1935	0.54	0/2621
All	All	0.34	0/17335	0.56	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 [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	1919	0	1840	12	0
1	B	1865	0	1790	14	0
1	C	1891	0	1809	16	0
1	D	1879	0	1800	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1809	0	1745	31	0
1	F	1865	0	1790	43	0
1	G	1879	0	1800	27	0
1	H	1835	0	1768	13	0
1	I	1877	0	1799	22	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	1	0
3	H	104	0	0	1	0
3	I	86	0	0	1	0
All	All	17583	0	16141	181	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 (181) 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:C:6:GLU:OE1	1:C:8:TRP:C	2.34	0.70
1:F:33:LYS:HA	1:F:106:MET:HE1	1.73	0.69
1:E:70:PHE:HA	1:E:73:ILE:HD12	1.77	0.67
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:F:32:CYS:C	1:F:106:MET:HE1	2.26	0.61
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:F:32:CYS:HB3	1:F:106:MET:HE3	1.85	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:D:209:GLU:H	1:D:209:GLU:CD	2.13	0.56
1:I:65:GLN:HE21	1:I:65:GLN:HA	1.70	0.56
1:G:154:LYS:NZ	3:G:401:HOH:O	2.36	0.56
1:E:60:THR:HA	1:E:203:LEU:HD11	1.88	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:33:LYS:CA	1:F:106:MET:HE1	2.38	0.54
1:I:94:ASP:OD2	1:I:105:LYS:NZ	2.40	0.53
1:F:57:ILE:HB	1:F:146:TYR:CE1	2.38	0.53
1:A:175:LYS:HE2	1:A:179:GLU:CD	2.33	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:E:175:LYS:HZ3	1:E:176:GLU:CD	2.17	0.53
1:I:58:TRP:CG	1:I:147:LYS:HE3	2.44	0.53
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:I:147:LYS:HB3	1:I:214:MET:HE1	1.91	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:85:MET:HE2	1:H:152:LYS:HE2	1.93	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
1:I:122:ASP:HB2	1:I:156:VAL:HB	1.94	0.49
1:B:61:TRP:H	1:B:61:TRP:CD1	2.30	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:D:163:ALA:HA	1:D:166:MET:HE3	1.95	0.48
1:B:178:LEU:HD23	1:B:190:VAL:HG21	1.95	0.48
1:E:213:THR:O	1:E:216:ASP:CB	2.56	0.48
1:E:57:ILE:HD12	1:E:57:ILE:C	2.39	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:F:149:PHE:CZ	1:F:214:MET:HE3	2.49	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:H:35:TRP:HB3	1:H:106:MET:HE1	1.96	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:F:33:LYS:N	1:F:106:MET:HE1	2.30	0.46
1:C:166:MET:HE3	1:F:161:PRO:HB2	1.96	0.46
1:G:58:TRP:HA	1:G:63:GLY:O	2.16	0.46
1:H:215:TYR:HA	1:H:218:MET:HE3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:75:LYS:HD3	1:G:75:LYS:C	2.41	0.45
1:G:176:GLU:H	1:G:176:GLU:CD	2.24	0.45
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:D:147:LYS:HB3	1:D:214:MET:HE1	1.99	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
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:E:219:LYS:HD2	1:E:219:LYS:N	2.33	0.44
1:E:35:TRP:HB3	1:E:106:MET:HE1	2.00	0.44
1:E:48:LYS:HA	1:E:67:ILE:HD11	2.00	0.44
1:G:61:TRP:H	1:G:61:TRP:CD1	2.35	0.44
1:E:149:PHE:CE2	1:E:215:TYR:HE2	2.36	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: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:D:31:LEU:HD23	1:D:31:LEU:C	2.44	0.42
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:96:ASN:HB2	1:C:222:MET:HE3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:225:LYS:HZ3	1:I:225:LYS:HG3	1.77	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: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:H:46:ASN:HD21	1:I:8:TRP:CD1	2.38	0.41
1:I:58:TRP:HZ2	1:I:230:HIS:HA	1.85	0.41
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: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:166:MET:HE3	1:I:162:THR:HA	2.03	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:D:106:MET:HE2	1:D:129:PHE:CD1	2.56	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:F:94:ASP:OD2	1:F:105:LYS:NZ	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	30	22
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%)	204 (100%)	0	100	100
1	B	198/204 (97%)	198 (100%)	0	100	100
1	C	200/204 (98%)	200 (100%)	0	100	100
1	D	199/204 (98%)	199 (100%)	0	100	100
1	E	192/204 (94%)	192 (100%)	0	100	100
1	F	198/204 (97%)	198 (100%)	0	100	100
1	G	199/204 (98%)	199 (100%)	0	100	100
1	H	195/204 (96%)	195 (100%)	0	100	100
1	I	199/204 (98%)	198 (100%)	1 (0%)	81	82
All	All	1784/1836 (97%)	1783 (100%)	1 (0%)	88	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	65	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	72	GLN
1	A	100	GLN
1	A	212	HIS
1	B	72	GLN
1	C	72	GLN
1	C	186	GLN
1	C	212	HIS
1	D	212	HIS
1	E	46	ASN
1	E	100	GLN
1	E	186	GLN
1	F	10	GLN
1	F	46	ASN
1	F	56	ASN
1	F	177	ASN
1	F	180	GLN

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Mol	Chain	Res	Type
1	F	192	GLN
1	G	10	GLN
1	G	72	GLN
1	G	165	ASN
1	G	177	ASN
1	G	192	GLN
1	G	194	ASN
1	H	10	GLN
1	H	72	GLN
1	H	100	GLN
1	H	177	ASN
1	I	19	ASN
1	I	65	GLN
1	I	138	ASN
1	I	165	ASN
1	I	180	GLN
1	I	212	HIS

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	231/231 (100%)	0.21	8 (3%) 47 53	21, 40, 81, 105	0
1	B	225/231 (97%)	0.52	21 (9%) 14 16	23, 43, 86, 129	0
1	C	227/231 (98%)	0.32	6 (2%) 57 64	29, 41, 78, 132	0
1	D	226/231 (97%)	0.12	3 (1%) 75 80	21, 36, 75, 92	0
1	E	219/231 (94%)	1.03	41 (18%) 3 3	25, 57, 141, 164	0
1	F	225/231 (97%)	1.08	50 (22%) 2 2	27, 56, 116, 152	0
1	G	226/231 (97%)	0.75	46 (20%) 3 2	22, 43, 85, 133	0
1	H	222/231 (96%)	0.39	19 (8%) 16 18	22, 39, 76, 133	0
1	I	226/231 (97%)	0.42	15 (6%) 24 27	20, 43, 82, 133	0
All	All	2027/2079 (97%)	0.53	209 (10%) 12 13	20, 43, 100, 164	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	70	PHE	6.0
1	G	81	GLY	5.8
1	E	60	THR	5.7
1	H	81	GLY	5.6
1	E	61	TRP	5.3
1	H	230	HIS	5.2
1	E	215	TYR	4.9
1	E	206	TRP	4.9
1	F	57	ILE	4.9
1	E	71	ILE	4.9
1	F	70	PHE	4.6
1	F	58	TRP	4.6
1	E	128	TYR	4.5
1	I	5	TYR	4.4
1	F	73	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	73	ILE	4.3
1	A	231	TRP	4.3
1	H	206	TRP	4.3
1	G	9	PRO	4.2
1	I	73	ILE	4.2
1	F	189	ALA	4.2
1	G	185	TYR	4.2
1	E	57	ILE	4.1
1	F	206	TRP	4.1
1	C	81	GLY	4.1
1	H	11	LEU	4.1
1	E	58	TRP	4.0
1	G	8	TRP	4.0
1	H	149	PHE	4.0
1	F	184	GLY	4.0
1	F	203	LEU	3.9
1	F	199	ILE	3.9
1	F	172	LEU	3.8
1	H	9	PRO	3.8
1	E	74	SER	3.8
1	E	59	THR	3.7
1	F	185	TYR	3.7
1	G	80	LYS	3.7
1	E	77	GLY	3.7
1	H	215	TYR	3.6
1	E	199	ILE	3.6
1	F	149	PHE	3.6
1	F	8	TRP	3.5
1	G	198	PRO	3.5
1	E	197	TYR	3.5
1	F	60	THR	3.4
1	A	81	GLY	3.4
1	E	11	LEU	3.4
1	F	64	ALA	3.4
1	A	5	TYR	3.3
1	C	5	TYR	3.3
1	G	193	ALA	3.3
1	G	61	TRP	3.3
1	G	197	TYR	3.3
1	H	207	LYS	3.3
1	G	63	GLY	3.3
1	F	197	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	211	TYR	3.2
1	G	189	ALA	3.2
1	E	214	MET	3.2
1	F	163	ALA	3.2
1	G	116	TYR	3.2
1	B	58	TRP	3.1
1	F	71	ILE	3.1
1	G	194	ASN	3.1
1	E	67	ILE	3.1
1	E	204	PRO	3.1
1	E	210	LEU	3.1
1	F	61	TRP	3.1
1	F	181	TYR	3.1
1	E	203	LEU	3.0
1	F	178	LEU	3.0
1	G	70	PHE	3.0
1	C	80	LYS	3.0
1	H	82	ALA	3.0
1	B	57	ILE	3.0
1	F	11	LEU	2.9
1	G	74	SER	2.9
1	H	197	TYR	2.9
1	A	73	ILE	2.9
1	G	172	LEU	2.9
1	F	56	ASN	2.9
1	F	79	ASP	2.9
1	B	185	TYR	2.9
1	E	64	ALA	2.9
1	B	73	ILE	2.8
1	A	78	LYS	2.8
1	H	163	ALA	2.8
1	F	173	PHE	2.8
1	E	78	LYS	2.8
1	F	162	THR	2.7
1	G	190	VAL	2.7
1	I	8	TRP	2.7
1	G	178	LEU	2.7
1	G	169	LEU	2.7
1	F	67	ILE	2.7
1	E	63	GLY	2.6
1	G	163	ALA	2.6
1	B	197	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	181	TYR	2.6
1	H	128	TYR	2.6
1	I	9	PRO	2.6
1	G	203	LEU	2.6
1	F	116	TYR	2.6
1	G	59	THR	2.6
1	G	137	SER	2.6
1	G	173	PHE	2.6
1	G	195	LEU	2.6
1	F	59	THR	2.6
1	F	74	SER	2.6
1	H	115	GLU	2.6
1	G	170	ALA	2.6
1	F	89	CYS	2.5
1	F	182	PRO	2.5
1	E	229	LEU	2.5
1	G	119	VAL	2.5
1	F	7	PRO	2.5
1	G	146	TYR	2.5
1	E	149	PHE	2.5
1	E	195	LEU	2.5
1	I	195	LEU	2.5
1	B	81	GLY	2.5
1	I	81	GLY	2.5
1	F	183	TRP	2.5
1	E	56	ASN	2.5
1	F	174	SER	2.5
1	E	190	VAL	2.5
1	E	205	THR	2.5
1	G	79	ASP	2.5
1	G	191	ALA	2.5
1	G	196	GLY	2.4
1	E	69	SER	2.4
1	E	66	THR	2.4
1	F	66	THR	2.4
1	I	170	ALA	2.4
1	B	77	GLY	2.4
1	H	200	ASP	2.4
1	F	69	SER	2.4
1	H	216	ASP	2.4
1	F	53	PRO	2.4
1	B	196	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	119	VAL	2.4
1	G	89	CYS	2.4
1	E	172	LEU	2.3
1	B	70	PHE	2.3
1	B	60	THR	2.3
1	G	73	ILE	2.3
1	G	199	ILE	2.3
1	F	161	PRO	2.3
1	G	77	GLY	2.3
1	H	177	ASN	2.3
1	F	78	LYS	2.3
1	E	216	ASP	2.3
1	D	167	GLU	2.3
1	G	183	TRP	2.3
1	G	75	LYS	2.3
1	E	227	ILE	2.3
1	F	214	MET	2.3
1	I	78	LYS	2.3
1	B	61	TRP	2.2
1	E	183	TRP	2.2
1	F	198	PRO	2.2
1	G	182	PRO	2.2
1	I	64	ALA	2.2
1	I	74	SER	2.2
1	H	10	GLN	2.2
1	E	213	THR	2.2
1	F	195	LEU	2.2
1	B	8	TRP	2.2
1	E	173	PHE	2.2
1	B	78	LYS	2.2
1	F	194	ASN	2.2
1	A	195	LEU	2.2
1	C	163	ALA	2.2
1	G	82	ALA	2.2
1	G	175	LYS	2.2
1	I	70	PHE	2.1
1	B	116	TYR	2.1
1	E	211	TYR	2.1
1	F	146	TYR	2.1
1	B	66	THR	2.1
1	H	205	THR	2.1
1	B	203	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	177	ASN	2.1
1	B	67	ILE	2.1
1	G	76	ASP	2.1
1	D	231	TRP	2.1
1	B	119	VAL	2.1
1	F	169	LEU	2.1
1	F	204	PRO	2.1
1	C	116	TYR	2.1
1	G	78	LYS	2.1
1	E	198	PRO	2.1
1	B	170	ALA	2.1
1	C	82	ALA	2.1
1	D	163	ALA	2.1
1	F	98	LYS	2.0
1	G	179	GLU	2.0
1	I	69	SER	2.0
1	A	230	HIS	2.0
1	G	177	ASN	2.0
1	B	195	LEU	2.0
1	I	80	LYS	2.0
1	A	74	SER	2.0
1	I	57	ILE	2.0
1	G	66	THR	2.0
1	F	215	TYR	2.0
1	I	197	TYR	2.0
1	F	160	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

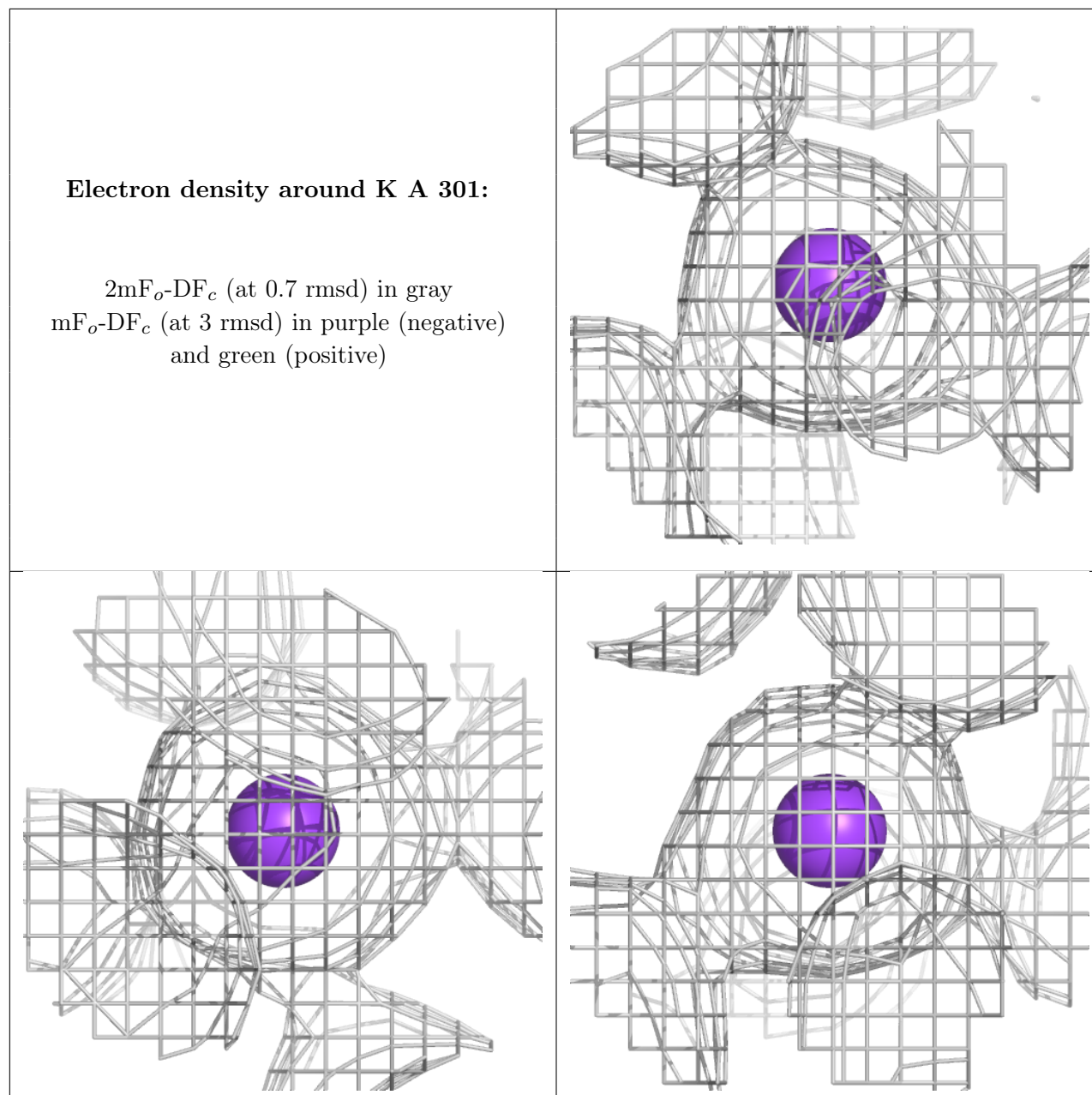
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

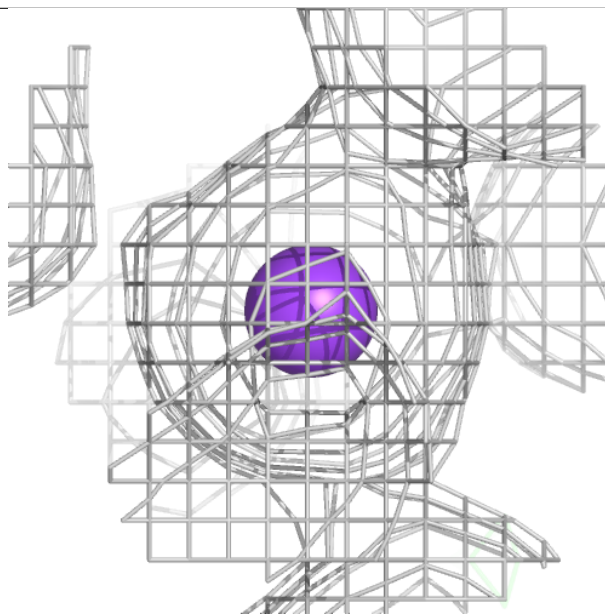
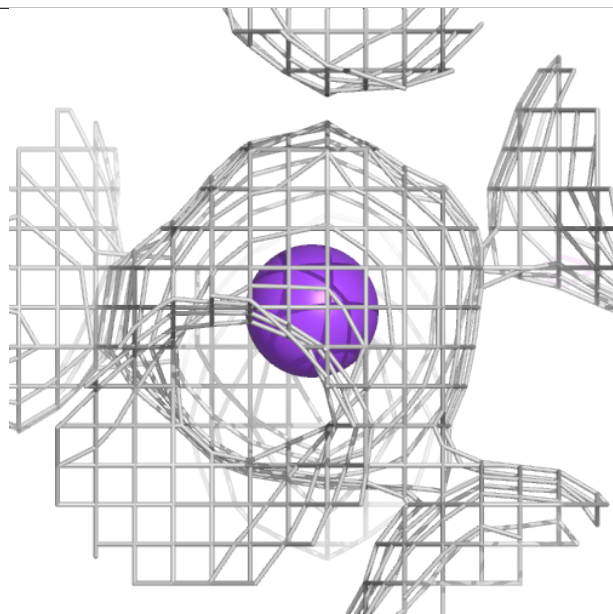
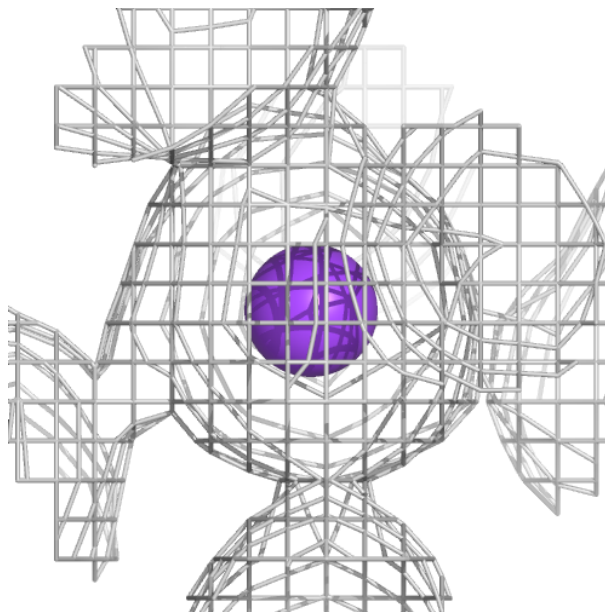
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	K	A	301	1/1	0.99	0.02	26,26,26,26	0
2	K	G	301	1/1	0.99	0.03	25,25,25,25	0
2	K	C	301	1/1	1.00	0.03	29,29,29,29	0

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.



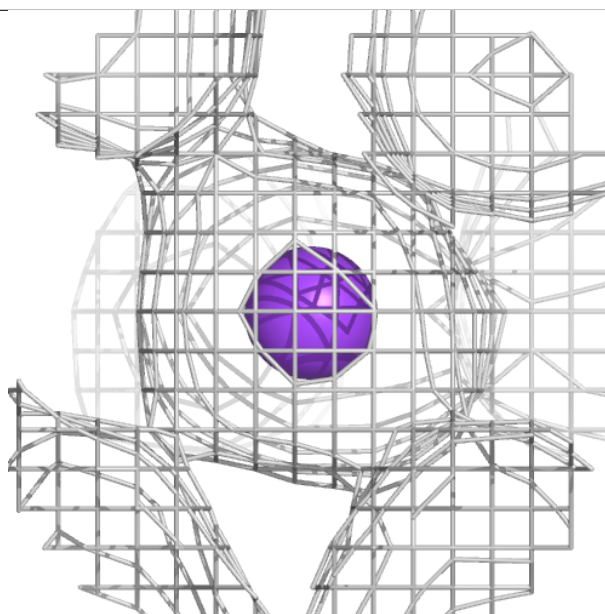
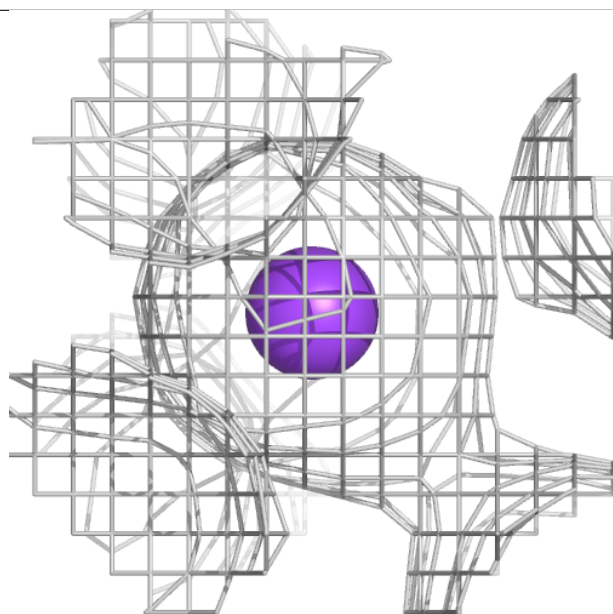
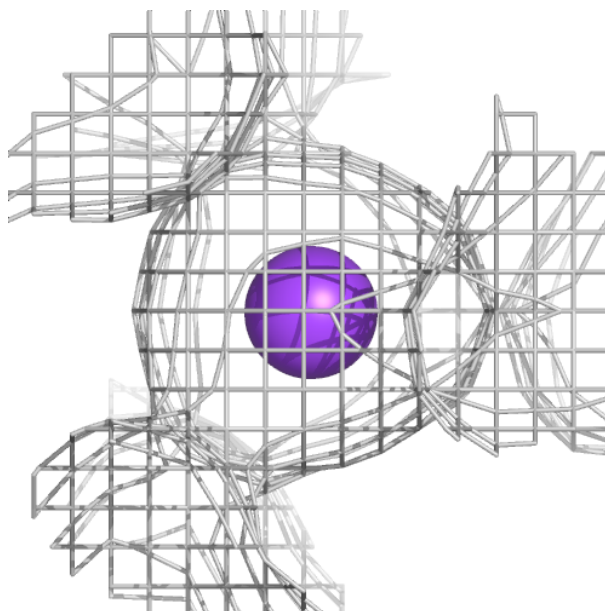
Electron density around K G 301:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.