



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2022 – 12:10 PM JST

PDB ID : 7E8O  
Title : Crystal structure of proteinaceous RNase P(PRORP) from Planctomycetes bacterium GWF2\_40\_8 complexed with Escherichia coli histidine pre-tRNA  
Authors : Li, Y.Y.; Gan, J.H.  
Deposited on : 2021-03-02  
Resolution : 2.80 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.

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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 : 2.26  
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) : 2.26

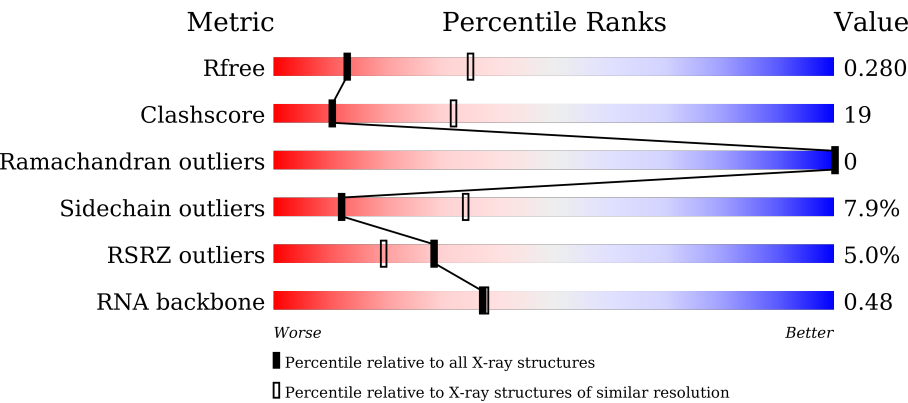
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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 <sub>free</sub>	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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	208	<div><div>2%</div><div>66%</div><div>26%</div><div>7%</div></div>
1	B	208	<div><div>%</div><div>55%</div><div>33%</div><div>8%</div></div>
1	C	208	<div><div>7%</div><div>46%</div><div>41%</div><div>9%</div></div>
1	D	208	<div><div>4%</div><div>46%</div><div>41%</div><div>11%</div></div>

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Mol	Chain	Length	Quality of chain
2	X	85	<div><div></div><div></div><div></div><div></div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7605 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 RNA-free ribonuclease P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1574	1012	265	290	7			
1	B	191	Total	C	N	O	S	0	0	0
			1547	996	259	285	7			
1	C	189	Total	C	N	O	S	0	0	0
			1525	981	258	279	7			
1	D	185	Total	C	N	O	S	0	0	0
			1501	967	254	273	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP A0A1G2XP69
A	-3	SER	-	expression tag	UNP A0A1G2XP69
A	-2	GLY	-	expression tag	UNP A0A1G2XP69
A	-1	GLY	-	expression tag	UNP A0A1G2XP69
A	0	GLY	-	expression tag	UNP A0A1G2XP69
B	-4	GLY	-	expression tag	UNP A0A1G2XP69
B	-3	SER	-	expression tag	UNP A0A1G2XP69
B	-2	GLY	-	expression tag	UNP A0A1G2XP69
B	-1	GLY	-	expression tag	UNP A0A1G2XP69
B	0	GLY	-	expression tag	UNP A0A1G2XP69
C	-4	GLY	-	expression tag	UNP A0A1G2XP69
C	-3	SER	-	expression tag	UNP A0A1G2XP69
C	-2	GLY	-	expression tag	UNP A0A1G2XP69
C	-1	GLY	-	expression tag	UNP A0A1G2XP69
C	0	GLY	-	expression tag	UNP A0A1G2XP69
D	-4	GLY	-	expression tag	UNP A0A1G2XP69
D	-3	SER	-	expression tag	UNP A0A1G2XP69
D	-2	GLY	-	expression tag	UNP A0A1G2XP69
D	-1	GLY	-	expression tag	UNP A0A1G2XP69
D	0	GLY	-	expression tag	UNP A0A1G2XP69

- Molecule 2 is a RNA chain called histidine pre-tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	68	Total	C	N	O	P	0	0	0
			1444	644	249	483	68			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	2	Total	Ca	0	0
			2	2		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

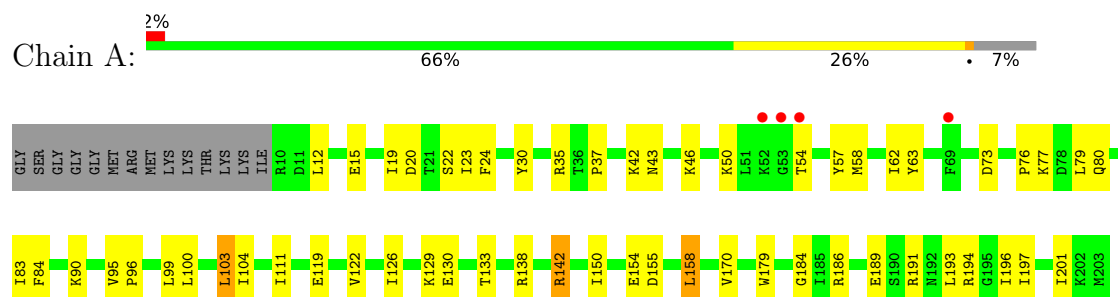
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	O	0	0
			4	4		
4	X	5	Total	O	0	0
			5	5		

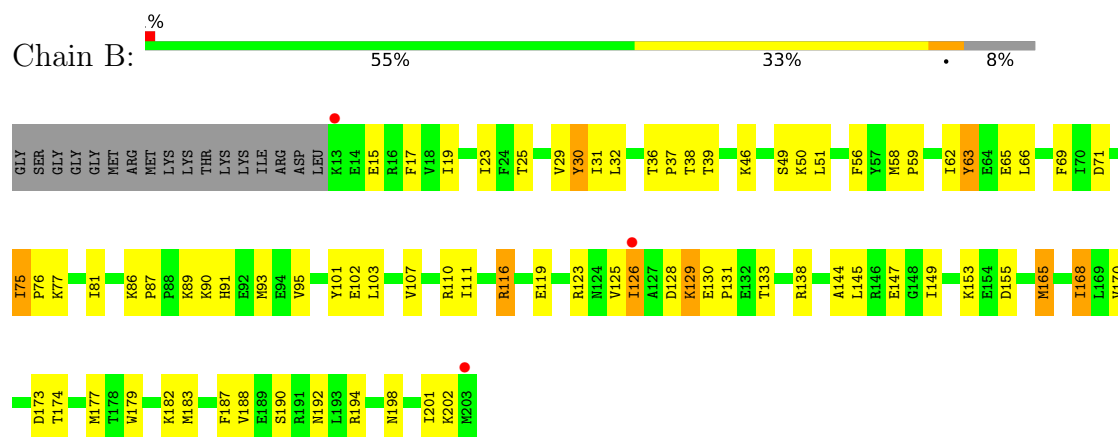
### 3 Residue-property plots

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.

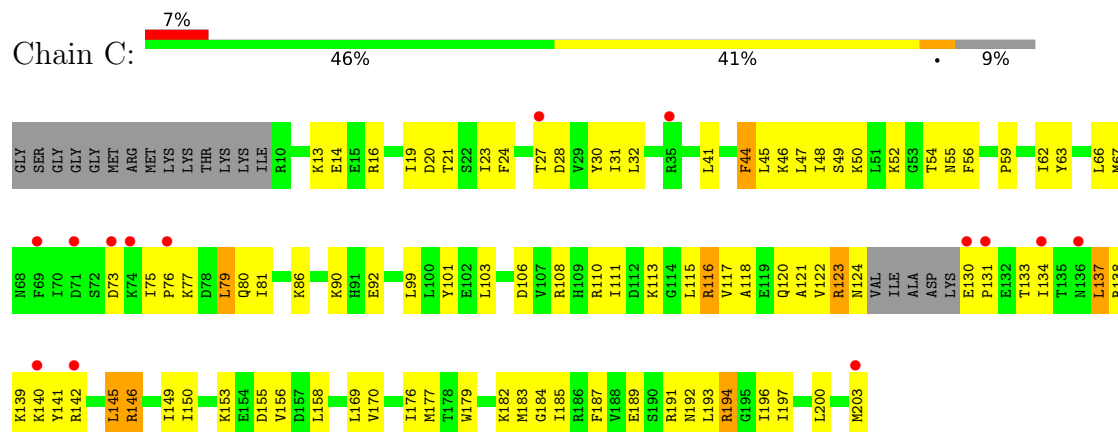
#### • Molecule 1: RNA-free ribonuclease P



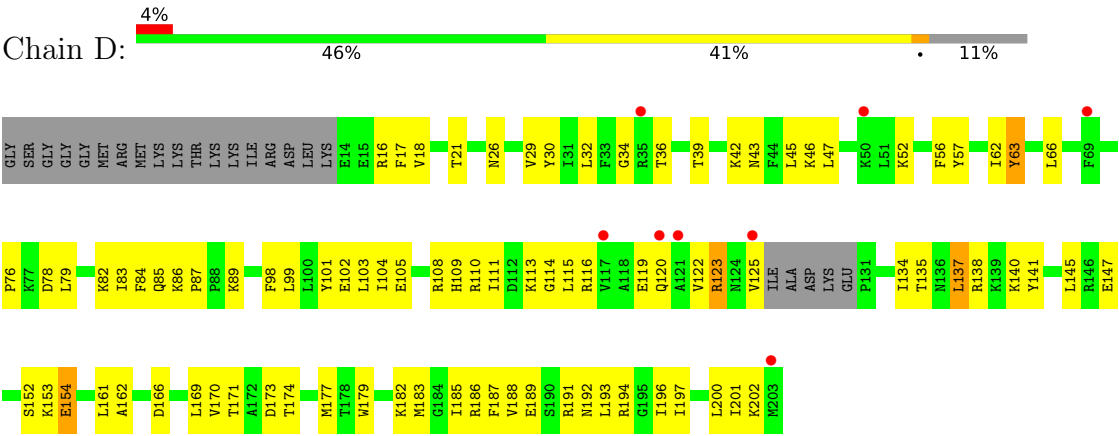
#### • Molecule 1: RNA-free ribonuclease P



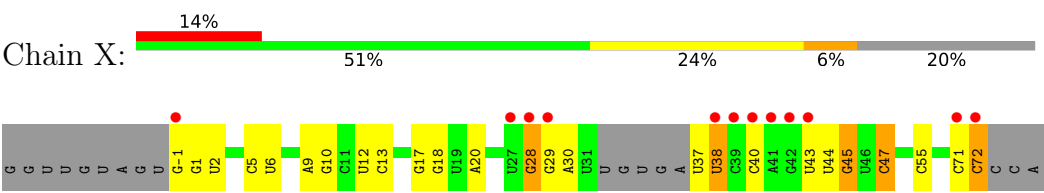
#### • Molecule 1: RNA-free ribonuclease P



● Molecule 1: RNA-free ribonuclease P



● Molecule 2: histidine pre-tRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.28Å 146.28Å 143.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.46 – 2.80 29.76 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.3 (29.46-2.80) 87.3 (29.76-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.230 , 0.284 0.231 , 0.280	Depositor DCC
$R_{free}$ test set	1678 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 35.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.039 for -h,-l,-k 0.034 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7605	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: 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	0/1599	0.76	0/2152
1	B	0.63	0/1572	0.77	0/2116
1	C	0.58	0/1549	0.88	0/2082
1	D	0.51	0/1525	0.73	0/2051
2	X	0.46	1/1610 (0.1%)	0.88	0/2504
All	All	0.58	1/7855 (0.0%)	0.81	0/10905

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	47	C	O3'-P	-6.60	1.53	1.61

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	1574	0	1640	48	0
1	B	1547	0	1612	62	0
1	C	1525	0	1578	97	0
1	D	1501	0	1567	83	0
2	X	1444	0	731	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	4	0	0	1	0
4	X	5	0	0	0	0
All	All	7605	0	7128	272	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 19.

All (272) 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:C:66:LEU:HD23	1:C:67:MET:CE	1.59	1.32
1:D:113:LYS:HA	1:D:116:ARG:HD3	1.19	1.16
1:C:66:LEU:HD23	1:C:67:MET:HE2	1.24	1.12
1:D:120:GLN:HA	1:D:123:ARG:HB2	1.34	1.09
1:C:66:LEU:HD23	1:C:67:MET:HE1	1.37	1.02
1:D:152:SER:OG	1:D:154:GLU:HG2	1.61	1.00
1:C:27:THR:HA	1:C:30:TYR:CE2	2.00	0.97
1:D:36:THR:HG23	1:D:39:THR:H	1.31	0.96
1:B:75:ILE:HD12	1:B:75:ILE:H	1.30	0.93
1:B:77:LYS:HB3	1:C:192:ASN:HB3	1.52	0.89
1:C:76:PRO:HG2	1:C:79:LEU:HD22	1.58	0.85
1:A:58:MET:HG3	1:A:83:ILE:HG21	1.57	0.84
1:D:47:LEU:HG	1:D:201:ILE:HD11	1.59	0.84
1:C:27:THR:HA	1:C:30:TYR:CD2	2.16	0.79
1:C:66:LEU:CD2	1:C:67:MET:HE1	2.15	0.77
1:C:59:PRO:HD2	1:C:62:ILE:HB	1.67	0.75
1:C:66:LEU:CD2	1:C:67:MET:CE	2.54	0.74
1:C:41:LEU:O	1:C:45:LEU:HD12	1.89	0.72
1:C:134:ILE:HG23	1:C:137:LEU:HD22	1.69	0.71
1:C:14:GLU:HA	1:C:54:THR:HG22	1.72	0.71
1:C:153:LYS:HD2	1:D:105:GLU:CD	2.11	0.71
1:A:122:VAL:HG13	1:B:125:VAL:HG11	1.71	0.71
1:C:45:LEU:CD2	1:C:80:GLN:HA	2.22	0.70
1:B:75:ILE:HD12	1:B:75:ILE:N	2.07	0.70
1:C:45:LEU:HD23	1:C:80:GLN:HA	1.71	0.70
1:D:16:ARG:HH21	1:D:166:ASP:HB3	1.57	0.69
1:B:36:THR:HG22	1:B:38:THR:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ARG:HG2	1:D:115:LEU:HD21	1.73	0.69
1:B:170:VAL:HG12	1:B:188:VAL:HG23	1.75	0.68
1:C:113:LYS:HA	1:C:116:ARG:HB2	1.75	0.67
1:B:81:ILE:HD11	1:C:196:ILE:CG1	2.24	0.67
1:C:66:LEU:CD2	1:C:67:MET:HE2	2.16	0.67
1:C:193:LEU:HD12	1:C:196:ILE:HG21	1.75	0.66
1:D:76:PRO:HB2	1:D:78:ASP:OD1	1.94	0.66
1:D:152:SER:HG	1:D:154:GLU:HG2	1.61	0.66
1:B:170:VAL:HG12	1:B:188:VAL:CG2	2.26	0.65
1:C:137:LEU:HD21	1:D:115:LEU:HD11	1.76	0.65
1:A:130:GLU:O	1:A:133:THR:HG22	1.97	0.64
1:A:58:MET:HG3	1:A:83:ILE:CG2	2.26	0.64
1:C:111:ILE:HD11	1:D:145:LEU:HD13	1.78	0.64
2:X:71:C:H2'	2:X:72:C:H5''	1.79	0.64
1:C:106:ASP:OD1	1:C:110:ARG:NH2	2.31	0.64
1:D:99:LEU:HD11	1:D:183:MET:HG2	1.80	0.64
1:B:19:ILE:HG22	1:B:170:VAL:CG2	2.28	0.64
1:B:116:ARG:NH2	1:B:119:GLU:OE1	2.29	0.64
1:C:54:THR:HG21	1:C:200:LEU:HD22	1.78	0.64
1:C:32:LEU:N	1:C:32:LEU:HD12	2.12	0.64
1:D:36:THR:HG22	1:D:39:THR:HB	1.78	0.63
1:D:26:ASN:HD22	1:D:29:VAL:HG23	1.63	0.63
1:B:19:ILE:HG22	1:B:170:VAL:HG22	1.81	0.63
1:B:58:MET:HB2	1:B:62:ILE:HD11	1.80	0.63
1:A:186:ARG:HG3	1:D:86:LYS:HD3	1.80	0.62
1:D:36:THR:HG22	1:D:39:THR:CB	2.29	0.62
1:D:78:ASP:OD1	1:D:78:ASP:N	2.27	0.62
1:A:15:GLU:CD	1:A:186:ARG:HH22	2.02	0.62
1:C:153:LYS:HD2	1:D:105:GLU:OE1	1.99	0.62
1:B:17:PHE:CE2	1:B:168:ILE:HD12	2.35	0.62
1:C:130:GLU:HG3	1:C:131:PRO:HD3	1.81	0.61
1:C:115:LEU:HB2	1:D:141:TYR:CE1	2.35	0.61
1:C:120:GLN:HA	1:C:123:ARG:HB2	1.82	0.61
2:X:-1:G:O5'	2:X:-1:G:H8	1.83	0.61
1:A:119:GLU:OE1	1:B:138:ARG:NH1	2.31	0.61
1:B:125:VAL:HG12	1:B:133:THR:OG1	2.01	0.60
1:A:95:VAL:HG12	1:A:99:LEU:HD12	1.83	0.60
1:A:62:ILE:HD11	1:A:154:GLU:O	2.02	0.60
1:B:102:GLU:OE1	1:B:182:LYS:HE3	2.02	0.59
1:C:23:ILE:HD11	1:C:170:VAL:HG12	1.84	0.59
1:C:137:LEU:O	1:C:141:TYR:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ILE:HD13	1:B:190:SER:HB3	1.85	0.59
1:A:19:ILE:HG22	1:A:170:VAL:HB	1.85	0.59
1:C:108:ARG:HA	1:C:111:ILE:HG22	1.84	0.59
1:C:75:ILE:HD12	1:C:75:ILE:O	2.03	0.58
1:C:193:LEU:O	1:C:196:ILE:HG22	2.04	0.58
1:D:113:LYS:HA	1:D:116:ARG:CD	2.11	0.58
1:B:17:PHE:HB2	1:B:56:PHE:CD1	2.38	0.58
1:C:134:ILE:HG23	1:C:137:LEU:CD2	2.33	0.58
1:C:76:PRO:HG2	1:C:79:LEU:CD2	2.32	0.58
1:D:47:LEU:HG	1:D:201:ILE:CD1	2.33	0.58
1:B:86:LYS:HD3	1:B:165:MET:HE1	1.86	0.58
2:X:71:C:H2'	2:X:72:C:C5'	2.33	0.58
1:C:113:LYS:HA	1:C:116:ARG:HD2	1.86	0.57
1:B:77:LYS:HB3	1:C:192:ASN:CB	2.32	0.57
1:C:193:LEU:HD12	1:C:196:ILE:CG2	2.34	0.57
1:B:63:TYR:O	1:B:66:LEU:HD23	2.05	0.57
1:C:146:ARG:HH12	1:D:108:ARG:HD3	1.70	0.57
1:D:63:TYR:CD2	1:D:85:GLN:HG3	2.40	0.57
1:C:197:ILE:O	1:C:200:LEU:HB2	2.04	0.56
1:A:58:MET:CE	1:A:63:TYR:CD2	2.89	0.56
1:B:86:LYS:HD3	1:B:165:MET:CE	2.35	0.56
1:C:63:TYR:O	1:C:66:LEU:HB3	2.06	0.56
2:X:37:U:H2'	2:X:38:U:C6	2.41	0.56
1:C:153:LYS:CD	1:D:105:GLU:OE1	2.53	0.56
1:D:137:LEU:HA	1:D:140:LYS:HE2	1.88	0.56
1:A:23:ILE:HD11	1:A:170:VAL:HG12	1.86	0.56
1:A:197:ILE:O	1:A:201:ILE:HG12	2.06	0.56
1:C:150:ILE:HD11	1:C:179:TRP:CD2	2.41	0.56
1:D:111:ILE:HA	1:D:145:LEU:HD21	1.88	0.56
1:C:146:ARG:HA	1:C:149:ILE:HD11	1.87	0.55
1:D:134:ILE:HA	1:D:137:LEU:HB3	1.88	0.55
1:D:17:PHE:HB2	1:D:56:PHE:CD2	2.42	0.55
1:C:21:THR:HG23	1:C:62:ILE:HG23	1.87	0.55
1:D:103:LEU:HB2	1:D:179:TRP:CH2	2.43	0.54
1:D:110:ARG:HB3	1:D:145:LEU:HD23	1.89	0.54
1:D:170:VAL:HA	1:D:188:VAL:O	2.08	0.54
1:D:86:LYS:HG3	1:D:161:LEU:HD11	1.89	0.54
1:A:20:ASP:HB3	1:A:158:LEU:HD11	1.90	0.53
1:A:103:LEU:O	1:A:103:LEU:HG	2.08	0.53
1:D:194:ARG:HG3	1:D:194:ARG:HH11	1.73	0.53
1:A:76:PRO:HG2	1:A:79:LEU:CD1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:ASN:ND2	1:D:29:VAL:HG23	2.22	0.53
1:A:20:ASP:OD1	1:A:22:SER:OG	2.26	0.53
1:C:117:VAL:CG1	1:C:140:LYS:HG3	2.39	0.53
1:B:51:LEU:HG	1:B:201:ILE:HG22	1.90	0.53
1:C:32:LEU:CD2	1:C:191:ARG:O	2.57	0.53
1:C:153:LYS:HG3	1:D:101:TYR:CE1	2.44	0.53
1:A:57:TYR:HE1	1:A:84:PHE:HD2	1.56	0.52
1:B:173:ASP:O	1:B:177:MET:HG3	2.09	0.52
1:C:32:LEU:N	1:C:32:LEU:CD1	2.73	0.52
1:C:44:PHE:O	1:C:48:ILE:HG12	2.09	0.52
1:C:193:LEU:HA	1:C:196:ILE:HG22	1.91	0.52
1:D:45:LEU:HD21	1:D:79:LEU:HD12	1.92	0.52
1:B:81:ILE:HD11	1:C:196:ILE:HG12	1.91	0.52
2:X:1:G:H1	2:X:71:C:H42	1.57	0.51
1:B:29:VAL:O	1:B:32:LEU:HD12	2.10	0.51
1:B:129:LYS:HB3	1:B:131:PRO:HD2	1.93	0.51
1:C:150:ILE:HG23	1:C:155:ASP:HB2	1.93	0.51
1:D:42:LYS:HG2	1:D:46:LYS:HE3	1.93	0.51
1:B:95:VAL:HG12	1:B:183:MET:CE	2.41	0.51
1:D:102:GLU:O	1:D:105:GLU:HB3	2.11	0.51
1:B:110:ARG:HG2	1:B:144:ALA:O	2.11	0.50
1:D:36:THR:HG22	1:D:39:THR:OG1	2.09	0.50
1:D:174:THR:HA	1:D:177:MET:HE3	1.93	0.50
1:B:110:ARG:NH1	1:B:147:GLU:O	2.38	0.50
1:D:196:ILE:O	1:D:200:LEU:HD22	2.11	0.50
1:C:118:ALA:O	1:C:121:ALA:HB3	2.11	0.50
1:B:75:ILE:HG22	1:B:76:PRO:HD2	1.93	0.50
1:B:103:LEU:HA	1:B:179:TRP:CH2	2.46	0.50
1:C:124:ASN:C	1:C:133:THR:HG21	2.32	0.50
1:D:174:THR:HA	1:D:177:MET:CE	2.42	0.50
1:D:63:TYR:O	1:D:66:LEU:HD23	2.12	0.50
2:X:44:U:O2'	2:X:45:G:H5'	2.12	0.50
1:C:117:VAL:HG11	1:C:140:LYS:HG3	1.93	0.49
1:D:137:LEU:O	1:D:137:LEU:HG	2.11	0.49
1:A:42:LYS:O	1:A:46:LYS:HG3	2.13	0.49
1:B:25:THR:HG21	1:B:69:PHE:HD2	1.76	0.49
1:C:77:LYS:O	1:C:81:ILE:HG23	2.12	0.49
1:D:34:GLY:HA3	1:D:39:THR:HG22	1.94	0.49
1:D:36:THR:CG2	1:D:39:THR:HB	2.43	0.49
2:X:29:G:C2	2:X:40:C:C4	3.00	0.49
1:C:92:GLU:O	1:C:92:GLU:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ARG:O	1:D:114:GLY:N	2.45	0.49
1:D:171:THR:HG22	1:D:173:ASP:N	2.27	0.49
1:A:189:GLU:OE1	1:A:191:ARG:N	2.39	0.48
1:C:45:LEU:O	1:C:49:SER:OG	2.29	0.48
1:D:162:ALA:HB2	1:D:169:LEU:HD13	1.95	0.48
1:B:59:PRO:HD2	1:B:62:ILE:HG12	1.94	0.48
1:D:183:MET:HE2	1:D:185:ILE:HD11	1.95	0.48
1:A:58:MET:CE	1:A:63:TYR:HA	2.44	0.48
1:A:58:MET:HE3	1:A:63:TYR:CD2	2.47	0.48
1:A:77:LYS:HA	1:A:80:GLN:HG3	1.95	0.48
1:D:171:THR:HG22	1:D:173:ASP:H	1.79	0.48
1:B:30:TYR:HE2	1:B:37:PRO:HG3	1.77	0.48
1:A:30:TYR:HE1	1:A:35:ARG:O	1.97	0.47
1:A:150:ILE:HD11	1:A:155:ASP:HB3	1.96	0.47
1:B:30:TYR:CE2	1:B:37:PRO:HG3	2.49	0.47
1:C:134:ILE:HG12	1:D:122:VAL:HG21	1.96	0.47
1:A:186:ARG:CG	1:D:86:LYS:HD3	2.44	0.47
1:C:179:TRP:HA	1:C:182:LYS:HB2	1.95	0.47
1:D:98:PHE:HD1	1:D:102:GLU:HG3	1.79	0.47
1:A:193:LEU:HD12	1:A:196:ILE:HD11	1.96	0.47
1:D:189:GLU:H	1:D:189:GLU:HG3	1.37	0.47
1:A:50:LYS:HB2	1:A:201:ILE:HD12	1.96	0.47
1:D:57:TYR:CD2	1:D:84:PHE:HB2	2.49	0.47
1:A:170:VAL:HG11	1:A:193:LEU:HD13	1.97	0.47
2:X:5:C:H2'	2:X:6:U:H6	1.79	0.46
1:C:32:LEU:CD1	1:C:32:LEU:H	2.29	0.46
1:C:66:LEU:HB3	1:C:67:MET:HE2	1.96	0.46
1:C:62:ILE:HG13	1:C:158:LEU:HD13	1.97	0.46
1:C:156:VAL:HG21	1:D:104:ILE:HG21	1.98	0.46
1:A:189:GLU:OE1	1:A:191:ARG:HD3	2.15	0.46
1:C:145:LEU:HD12	1:C:145:LEU:H	1.80	0.46
1:C:193:LEU:HA	1:C:196:ILE:CG2	2.45	0.46
1:A:43:ASN:HA	1:A:46:LYS:HE2	1.97	0.46
1:B:89:LYS:O	1:B:93:MET:HG3	2.15	0.46
1:A:58:MET:HE1	1:A:63:TYR:HA	1.97	0.46
2:X:29:G:C6	2:X:40:C:N4	2.83	0.46
1:D:135:THR:HA	1:D:138:ARG:HH21	1.80	0.45
1:D:191:ARG:HH11	1:D:192:ASN:HD21	1.64	0.45
1:C:179:TRP:HE3	1:C:183:MET:HE2	1.81	0.45
1:D:42:LYS:HA	1:D:45:LEU:HD12	1.98	0.45
1:C:45:LEU:HD12	1:C:45:LEU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ILE:HG22	1:C:138:ARG:HG3	1.97	0.45
1:A:184:GLY:HA3	1:D:89:LYS:HG2	1.98	0.45
1:B:15:GLU:OE1	1:B:15:GLU:HA	2.14	0.45
1:D:43:ASN:HD22	1:D:46:LYS:NZ	2.14	0.45
1:B:51:LEU:HD23	1:B:51:LEU:HA	1.70	0.45
1:C:150:ILE:HG13	1:C:179:TRP:CD1	2.52	0.45
1:B:81:ILE:HD11	1:C:196:ILE:HG13	1.98	0.45
1:C:155:ASP:OD1	1:C:176:ILE:HD11	2.16	0.45
1:D:36:THR:CG2	1:D:39:THR:CB	2.95	0.45
1:D:18:VAL:HG13	1:D:161:LEU:HD23	1.99	0.45
1:B:119:GLU:O	1:B:123:ARG:HG3	2.17	0.44
1:B:130:GLU:O	1:B:131:PRO:C	2.54	0.44
1:B:30:TYR:HE2	1:B:37:PRO:CG	2.31	0.44
1:C:101:TYR:CZ	1:D:153:LYS:HG3	2.53	0.44
1:D:18:VAL:HG21	1:D:162:ALA:HA	1.99	0.44
1:A:76:PRO:HG2	1:A:79:LEU:HD13	1.98	0.44
1:B:29:VAL:HA	1:B:32:LEU:HD12	1.99	0.44
1:C:50:LYS:HE3	1:C:50:LYS:HB3	1.65	0.44
1:B:95:VAL:HG12	1:B:183:MET:HE1	1.99	0.44
1:C:76:PRO:O	1:C:79:LEU:HD23	2.17	0.44
1:A:90:LYS:HD3	1:B:101:TYR:CD2	2.53	0.44
1:B:91:HIS:CE1	1:C:99:LEU:HD21	2.53	0.44
1:B:116:ARG:HH22	1:B:119:GLU:CD	2.20	0.44
1:D:177:MET:HB3	1:D:187:PHE:CE1	2.53	0.44
1:B:107:VAL:O	1:B:111:ILE:HG13	2.17	0.44
1:C:55:ASN:C	1:C:56:PHE:HD1	2.21	0.44
2:X:28:G:N2	2:X:29:G:H1'	2.33	0.44
1:C:76:PRO:O	1:C:79:LEU:CD2	2.66	0.43
1:B:62:ILE:HA	1:B:65:GLU:HB2	1.99	0.43
1:B:177:MET:HB3	1:B:187:PHE:CE2	2.53	0.43
1:C:108:ARG:O	1:C:111:ILE:HG22	2.18	0.43
2:X:5:C:H2'	2:X:6:U:C6	2.53	0.43
1:B:201:ILE:HD12	1:B:202:LYS:HG2	2.00	0.43
1:A:58:MET:HE2	1:A:63:TYR:CD2	2.54	0.43
1:A:122:VAL:CG1	1:B:125:VAL:HG11	2.46	0.43
1:A:100:LEU:O	1:A:104:ILE:HG12	2.18	0.43
1:C:76:PRO:CG	1:C:79:LEU:HD22	2.41	0.43
1:A:184:GLY:HA2	1:D:87:PRO:HG2	2.00	0.43
1:D:108:ARG:HG3	1:D:109:HIS:CD2	2.53	0.43
1:C:27:THR:HA	1:C:30:TYR:HE2	1.71	0.42
1:C:90:LYS:H	1:C:90:LYS:HG2	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ARG:NH1	1:B:198:ASN:OD1	2.52	0.42
1:A:42:LYS:HE3	1:A:46:LYS:HD3	2.01	0.42
1:A:150:ILE:CD1	1:A:155:ASP:HB3	2.49	0.42
1:B:36:THR:HB	1:B:39:THR:H	1.84	0.42
1:B:46:LYS:HD2	1:B:46:LYS:HA	1.84	0.42
1:B:149:ILE:HG13	1:B:179:TRP:HE1	1.84	0.42
1:C:19:ILE:HD13	1:C:56:PHE:HB3	2.00	0.42
1:C:122:VAL:CG1	1:D:125:VAL:HG21	2.49	0.42
1:D:78:ASP:OD2	1:D:82:LYS:HE2	2.19	0.42
1:C:134:ILE:HD13	1:D:119:GLU:HB2	2.01	0.42
1:D:99:LEU:CD1	1:D:183:MET:HG2	2.49	0.42
1:D:193:LEU:O	1:D:197:ILE:HG13	2.19	0.42
1:B:87:PRO:HG2	1:C:184:GLY:HA2	2.01	0.42
1:C:101:TYR:OH	1:D:153:LYS:HG3	2.20	0.42
1:C:20:ASP:HB2	1:C:158:LEU:HD21	2.02	0.42
1:D:63:TYR:OH	1:D:83:ILE:O	2.37	0.42
1:D:119:GLU:O	1:D:122:VAL:HG22	2.20	0.42
1:A:111:ILE:HD13	1:B:145:LEU:HB3	2.00	0.41
2:X:9:A:O2'	2:X:10:G:N7	2.53	0.41
1:A:24:PHE:HA	1:A:30:TYR:HB3	2.03	0.41
1:A:196:ILE:HD13	1:A:196:ILE:HG21	1.85	0.41
1:A:95:VAL:HG12	1:A:96:PRO:HD2	2.02	0.41
1:B:168:ILE:HG22	1:B:187:PHE:HA	2.03	0.41
1:D:62:ILE:HD13	1:D:62:ILE:HA	1.88	0.41
1:D:110:ARG:NH2	1:D:147:GLU:O	2.53	0.41
1:A:126:ILE:HB	1:A:129:LYS:HB2	2.03	0.41
1:B:126:ILE:HB	4:B:401:HOH:O	2.20	0.41
1:B:174:THR:HA	1:B:177:MET:HE2	2.02	0.41
1:C:20:ASP:OD1	1:C:21:THR:N	2.54	0.41
1:C:24:PHE:CZ	1:C:44:PHE:HD2	2.39	0.41
1:C:169:LEU:HD11	1:C:185:ILE:HG21	2.02	0.41
2:X:40:C:O2	2:X:40:C:H2'	2.20	0.41
1:A:30:TYR:CE1	1:A:37:PRO:HD3	2.55	0.41
1:A:138:ARG:O	1:A:142:ARG:HB2	2.21	0.41
1:D:21:THR:HG22	1:D:66:LEU:HB3	2.03	0.41
1:C:55:ASN:O	1:C:56:PHE:HD1	2.04	0.40
1:C:177:MET:HB3	1:C:187:PHE:CE2	2.56	0.40
1:D:32:LEU:HB3	1:D:194:ARG:HD3	2.04	0.40
1:D:166:ASP:O	1:D:186:ARG:NH1	2.54	0.40
1:C:47:LEU:HD11	1:C:194:ARG:HH22	1.86	0.40

There are no symmetry-related clashes.

## 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	192/208 (92%)	188 (98%)	4 (2%)	0	100	100
1	B	189/208 (91%)	184 (97%)	5 (3%)	0	100	100
1	C	185/208 (89%)	179 (97%)	6 (3%)	0	100	100
1	D	181/208 (87%)	178 (98%)	3 (2%)	0	100	100
All	All	747/832 (90%)	729 (98%)	18 (2%)	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	176/187 (94%)	168 (96%)	8 (4%)	27	60
1	B	173/187 (92%)	156 (90%)	17 (10%)	8	24
1	C	168/187 (90%)	147 (88%)	21 (12%)	4	14
1	D	168/187 (90%)	160 (95%)	8 (5%)	25	58
All	All	685/748 (92%)	631 (92%)	54 (8%)	12	34

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	54	THR

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Mol	Chain	Res	Type
1	A	73	ASP
1	A	103	LEU
1	A	142	ARG
1	A	158	LEU
1	A	179	TRP
1	A	194	ARG
1	B	30	TYR
1	B	31	ILE
1	B	49	SER
1	B	50	LYS
1	B	63	TYR
1	B	71	ASP
1	B	75	ILE
1	B	90	LYS
1	B	116	ARG
1	B	126	ILE
1	B	128	ASP
1	B	129	LYS
1	B	153	LYS
1	B	155	ASP
1	B	165	MET
1	B	168	ILE
1	B	192	ASN
1	C	13	LYS
1	C	16	ARG
1	C	28	ASP
1	C	31	ILE
1	C	44	PHE
1	C	46	LYS
1	C	52	LYS
1	C	73	ASP
1	C	79	LEU
1	C	86	LYS
1	C	103	LEU
1	C	116	ARG
1	C	123	ARG
1	C	137	LEU
1	C	139	LYS
1	C	142	ARG
1	C	145	LEU
1	C	146	ARG
1	C	189	GLU

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Mol	Chain	Res	Type
1	C	194	ARG
1	C	203	MET
1	D	30	TYR
1	D	52	LYS
1	D	63	TYR
1	D	123	ARG
1	D	137	LEU
1	D	154	GLU
1	D	182	LYS
1	D	202	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	85	GLN
1	A	198	ASN
1	C	43	ASN
1	C	85	GLN
1	D	26	ASN
1	D	43	ASN
1	D	109	HIS
1	D	192	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	X	66/85 (77%)	14 (21%)	0

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	X	2	U
2	X	12	U
2	X	13	C
2	X	17	G
2	X	18	G
2	X	20	A
2	X	28	G
2	X	30	A

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Mol	Chain	Res	Type
2	X	38	U
2	X	43	U
2	X	45	G
2	X	47	C
2	X	55	C
2	X	72	C

There are no RNA pucker outliers to report.

## 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 5 ligands modelled in this entry, 5 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	194/208 (93%)	-0.33	4 (2%) 63 54	16, 36, 72, 123	0
1	B	191/208 (91%)	-0.25	3 (1%) 72 66	20, 56, 92, 122	0
1	C	189/208 (90%)	0.38	14 (7%) 14 8	28, 83, 142, 165	0
1	D	185/208 (88%)	-0.03	8 (4%) 35 25	27, 56, 119, 156	0
2	X	68/85 (80%)	0.51	12 (17%) 1 1	25, 73, 154, 171	0
All	All	827/917 (90%)	-0.01	41 (4%) 28 19	16, 56, 129, 171	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	73	ASP	5.6
1	C	71	ASP	5.3
1	C	69	PHE	5.2
1	C	203	MET	4.9
1	D	121	ALA	4.6
2	X	72	C	4.3
1	C	35	ARG	4.2
1	D	203	MET	3.9
1	C	74	LYS	3.8
1	A	54	THR	3.6
1	D	120	GLN	3.3
1	C	131	PRO	3.3
1	D	125	VAL	3.2
1	C	140	LYS	3.2
1	B	203	MET	3.1
1	C	142	ARG	3.0
2	X	29	G	3.0
2	X	71	C	3.0
2	X	38	U	2.9
2	X	28	G	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	69	PHE	2.8
2	X	41	A	2.8
1	D	50	LYS	2.8
1	C	27	THR	2.8
2	X	-1	G	2.7
1	D	35	ARG	2.4
1	C	134	ILE	2.4
1	D	117	VAL	2.4
2	X	39	C	2.4
1	C	130	GLU	2.4
1	C	136	ASN	2.3
1	A	53	GLY	2.3
2	X	42	G	2.3
1	A	52	LYS	2.2
1	D	69	PHE	2.2
2	X	27	U	2.2
1	B	126	ILE	2.2
2	X	43	U	2.2
1	B	13	LYS	2.1
1	C	76	PRO	2.1
2	X	40	C	2.1

## 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.

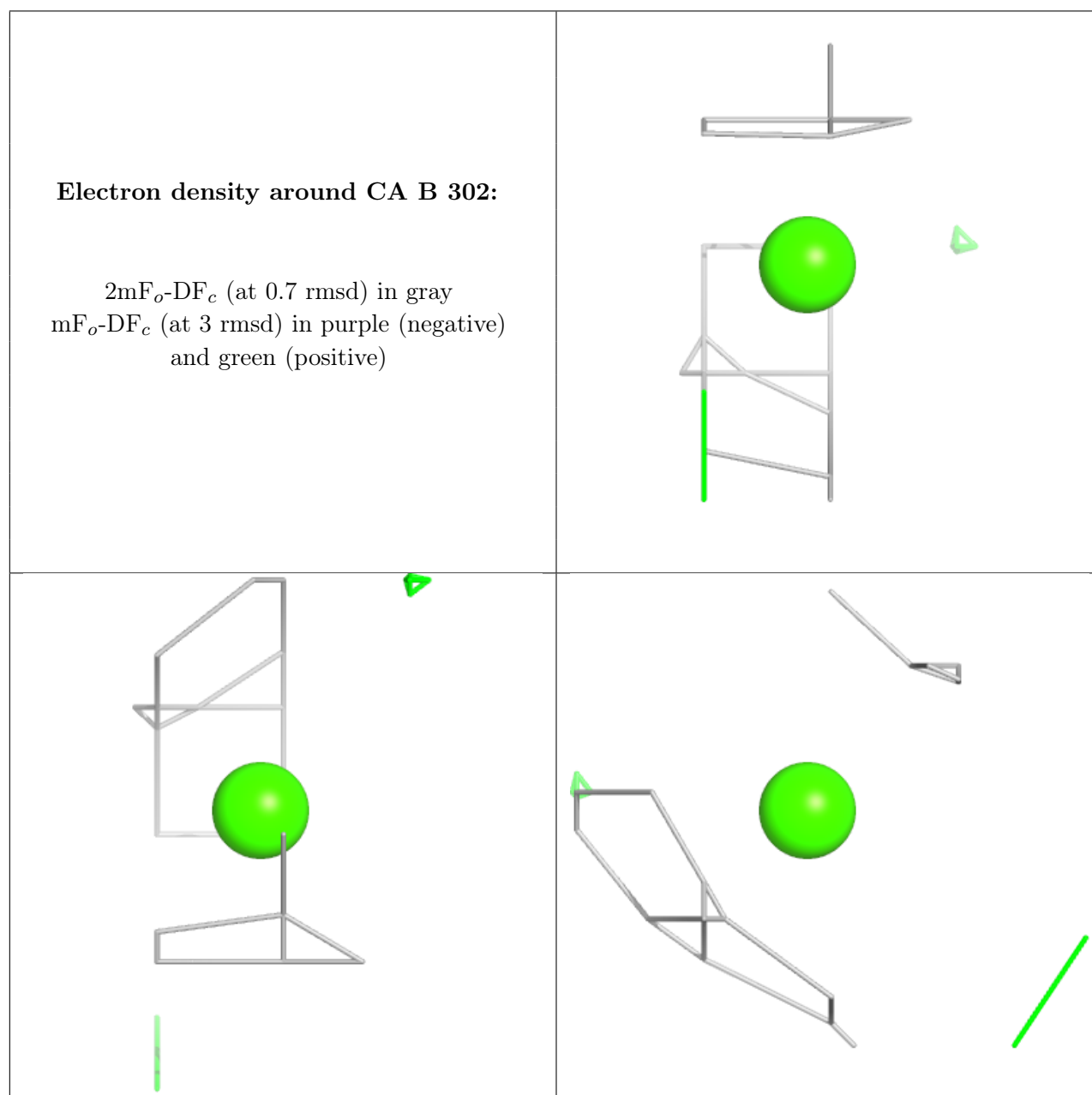
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	B	302	1/1	0.83	0.23	115,115,115,115	0
3	CA	A	301	1/1	0.96	0.10	76,76,76,76	0

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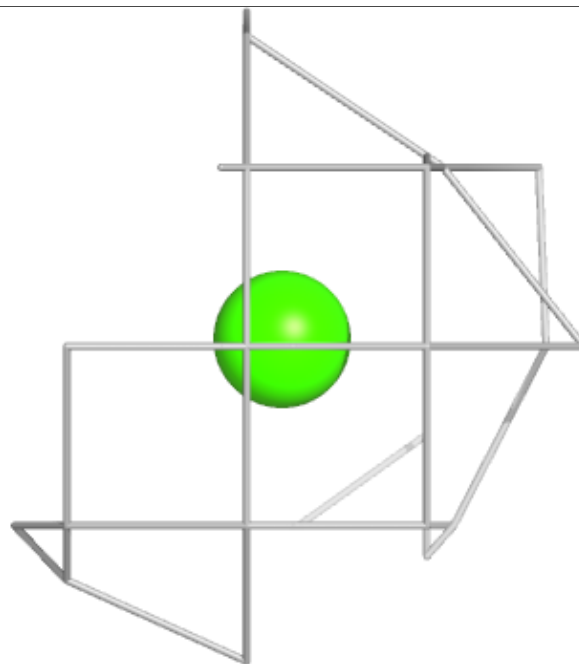
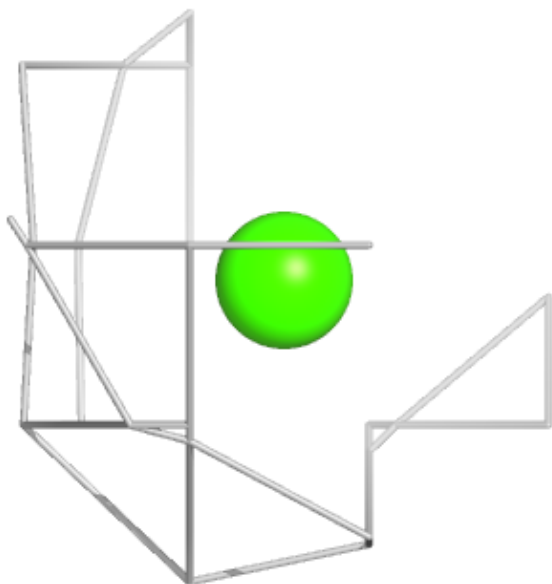
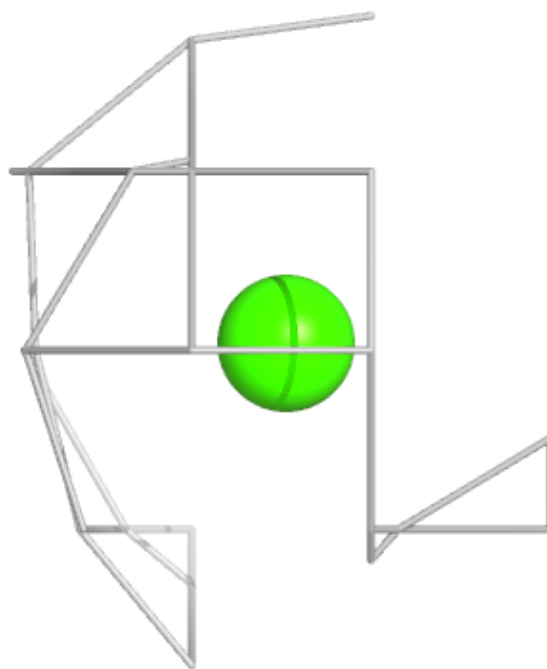
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	C	301	1/1	0.97	0.30	86,86,86,86	0
3	CA	D	301	1/1	0.97	0.04	92,92,92,92	0
3	CA	B	301	1/1	0.98	0.09	59,59,59,59	0

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.



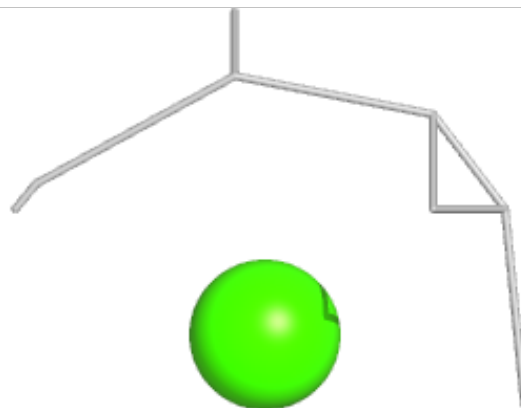
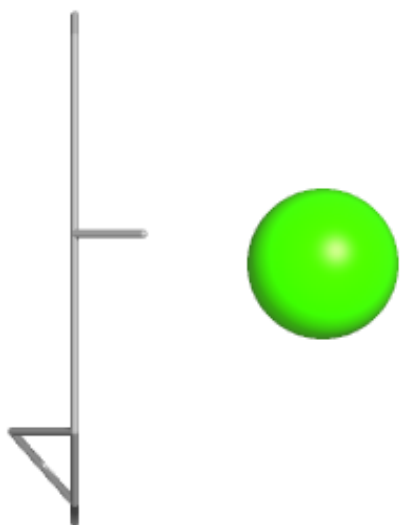
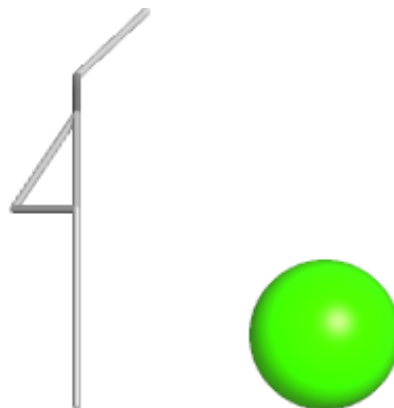
**Electron density around CA A 301:**

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



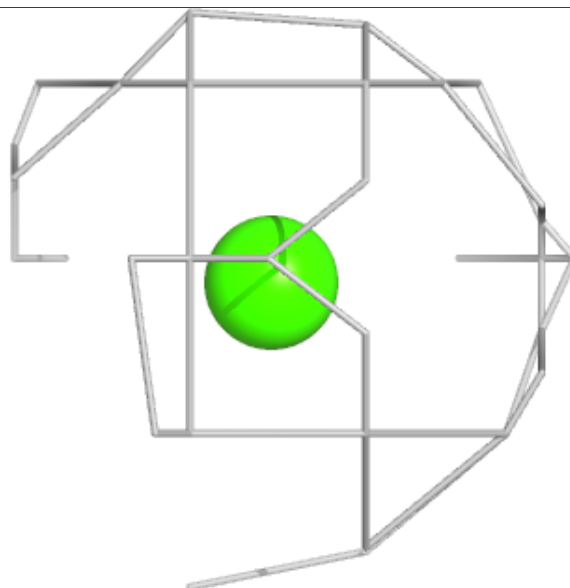
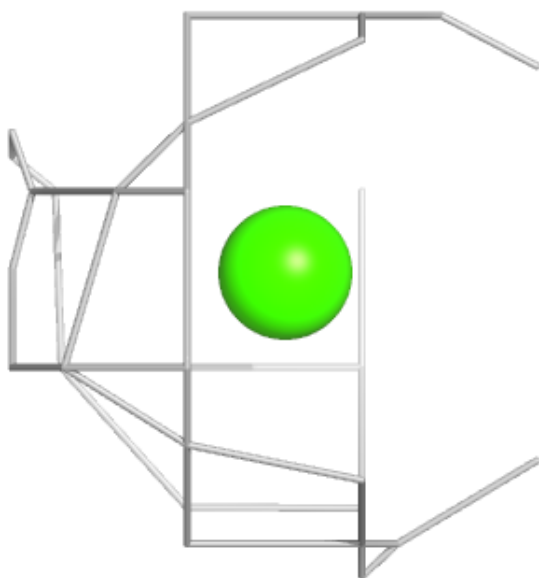
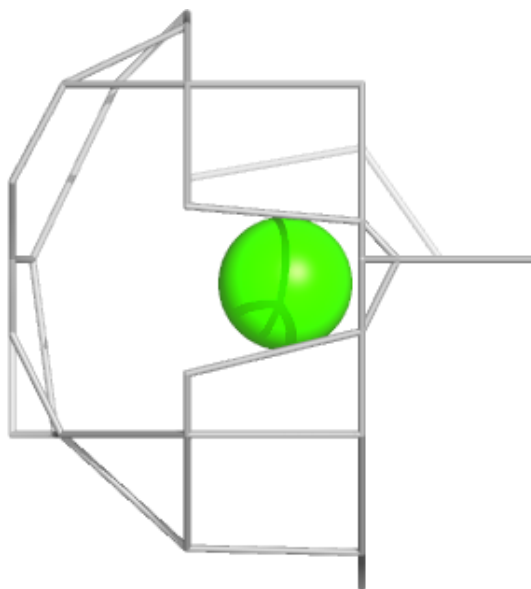
**Electron density around CA C 301:**

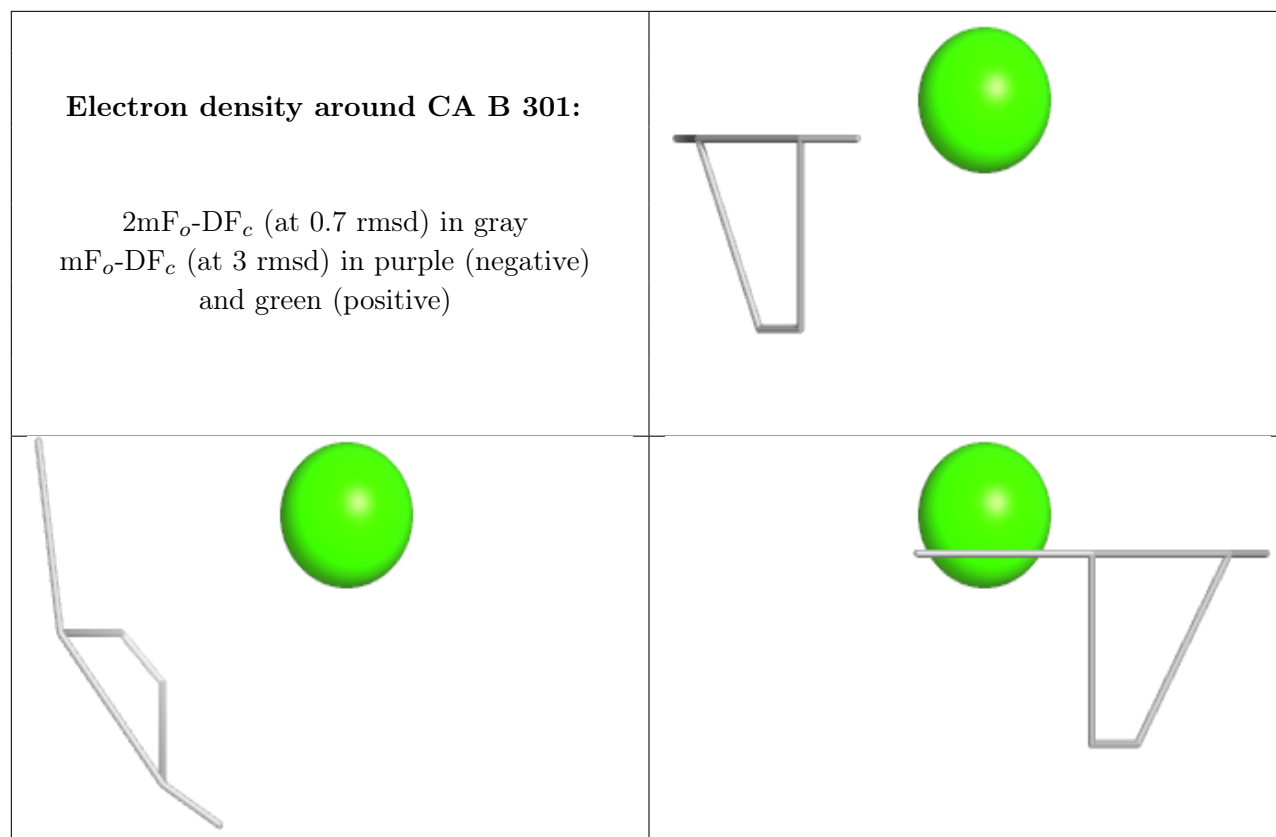
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CA D 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.