



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:10 AM UTC

PDB ID : 9BW0 / pdb_00009bw0
Title : RNA Polymerase II - No ATP
Authors : Calero, G.
Deposited on : 2024-05-20
Resolution : 3.51 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

i

X-RAY DIFFRACTION

A.

Metric	Percentile Rank	Value
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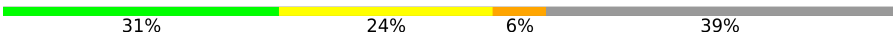
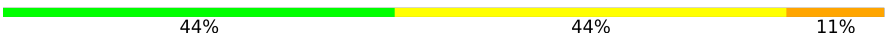


Similar resolution
(#Entries, resolution range(Å))

Quality of chain

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	R	9	
14	T	13	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 30691 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1398	Total	C	N	O	S	0	0	0
			10974	6926	1915	2071	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1062	Total	C	N	O	S	0	0	0
			8438	5354	1477	1552	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	162	Total	C	N	O	S	0	0	0
			1287	799	224	262	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	208	Total	C	N	O	S	0	0	0
			1713	1089	303	312	9			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1338	860	222	248	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	117	Total	C	N	O	S	0	0	0
			951	605	158	184	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	117	Total	C	N	O	S	0	0	0
			955	587	176	182	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	43	Total	C	N	O	S	0	0	0
			343	211	69	59	4			

- Molecule 13 is a RNA chain called RNA (5'-R(P*UP*CP*GP*AP*GP*AP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	9	Total	C	N	O	P	0	0	0
			198	88	40	61	9			

- Molecule 14 is a DNA chain called DNA (5'-D(P*AP*CP*GP*TP*CP*CP*CP*TP*CP*T

P*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	13	Total 260	C 124	N 44	O 79	P 13	0	0	0

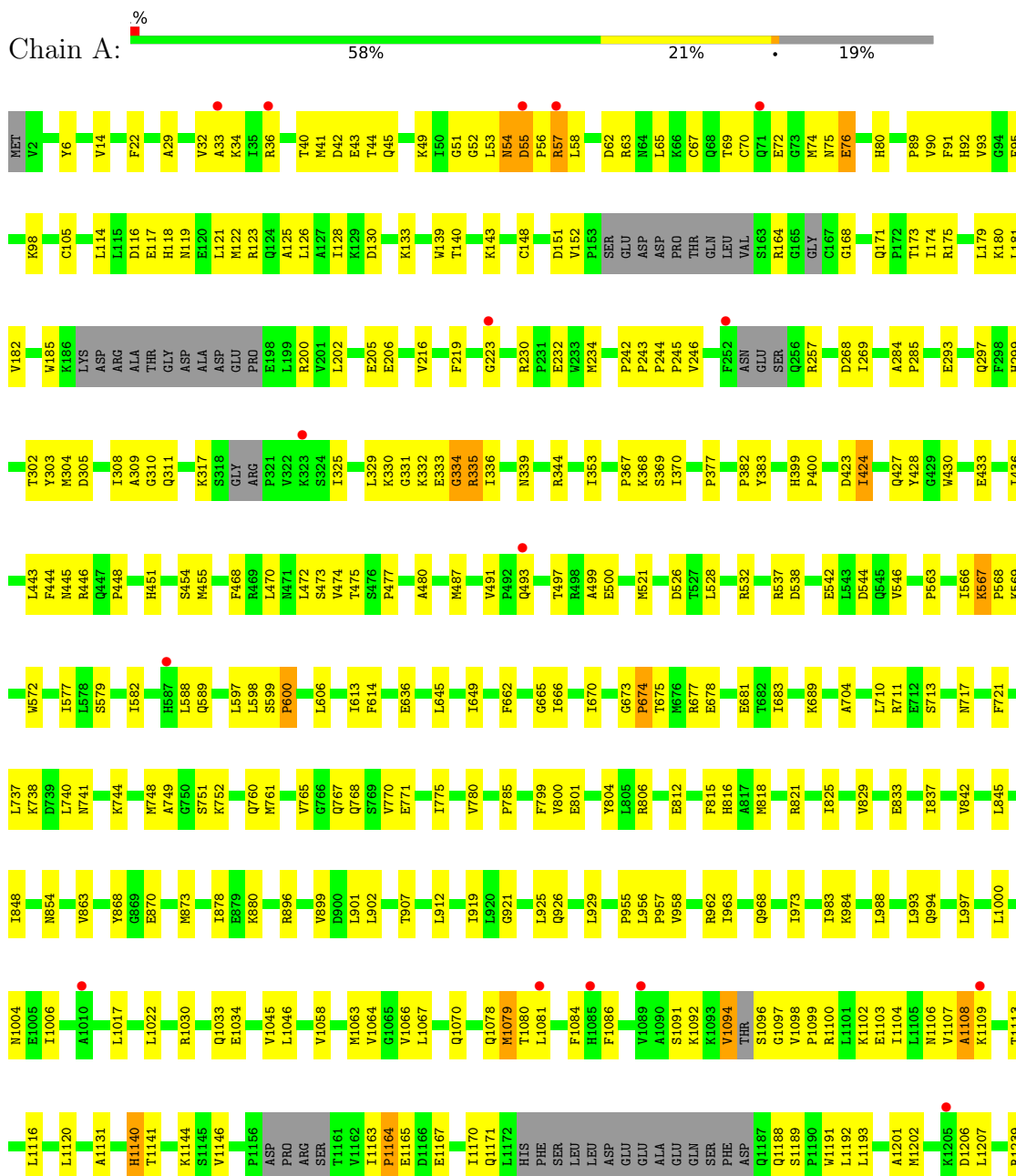
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

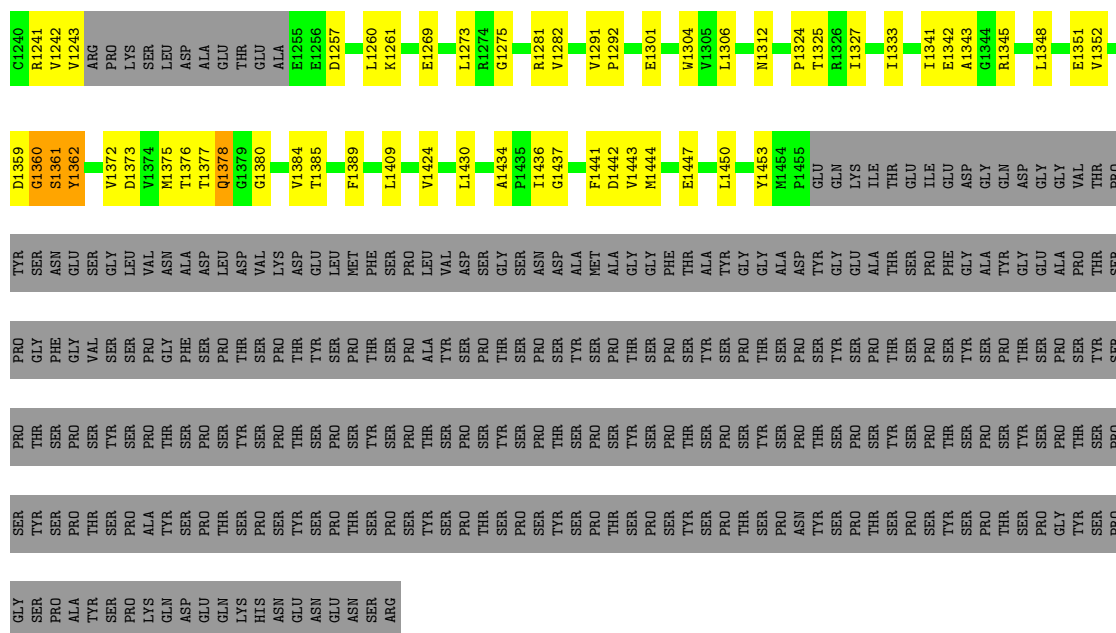
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total 2	Zn 2	0	0
15	B	1	Total 1	Zn 1	0	0
15	C	1	Total 1	Zn 1	0	0
15	I	2	Total 2	Zn 2	0	0
15	J	1	Total 1	Zn 1	0	0
15	L	1	Total 1	Zn 1	0	0

3 Residue-property plots

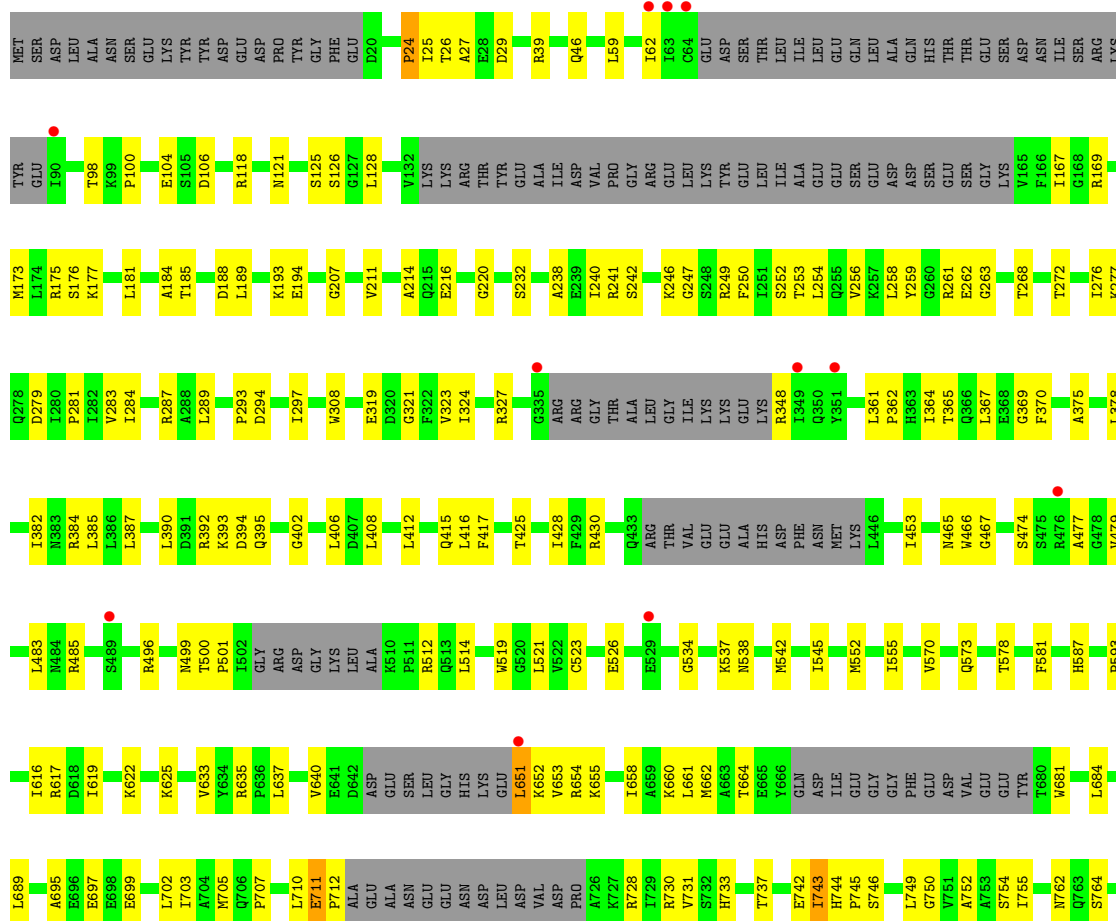
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

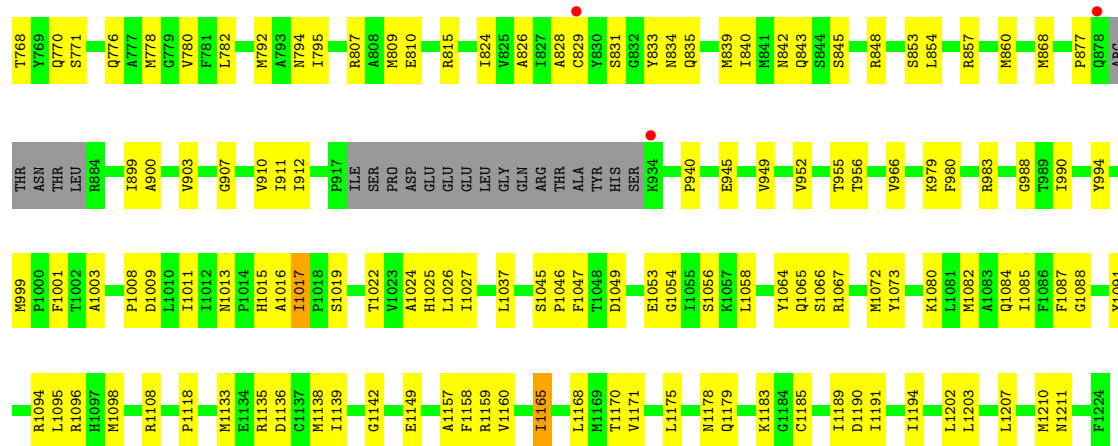
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



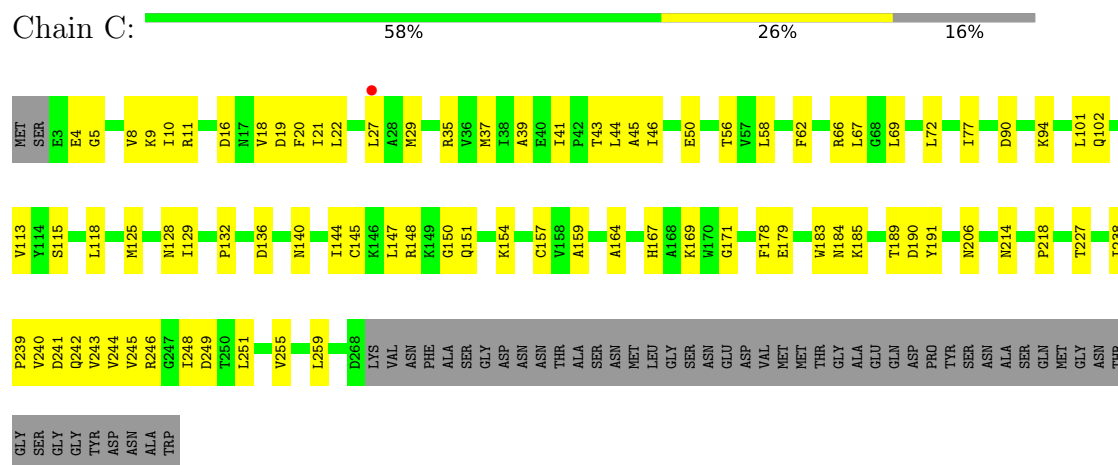


• Molecule 2: DNA-directed RNA polymerase subunit beta

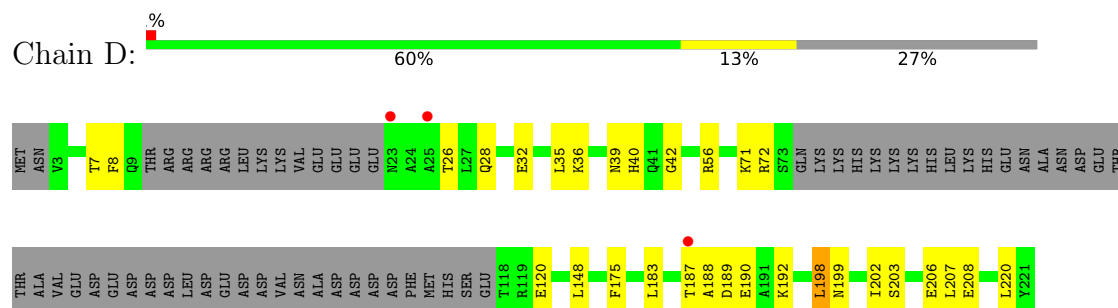




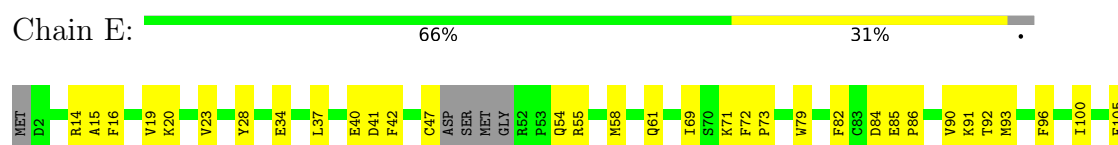
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



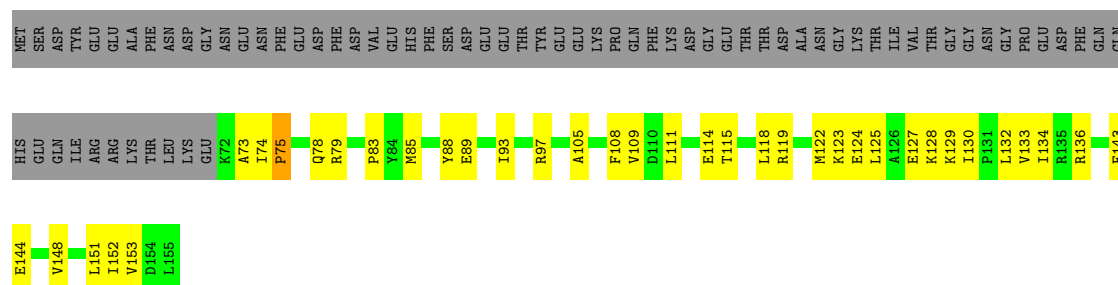
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1





- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 30% 23% 46%



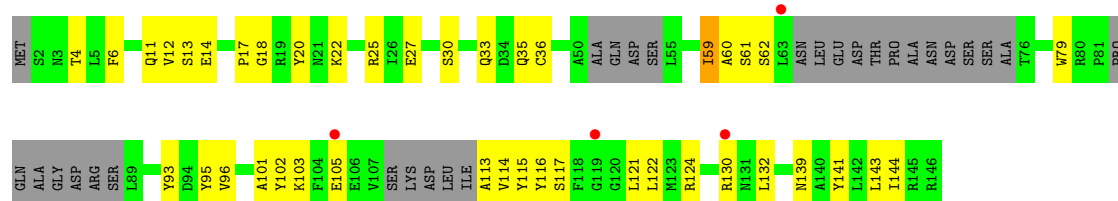
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G: 78% 20%



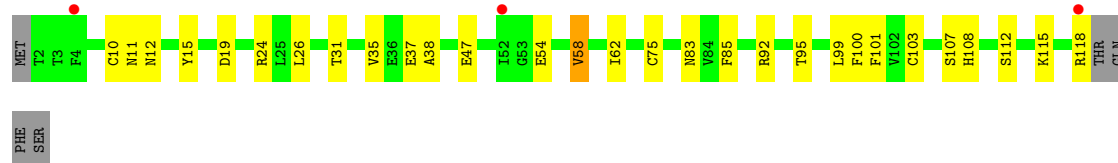
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 3% 51% 28% 20%



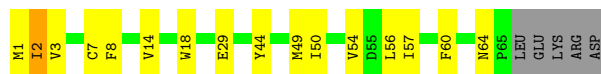
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 2% 72% 23%



- Molecule 10: DNA-directed RNA polymerases II subunit RPABC5

Chain J:  70% 21% 7%



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:  74% 22%



- Molecule 12: DNA-directed RNA polymerases II subunit RPABC4

Chain L:  31% 24% 6% 39%



- Molecule 13: RNA (5'-R(P*UP*CP*GP*AP*GP*AP*AP*GP*G)-3')

Chain R:  44% 44% 11%



- Molecule 14: DNA (5'-D(P*AP*CP*GP*TP*CP*CP*CP*TP*CP*TP*CP*GP*A)-3')

Chain T:  77% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	219.09Å 390.92Å 281.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.08 – 3.51 35.08 – 3.51	Depositor EDS
% Data completeness (in resolution range)	89.3 (35.08-3.51) 94.3 (35.08-3.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.219 , 0.246 0.228 , 0.253	Depositor DCC
R_{free} test set	5586 reflections (3.69%)	wwPDB-VP
Wilson B-factor (Å ²)	128.7	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 175.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.075 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.084 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30691	wwPDB-VP
Average B, all atoms (Å ²)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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: ZN

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	0.15	0/11165	0.43	0/15092
2	B	0.14	0/8604	0.39	0/11602
3	C	0.14	0/2133	0.37	0/2891
4	D	0.11	0/1296	0.32	0/1741
5	E	0.14	0/1747	0.39	0/2349
6	F	0.15	0/691	0.37	0/933
7	G	0.14	0/1366	0.37	0/1841
8	H	0.16	0/965	0.43	0/1302
9	I	0.14	0/973	0.46	1/1309 (0.1%)
10	J	0.11	0/541	0.38	0/727
11	K	0.11	0/938	0.35	0/1267
12	L	0.18	0/345	0.51	0/457
13	R	0.11	0/222	0.32	0/345
14	T	0.17	0/289	0.34	0/442
All	All	0.15	0/31275	0.40	1/42298 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	58	VAL	N-CA-C	-5.64	107.79	113.20

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	10974	0	11038	297	0
2	B	8438	0	8469	236	0
3	C	2095	0	2051	62	0
4	D	1287	0	1296	21	0
5	E	1713	0	1739	47	0
6	F	679	0	701	31	0
7	G	1338	0	1353	35	0
8	H	951	0	926	30	0
9	I	955	0	914	23	0
10	J	532	0	542	18	0
11	K	920	0	929	21	0
12	L	343	0	364	16	0
13	R	198	0	99	4	0
14	T	260	0	147	2	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
All	All	30691	0	30568	729	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 12.

All (729) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:ILE:HD13	2:B:1067:ARG:NH1	1.84	0.91
1:A:148:CYS:HB2	1:A:168:GLY:HA2	1.56	0.88
5:E:37:LEU:HD13	5:E:42:PHE:HB2	1.58	0.85
1:A:123:ARG:HD3	1:A:123:ARG:N	1.91	0.84
12:L:55:ILE:HG13	12:L:56:LEU:H	1.42	0.84
12:L:47:ARG:HG3	12:L:54:ARG:HG2	1.60	0.83
1:A:919:ILE:HD11	1:A:925:LEU:HD22	1.60	0.82
3:C:148:ARG:HG2	3:C:151:GLN:HG3	1.62	0.82
1:A:1096:SER:HB3	1:A:1100:ARG:HB2	1.60	0.82
1:A:1098:VAL:HG13	1:A:1099:PRO:HD3	1.62	0.82
1:A:119:ASN:H	1:A:123:ARG:HH21	1.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:HG3	1:A:448:PRO:HD2	1.62	0.81
1:A:443:LEU:HD11	2:B:1138:MET:HE3	1.62	0.81
5:E:37:LEU:CD1	5:E:42:PHE:HB2	2.11	0.81
1:A:968:GLN:HA	1:A:973:ILE:HD13	1.61	0.80
1:A:683:ILE:HG12	1:A:801:GLU:HG3	1.64	0.80
8:H:14:GLU:HB2	8:H:27:GLU:HB3	1.66	0.78
8:H:4:THR:HA	8:H:60:ALA:HB2	1.64	0.78
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.66	0.77
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.66	0.77
2:B:635:ARG:NH2	2:B:637:LEU:HD21	1.99	0.77
1:A:1063:MET:HE3	1:A:1436:ILE:HG23	1.67	0.77
2:B:367:LEU:HD12	2:B:369:GLY:H	1.51	0.76
2:B:1082:MET:HE3	3:C:190:ASP:HB2	1.68	0.76
1:A:41:MET:HA	1:A:49:LYS:HA	1.68	0.75
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.69	0.74
2:B:776:GLN:HG3	2:B:1096:ARG:HH11	1.52	0.74
12:L:30:ILE:HG22	12:L:31:CYS:H	1.53	0.73
1:A:1144:LYS:HD2	1:A:1269:GLU:HG2	1.70	0.73
1:A:40:THR:OG1	1:A:41:MET:N	2.19	0.73
1:A:1063:MET:HG2	2:B:1139:ILE:HG22	1.71	0.72
1:A:579:SER:HA	1:A:582:ILE:HD12	1.70	0.72
1:A:901:LEU:HA	1:A:907:THR:HG23	1.70	0.72
1:A:41:MET:HE1	1:A:257:ARG:HG3	1.71	0.72
11:K:81:TYR:HE1	11:K:86:ALA:HB2	1.54	0.72
2:B:635:ARG:HH21	2:B:637:LEU:HD21	1.53	0.72
4:D:40:HIS:HE1	7:G:73:LYS:HD2	1.53	0.72
2:B:323:VAL:HG12	2:B:324:ILE:HD12	1.72	0.71
2:B:1053:GLU:OE1	2:B:1067:ARG:NH2	2.23	0.71
1:A:116:ASP:O	1:A:123:ARG:NH1	2.23	0.71
7:G:116:PRO:HG2	7:G:119:LEU:HD23	1.73	0.70
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.72	0.70
1:A:1447:GLU:HA	1:A:1450:LEU:HD12	1.73	0.70
9:I:12:ASN:ND2	9:I:31:THR:OG1	2.25	0.70
5:E:55:ARG:NH2	5:E:137:GLU:OE1	2.21	0.70
3:C:66:ARG:NH2	10:J:3:VAL:O	2.25	0.69
12:L:57:LEU:HD23	12:L:58:LYS:H	1.56	0.69
2:B:387:LEU:HD22	2:B:393:LYS:HB2	1.73	0.69
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.74	0.69
3:C:102:GLN:HB3	3:C:154:LYS:HE3	1.74	0.69
2:B:581:PHE:HB2	2:B:625:LYS:HG2	1.75	0.69
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.76	0.68
3:C:37:MET:HA	3:C:41:ILE:HD11	1.75	0.67
1:A:1239:ARG:HH22	1:A:1241:ARG:NH2	1.93	0.67
1:A:98:LYS:HB3	1:A:234:MET:HE1	1.77	0.66
1:A:614:PHE:HB3	8:H:122:LEU:HD21	1.76	0.66
1:A:673:GLY:O	1:A:675:THR:N	2.29	0.66
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.78	0.66
3:C:56:THR:HG21	3:C:145:CYS:SG	2.36	0.66
1:A:114:LEU:HD21	1:A:171:GLN:HG3	1.78	0.66
1:A:670:ILE:HD13	2:B:1067:ARG:CZ	2.24	0.66
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.77	0.66
5:E:127:ILE:HD11	5:E:132:ILE:HD11	1.77	0.66
2:B:465:ASN:HA	2:B:477:ALA:HA	1.77	0.66
2:B:249:ARG:HD3	2:B:415:GLN:HG3	1.78	0.66
2:B:1022:THR:HG22	2:B:1025:HIS:HB2	1.76	0.66
9:I:92:ARG:HB2	9:I:95:THR:HG23	1.78	0.65
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.78	0.65
12:L:57:LEU:HD23	12:L:59:ALA:H	1.60	0.65
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.79	0.65
5:E:14:ARG:HH12	5:E:142:VAL:HG22	1.60	0.65
3:C:94:LYS:HE3	3:C:125:MET:HE1	1.78	0.65
2:B:1160:VAL:HG23	2:B:1194:ILE:HG13	1.79	0.65
1:A:806:ARG:HD3	2:B:728:ARG:HA	1.79	0.65
5:E:85:GLU:OE1	5:E:91:LYS:NZ	2.24	0.65
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.79	0.64
4:D:175:PHE:HE1	7:G:1:MET:HB3	1.62	0.64
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.79	0.64
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.79	0.64
1:A:683:ILE:HD11	1:A:799:PHE:CE2	2.33	0.64
1:A:43:GLU:HG3	1:A:44:THR:H	1.63	0.64
1:A:76:GLU:HB2	2:B:1159:ARG:HH22	1.63	0.64
2:B:128:LEU:HB3	2:B:167:ILE:HG23	1.78	0.64
2:B:46:GLN:HE22	2:B:496:ARG:HG2	1.61	0.64
2:B:319:GLU:HG2	9:I:15:TYR:HE1	1.61	0.64
2:B:526:GLU:HG3	2:B:771:SER:HB2	1.80	0.64
1:A:119:ASN:H	1:A:123:ARG:NH2	1.95	0.64
1:A:383:TYR:HB3	6:F:115:THR:HA	1.78	0.64
1:A:1098:VAL:CG1	1:A:1099:PRO:HD3	2.28	0.64
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.13	0.63
2:B:899:ILE:HD12	2:B:949:VAL:HG21	1.80	0.63
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:LEU:HD21	8:H:103:LYS:HB3	1.81	0.63
6:F:133:VAL:HG11	7:G:58:ARG:HH11	1.63	0.63
1:A:122:MET:HB3	1:A:123:ARG:NH1	2.13	0.62
3:C:46:ILE:HD12	3:C:46:ILE:H	1.64	0.62
2:B:184:ALA:HB1	2:B:188:ASP:HB2	1.80	0.62
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.81	0.62
1:A:1120:LEU:HD21	1:A:1131:ALA:HB2	1.81	0.62
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.81	0.62
2:B:1168:LEU:HD12	2:B:1170:THR:HG23	1.79	0.62
1:A:665:GLY:HA2	2:B:1026:LEU:HD22	1.81	0.62
2:B:193:LYS:HE2	10:J:64:ASN:HB3	1.81	0.62
8:H:6:PHE:HB3	8:H:59:ILE:HG13	1.82	0.62
2:B:1016:ALA:C	2:B:1017:ILE:HD12	2.25	0.62
1:A:1096:SER:CB	1:A:1100:ARG:HB2	2.30	0.62
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.81	0.62
1:A:91:PHE:HE2	1:A:180:LYS:HG3	1.65	0.62
1:A:377:PRO:HD3	1:A:493:GLN:NE2	2.15	0.61
1:A:683:ILE:HD11	1:A:799:PHE:HE2	1.64	0.61
2:B:900:ALA:HA	12:L:58:LYS:HD2	1.82	0.61
3:C:115:SER:HB3	3:C:132:PRO:HB2	1.82	0.61
7:G:125:SER:HB3	7:G:128:PRO:HA	1.81	0.61
1:A:174:ILE:O	1:A:175:ARG:NH1	2.26	0.61
7:G:1:MET:HE1	7:G:80:LYS:N	2.14	0.61
9:I:101:PHE:HE1	9:I:112:SER:HB2	1.64	0.61
1:A:69:THR:OG1	1:A:70:CYS:N	2.28	0.61
1:A:118:HIS:H	1:A:123:ARG:NH2	1.98	0.61
7:G:138:THR:HG22	7:G:139:ILE:H	1.66	0.61
1:A:329:LEU:HD22	2:B:1203:LEU:HD12	1.83	0.60
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.84	0.60
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.83	0.60
1:A:670:ILE:CD1	2:B:1067:ARG:NH1	2.60	0.60
8:H:30:SER:HB3	8:H:36:CYS:HB3	1.82	0.60
8:H:11:GLN:CD	8:H:12:VAL:H	2.10	0.60
1:A:174:ILE:HD11	1:A:181:LEU:HB3	1.83	0.59
1:A:1100:ARG:HA	1:A:1103:GLU:HB2	1.85	0.59
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.83	0.59
4:D:40:HIS:CE1	7:G:73:LYS:HD2	2.37	0.59
5:E:180:ARG:HG2	5:E:186:LEU:HD21	1.85	0.59
3:C:10:ILE:HG12	11:K:108:GLU:HB3	1.85	0.59
2:B:730:ARG:NH2	2:B:1049:ASP:OD1	2.34	0.59
7:G:1:MET:HE1	7:G:80:LYS:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:61:GLN:HB3	5:E:79:TRP:HE3	1.67	0.58
14:T:24:DT:H2"	14:T:25:DC:H5"	1.84	0.58
2:B:214:ALA:HB1	2:B:406:LEU:HD13	1.84	0.58
2:B:743:ILE:HG13	2:B:744:HIS:H	1.68	0.58
7:G:108:VAL:HG22	7:G:159:ALA:HB3	1.85	0.58
1:A:599:SER:O	8:H:25:ARG:NH2	2.37	0.58
1:A:711:ARG:NH1	9:I:92:ARG:O	2.37	0.58
1:A:14:VAL:HG21	1:A:1430:LEU:HD22	1.85	0.58
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.86	0.58
1:A:451:HIS:NE2	1:A:477:PRO:O	2.33	0.58
1:A:180:LYS:NZ	1:A:293:GLU:OE1	2.36	0.58
1:A:896:ARG:NH1	1:A:1034:GLU:OE2	2.37	0.58
2:B:485:ARG:NH1	2:B:782:LEU:HD11	2.19	0.58
2:B:824:ILE:HD11	10:J:44:TYR:HE2	1.69	0.58
2:B:1037:LEU:HD21	2:B:1064:TYR:HE2	1.67	0.58
2:B:652:LYS:HG3	2:B:689:LEU:HD23	1.86	0.57
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.84	0.57
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.86	0.57
1:A:1079:MET:O	1:A:1081:LEU:N	2.37	0.57
10:J:1:MET:N	10:J:54:VAL:O	2.37	0.57
1:A:54:ASN:C	1:A:56:PRO:HD3	2.29	0.57
1:A:563:PRO:HB3	1:A:572:TRP:CE2	2.40	0.57
1:A:1106:ASN:HB3	1:A:1385:THR:HG21	1.85	0.57
2:B:810:GLU:HA	2:B:815:ARG:HH22	1.70	0.57
1:A:868:TYR:HD2	1:A:1058:VAL:HG11	1.70	0.57
2:B:542:MET:HG3	2:B:743:ILE:HD12	1.85	0.57
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.70	0.57
2:B:824:ILE:HD11	10:J:44:TYR:CE2	2.40	0.57
2:B:542:MET:HG3	2:B:743:ILE:CD1	2.35	0.57
2:B:1171:VAL:HG11	2:B:1191:ILE:HG21	1.86	0.57
1:A:761:MET:HA	1:A:804:TYR:HB2	1.86	0.56
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.39	0.56
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.86	0.56
1:A:1140:HIS:H	1:A:1275:GLY:HA3	1.70	0.56
2:B:1084:GLN:HE22	3:C:191:TYR:HA	1.70	0.56
6:F:79:ARG:HD3	6:F:144:GLU:HG2	1.86	0.56
9:I:75:CYS:SG	9:I:108:HIS:NE2	2.77	0.56
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.87	0.56
9:I:103:CYS:SG	9:I:107:SER:N	2.79	0.56
1:A:284:ALA:N	1:A:285:PRO:HD3	2.20	0.56
2:B:1158:PHE:HD2	2:B:1160:VAL:HG13	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:100:PHE:HE2	9:I:118:ARG:HH21	1.54	0.56
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.87	0.56
4:D:40:HIS:CE1	7:G:73:LYS:HB3	2.40	0.56
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.37	0.56
2:B:651:LEU:HD23	2:B:652:LYS:H	1.70	0.56
2:B:730:ARG:HG3	2:B:731:VAL:N	2.21	0.56
5:E:180:ARG:O	5:E:186:LEU:HD23	2.06	0.56
1:A:837:ILE:HD11	1:A:1102:LYS:HG2	1.87	0.55
7:G:1:MET:HE2	7:G:2:PHE:H	1.72	0.55
1:A:119:ASN:N	1:A:123:ARG:HE	2.04	0.55
1:A:174:ILE:C	1:A:175:ARG:HH11	2.13	0.55
2:B:125:SER:HB3	2:B:169:ARG:HD2	1.87	0.55
1:A:711:ARG:NH2	9:I:95:THR:OG1	2.39	0.55
1:A:499:ALA:HB2	6:F:118:LEU:HD11	1.88	0.54
1:A:1443:VAL:HG12	6:F:132:LEU:HD22	1.88	0.54
2:B:408:LEU:HD21	2:B:545:ILE:HG12	1.88	0.54
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.73	0.54
3:C:35:ARG:HH11	11:K:41:THR:HB	1.71	0.54
5:E:47:CYS:O	5:E:54:GLN:NE2	2.41	0.54
6:F:85:MET:HE1	6:F:125:LEU:HD11	1.89	0.54
1:A:202:LEU:HD22	1:A:206:GLU:OE2	2.07	0.54
2:B:1158:PHE:CD2	2:B:1160:VAL:HG13	2.43	0.54
3:C:50:GLU:HG3	12:L:66:GLN:HB3	1.90	0.54
3:C:238:ILE:HD12	3:C:239:PRO:HD2	1.89	0.54
1:A:768:GLN:HG3	1:A:816:HIS:HA	1.89	0.54
1:A:818:MET:HG3	2:B:514:LEU:HD23	1.89	0.54
2:B:1171:VAL:HG21	2:B:1191:ILE:HG23	1.89	0.54
1:A:526:ASP:OD2	2:B:835:GLN:HG2	2.07	0.54
1:A:1146:VAL:HG12	1:A:1201:ALA:HB1	1.88	0.54
1:A:174:ILE:C	1:A:175:ARG:HD2	2.32	0.54
1:A:1376:THR:HG22	5:E:212:ARG:HH22	1.73	0.54
2:B:710:LEU:HD22	2:B:733:HIS:HB3	1.90	0.54
2:B:1133:MET:HG3	14:T:19:DC:H4'	1.88	0.53
1:A:123:ARG:N	1:A:123:ARG:CD	2.68	0.53
1:A:34:LYS:HB3	1:A:36:ARG:HH21	1.72	0.53
10:J:8:PHE:H	10:J:49:MET:HE3	1.74	0.53
1:A:116:ASP:OD2	1:A:164:ARG:HD2	2.08	0.53
2:B:730:ARG:HG3	2:B:731:VAL:H	1.72	0.53
3:C:8:VAL:HG22	3:C:22:LEU:HD12	1.90	0.53
3:C:46:ILE:HD12	3:C:72:LEU:HD11	1.90	0.53
8:H:96:VAL:HG22	8:H:143:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HG23	1:A:33:ALA:H	1.74	0.53
2:B:1142:GLY:HA3	6:F:88:TYR:HE1	1.73	0.53
1:A:335:ARG:NH1	1:A:339:ASN:OD1	2.42	0.53
1:A:666:ILE:HG23	2:B:1026:LEU:CB	2.39	0.53
3:C:27:LEU:H	3:C:27:LEU:HD23	1.73	0.53
2:B:552:MET:HA	2:B:555:ILE:HG22	1.90	0.53
2:B:653:VAL:HA	2:B:689:LEU:HD22	1.91	0.53
5:E:128:PRO:HA	5:E:130:ALA:H	1.73	0.52
7:G:1:MET:CE	7:G:2:PHE:H	2.22	0.52
10:J:1:MET:H2	10:J:56:LEU:H	1.57	0.52
2:B:384:ARG:HH12	2:B:393:LYS:HE2	1.73	0.52
3:C:10:ILE:HB	11:K:112:GLN:NE2	2.24	0.52
6:F:111:LEU:HD21	6:F:114:GLU:H	1.74	0.52
4:D:192:LYS:HA	4:D:198:LEU:HD12	1.90	0.52
1:A:62:ASP:OD1	1:A:63:ARG:N	2.43	0.52
1:A:902:LEU:HG	1:A:926:GLN:HG2	1.91	0.52
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.91	0.52
2:B:62:ILE:HD13	2:B:417:PHE:HD2	1.75	0.52
1:A:1120:LEU:HD13	1:A:1304:TRP:O	2.10	0.52
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.42	0.52
3:C:113:VAL:HG12	3:C:144:ILE:HD12	1.92	0.52
7:G:20:PRO:C	7:G:22:MET:H	2.18	0.52
1:A:563:PRO:HG2	1:A:566:ILE:HG13	1.92	0.52
2:B:412:LEU:HD21	2:B:479:VAL:HG11	1.91	0.52
2:B:635:ARG:HH22	2:B:742:GLU:CD	2.17	0.52
1:A:269:ILE:HD11	1:A:303:TYR:HB2	1.92	0.52
1:A:919:ILE:HG12	1:A:983:ILE:HD13	1.92	0.52
8:H:13:SER:HB2	8:H:27:GLU:O	2.10	0.52
10:J:14:VAL:HG22	10:J:50:ILE:HD11	1.92	0.52
1:A:1257:ASP:OD1	1:A:1257:ASP:N	2.36	0.52
2:B:294:ASP:OD1	9:I:12:ASN:HA	2.09	0.52
1:A:606:LEU:HG	1:A:613:ILE:HD13	1.92	0.52
2:B:903:VAL:O	2:B:949:VAL:HG23	2.10	0.52
1:A:1106:ASN:HB3	1:A:1385:THR:CG2	2.41	0.51
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.45	0.51
8:H:102:TYR:CZ	8:H:115:TYR:HB3	2.45	0.51
1:A:1192:LEU:HD22	1:A:1239:ARG:HH21	1.75	0.51
1:A:1325:THR:HA	5:E:147:HIS:HA	1.92	0.51
6:F:105:ALA:HA	7:G:16:SER:HA	1.92	0.51
9:I:12:ASN:HD22	9:I:31:THR:CB	2.22	0.51
1:A:472:LEU:O	1:A:475:THR:OG1	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:ARG:HG2	1:A:896:ARG:HH11	1.75	0.51
1:A:1202:MET:HE3	1:A:1207:LEU:HB2	1.93	0.51
2:B:980:PHE:CE2	2:B:990:ILE:HD11	2.45	0.51
2:B:994:TYR:HB2	2:B:999:MET:HE2	1.92	0.51
3:C:22:LEU:HD11	11:K:101:LEU:HD21	1.92	0.51
2:B:39:ARG:HD3	2:B:664:THR:HG21	1.91	0.51
2:B:1082:MET:HA	3:C:189:THR:HA	1.93	0.51
1:A:538:ASP:OD1	8:H:22:LYS:HB2	2.10	0.51
2:B:831:SER:HB2	2:B:833:TYR:HD2	1.76	0.51
1:A:330:LYS:HD2	1:A:331:GLY:H	1.74	0.51
2:B:651:LEU:HB3	2:B:654:ARG:HH22	1.75	0.51
5:E:90:VAL:HA	5:E:93:MET:HB3	1.93	0.51
2:B:216:GLU:HB3	2:B:500:THR:HG23	1.93	0.51
6:F:85:MET:HE2	6:F:153:VAL:HG22	1.93	0.51
1:A:179:LEU:HG	1:A:297:GLN:HG3	1.93	0.51
1:A:1342:GLU:HG3	5:E:198:ILE:HG12	1.92	0.51
1:A:1345:ARG:NH1	1:A:1373:ASP:OD1	2.44	0.51
6:F:124:GLU:HB3	6:F:130:ILE:HG12	1.93	0.51
12:L:68:GLU:CD	12:L:68:GLU:H	2.19	0.51
2:B:412:LEU:HD21	2:B:479:VAL:CG1	2.41	0.50
3:C:16:ASP:C	3:C:240:VAL:HG11	2.36	0.50
7:G:112:LYS:HA	7:G:115:MET:HE3	1.93	0.50
1:A:244:PRO:N	1:A:245:PRO:HD2	2.26	0.50
1:A:821:ARG:O	1:A:825:ILE:HD12	2.11	0.50
2:B:262:GLU:O	2:B:262:GLU:HG3	2.11	0.50
2:B:593:PRO:HG2	2:B:617:ARG:HH21	1.76	0.50
7:G:62:LEU:HB3	7:G:63:PRO:HD2	1.93	0.50
12:L:47:ARG:NH1	12:L:52:GLY:O	2.44	0.50
2:B:1065:GLN:CD	2:B:1067:ARG:H	2.18	0.50
3:C:46:ILE:HD13	3:C:67:LEU:O	2.12	0.50
6:F:133:VAL:HG11	7:G:58:ARG:NH1	2.26	0.50
1:A:75:ASN:O	1:A:76:GLU:HB3	2.11	0.50
2:B:640:VAL:HG13	2:B:651:LEU:N	2.27	0.50
1:A:738:LYS:HB3	1:A:740:LEU:HD12	1.94	0.50
2:B:824:ILE:HG23	2:B:1008:PRO:HA	1.93	0.50
3:C:244:VAL:O	3:C:248:ILE:HG13	2.10	0.50
1:A:956:LEU:HD11	1:A:1017:LEU:HG	1.94	0.50
1:A:1004:ASN:H	1:A:1004:ASN:ND2	2.09	0.50
2:B:365:THR:HG21	2:B:370:PHE:HB2	1.94	0.50
2:B:776:GLN:HE22	13:R:9:G:H5'	1.77	0.50
1:A:335:ARG:HD2	2:B:1202:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:MET:C	1:A:123:ARG:HD3	2.36	0.50
1:A:544:ASP:HB2	11:K:47:ARG:HH12	1.76	0.50
1:A:546:VAL:HG13	1:A:577:ILE:HD12	1.93	0.50
5:E:185:ALA:HA	5:E:190:LEU:HD13	1.93	0.50
1:A:1376:THR:O	1:A:1378:GLN:N	2.44	0.49
2:B:1142:GLY:HA3	6:F:88:TYR:CE1	2.47	0.49
3:C:62:PHE:HE2	10:J:1:MET:HE2	1.77	0.49
1:A:130:ASP:HB3	1:A:133:LYS:HE3	1.94	0.49
1:A:800:VAL:HG22	1:A:812:GLU:HB2	1.94	0.49
2:B:367:LEU:HD12	2:B:369:GLY:N	2.24	0.49
1:A:55:ASP:N	1:A:56:PRO:HD3	2.27	0.49
1:A:588:LEU:HD23	1:A:589:GLN:N	2.27	0.49
2:B:294:ASP:OD1	9:I:12:ASN:OD1	2.30	0.49
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.47	0.49
2:B:453:ILE:HD12	2:B:453:ILE:H	1.77	0.49
4:D:26:THR:C	4:D:28:GLN:H	2.20	0.49
5:E:190:LEU:HA	5:E:194:GLU:OE1	2.13	0.49
1:A:475:THR:HG23	1:A:480:ALA:O	2.13	0.49
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.13	0.49
3:C:136:ASP:HB3	3:C:140:ASN:H	1.78	0.49
1:A:1348:LEU:HD21	1:A:1375:MET:HE3	1.94	0.49
2:B:526:GLU:OE2	2:B:538:ASN:ND2	2.46	0.49
2:B:655:LYS:HA	2:B:658:ILE:HD12	1.93	0.49
1:A:173:THR:HG22	1:A:175:ARG:NE	2.28	0.48
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.48	0.48
1:A:713:SER:O	1:A:717:ASN:ND2	2.46	0.48
1:A:1164:PRO:HB2	1:A:1165:GLU:OE1	2.12	0.48
2:B:128:LEU:HB3	2:B:167:ILE:CG2	2.44	0.48
8:H:33:GLN:HB3	8:H:35:GLN:NE2	2.28	0.48
1:A:1104:ILE:HD13	1:A:1352:VAL:HG12	1.95	0.48
2:B:348:ARG:C	2:B:348:ARG:HD2	2.38	0.48
2:B:1087:PHE:HD1	2:B:1088:GLY:H	1.60	0.48
3:C:45:ALA:HA	3:C:72:LEU:HD13	1.95	0.48
5:E:19:VAL:HG22	5:E:140:LEU:HD22	1.95	0.48
3:C:58:LEU:HD23	3:C:58:LEU:H	1.77	0.48
1:A:770:VAL:HG12	1:A:771:GLU:HG2	1.95	0.48
3:C:4:GLU:OE2	11:K:104:ASN:ND2	2.30	0.48
4:D:183:LEU:HD23	7:G:144:ARG:HE	1.78	0.48
10:J:1:MET:N	10:J:56:LEU:H	2.12	0.48
1:A:912:LEU:HD22	1:A:1033:GLN:HA	1.95	0.48
1:A:1343:ALA:HB1	5:E:149:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.95	0.48
9:I:83:ASN:HB3	9:I:103:CYS:HA	1.95	0.48
1:A:842:VAL:HG13	1:A:1066:VAL:HG23	1.95	0.48
1:A:760:GLN:HG2	1:A:765:VAL:HA	1.95	0.48
2:B:519:TRP:HE1	2:B:635:ARG:HH12	1.62	0.48
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.95	0.48
3:C:62:PHE:CE2	10:J:1:MET:HE2	2.49	0.48
6:F:119:ARG:HA	6:F:122:MET:HE3	1.95	0.48
1:A:122:MET:O	1:A:126:LEU:HD12	2.14	0.48
1:A:532:ARG:HD3	1:A:749:ALA:HB2	1.96	0.48
1:A:537:ARG:HD3	8:H:121:LEU:HA	1.96	0.48
5:E:178:ILE:HG13	5:E:182:ASP:OD2	2.14	0.48
12:L:48:CYS:HB2	12:L:52:GLY:H	1.79	0.48
2:B:425:THR:HA	2:B:428:ILE:HD12	1.96	0.47
2:B:955:THR:OG1	2:B:956:THR:N	2.43	0.47
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.96	0.47
1:A:29:ALA:O	2:B:1183:LYS:HE3	2.13	0.47
1:A:854:ASN:HB2	1:A:1000:LEU:HD21	1.96	0.47
1:A:1096:SER:C	1:A:1099:PRO:HD2	2.39	0.47
2:B:289:LEU:HD13	2:B:375:ALA:HB2	1.94	0.47
2:B:1165:ILE:HD13	2:B:1185:CYS:HB2	1.96	0.47
3:C:101:LEU:HD13	3:C:118:LEU:HG	1.97	0.47
8:H:95:TYR:HD2	8:H:144:ILE:HD13	1.79	0.47
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.47	0.47
1:A:53:LEU:HD12	1:A:54:ASN:H	1.80	0.47
1:A:1170:ILE:HG13	1:A:1170:ILE:O	2.14	0.47
2:B:619:ILE:HD12	2:B:619:ILE:H	1.79	0.47
1:A:497:THR:HA	1:A:500:GLU:HB2	1.95	0.47
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.96	0.47
2:B:1084:GLN:NE2	3:C:191:TYR:HA	2.29	0.47
3:C:35:ARG:NH1	11:K:41:THR:HB	2.30	0.47
5:E:91:LYS:HD2	5:E:92:THR:N	2.29	0.47
3:C:248:ILE:HD13	11:K:101:LEU:HD12	1.96	0.47
8:H:11:GLN:OE1	8:H:12:VAL:N	2.47	0.47
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.95	0.47
1:A:367:PRO:HD2	1:A:370:ILE:HD12	1.97	0.47
1:A:825:ILE:O	1:A:829:VAL:HG22	2.15	0.47
1:A:880:LYS:HA	1:A:955:PRO:HA	1.97	0.47
1:A:984:LYS:O	1:A:988:LEU:HB2	2.15	0.47
4:D:192:LYS:HG2	4:D:198:LEU:HB2	1.95	0.47
5:E:19:VAL:O	5:E:23:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:114:GLU:HG3	6:F:119:ARG:CZ	2.45	0.47
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.45	0.47
13:R:4:G:H2'	13:R:5:A:H8	1.78	0.47
1:A:382:PRO:HG3	1:A:428:TYR:CZ	2.50	0.47
1:A:473:SER:C	1:A:475:THR:H	2.23	0.47
2:B:824:ILE:CG2	2:B:1009:ASP:H	2.28	0.47
1:A:1242:VAL:O	1:A:1243:VAL:HB	2.14	0.47
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.97	0.47
6:F:73:ALA:O	6:F:74:ILE:HB	2.14	0.47
11:K:47:ARG:HD3	11:K:61:TYR:HD1	1.79	0.47
2:B:408:LEU:HD23	2:B:545:ILE:HG21	1.96	0.47
2:B:842:ASN:HB3	2:B:845:SER:HB2	1.96	0.47
2:B:848:ARG:HD3	10:J:7:CYS:O	2.15	0.47
1:A:613:ILE:HG23	8:H:117:SER:HB2	1.96	0.46
1:A:868:TYR:CD2	1:A:1058:VAL:HG11	2.48	0.46
1:A:1189:SER:HB2	1:A:1243:VAL:H	1.80	0.46
2:B:26:THR:HG22	2:B:27:ALA:N	2.29	0.46
5:E:170:LEU:C	5:E:171:LYS:HD3	2.40	0.46
2:B:616:ILE:CG2	2:B:697:GLU:HA	2.46	0.46
2:B:780:VAL:HG22	2:B:795:ILE:HG23	1.97	0.46
2:B:1135:ARG:O	2:B:1139:ILE:HG13	2.16	0.46
9:I:10:CYS:HB3	9:I:12:ASN:HB2	1.97	0.46
9:I:58:VAL:HA	9:I:62:ILE:HD13	1.97	0.46
1:A:174:ILE:HD12	1:A:182:VAL:C	2.40	0.46
1:A:689:LYS:HE3	1:A:721:PHE:CE1	2.50	0.46
1:A:704:ALA:HB2	1:A:710:LEU:HG	1.97	0.46
1:A:1384:VAL:HA	1:A:1389:PHE:HD2	1.80	0.46
2:B:711:GLU:HB2	2:B:712:PRO:CD	2.46	0.46
1:A:662:PHE:HB3	2:B:829:CYS:SG	2.56	0.46
2:B:361:LEU:HB3	2:B:364:ILE:HD12	1.96	0.46
4:D:8:PHE:CE2	7:G:6:ASP:HB2	2.51	0.46
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.98	0.46
2:B:412:LEU:HG	2:B:466:TRP:CZ2	2.51	0.46
7:G:88:ASP:OD1	7:G:144:ARG:HG3	2.16	0.46
2:B:810:GLU:HA	2:B:815:ARG:NH2	2.30	0.46
6:F:109:VAL:HB	6:F:124:GLU:HG2	1.96	0.46
1:A:330:LYS:HD2	1:A:331:GLY:N	2.30	0.46
1:A:775:ILE:HG21	1:A:815:PHE:CD1	2.51	0.46
1:A:825:ILE:HG12	2:B:512:ARG:HB3	1.98	0.46
1:A:1141:THR:HB	1:A:1273:LEU:HB2	1.98	0.46
2:B:100:PRO:HG3	2:B:126:SER:OG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:SER:OG	2:B:252:SER:O	2.33	0.46
2:B:911:ILE:HD12	2:B:912:ILE:HG13	1.98	0.46
4:D:35:LEU:HD23	4:D:36:LYS:HG3	1.98	0.46
8:H:93:TYR:CG	8:H:143:LEU:HB3	2.49	0.46
1:A:216:VAL:HA	1:A:219:PHE:HE1	1.81	0.46
10:J:1:MET:O	10:J:2:ILE:HG22	2.15	0.46
1:A:863:VAL:HG23	5:E:170:LEU:HD21	1.98	0.46
2:B:828:ALA:HB2	2:B:1085:ILE:HG23	1.98	0.46
6:F:93:ILE:HG23	6:F:132:LEU:HD12	1.98	0.46
8:H:132:LEU:HD23	8:H:132:LEU:H	1.80	0.46
6:F:111:LEU:CD2	6:F:114:GLU:H	2.29	0.45
10:J:2:ILE:HD13	10:J:57:ILE:HD13	1.98	0.45
1:A:334:GLY:O	1:A:336:ILE:N	2.49	0.45
5:E:20:LYS:HE2	5:E:34:GLU:HG2	1.97	0.45
3:C:183:TRP:O	3:C:185:LYS:N	2.49	0.45
5:E:180:ARG:HG2	5:E:186:LEU:CD2	2.45	0.45
1:A:90:VAL:HG13	1:A:297:GLN:OE1	2.17	0.45
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.98	0.45
3:C:238:ILE:HG23	3:C:243:VAL:HG22	1.99	0.45
5:E:16:PHE:CD1	5:E:58:MET:HE3	2.51	0.45
7:G:26:LEU:HD13	7:G:56:ILE:HD11	1.97	0.45
7:G:44:TYR:HE2	7:G:106:MET:HB2	1.81	0.45
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.97	0.45
2:B:185:THR:HG22	2:B:188:ASP:OD1	2.17	0.45
2:B:824:ILE:HG22	2:B:1009:ASP:H	1.82	0.45
2:B:1024:ALA:HA	2:B:1027:ILE:HD12	1.98	0.45
2:B:1168:LEU:CD1	2:B:1170:THR:HG23	2.46	0.45
1:A:542:GLU:O	1:A:546:VAL:HG23	2.17	0.45
1:A:1091:SER:HB2	1:A:1094:VAL:HB	1.99	0.45
1:A:1360:GLY:O	1:A:1362:TYR:N	2.50	0.45
2:B:173:MET:HG3	2:B:176:SER:HB3	1.99	0.45
3:C:46:ILE:CD1	3:C:72:LEU:HD11	2.47	0.45
3:C:164:ALA:HB2	3:C:171:GLY:HA2	1.98	0.45
1:A:444:PHE:HE1	1:A:470:LEU:HD13	1.81	0.45
1:A:472:LEU:HD11	2:B:835:GLN:HE22	1.80	0.45
2:B:287:ARG:O	2:B:327:ARG:HG3	2.17	0.45
2:B:705:MET:HE3	2:B:742:GLU:HG2	1.98	0.45
1:A:304:MET:HE2	2:B:1210:MET:HA	1.99	0.45
2:B:232:SER:O	2:B:261:ARG:NH1	2.49	0.45
2:B:24:PRO:O	2:B:25:ILE:HG13	2.17	0.45
2:B:294:ASP:OD1	2:B:294:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:860:MET:HE3	2:B:860:MET:HB3	1.90	0.45
3:C:11:ARG:HB3	3:C:19:ASP:HB3	1.99	0.45
1:A:92:HIS:HB3	1:A:95:PHE:HB2	1.98	0.45
1:A:845:LEU:HA	1:A:848:ILE:HD13	1.98	0.45
2:B:387:LEU:HD22	2:B:393:LYS:CB	2.44	0.45
2:B:752:ALA:O	2:B:755:ILE:HG13	2.17	0.45
3:C:164:ALA:HA	3:C:167:HIS:O	2.17	0.45
5:E:71:LYS:O	5:E:73:PRO:HD3	2.17	0.45
11:K:21:ILE:HD12	11:K:21:ILE:O	2.17	0.44
1:A:67:CYS:HB3	1:A:70:CYS:O	2.17	0.44
1:A:70:CYS:O	1:A:72:GLU:N	2.50	0.44
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.52	0.44
1:A:1450:LEU:HD23	6:F:108:PHE:CZ	2.52	0.44
2:B:240:ILE:O	2:B:253:THR:OG1	2.30	0.44
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.98	0.44
2:B:1003:ALA:HA	3:C:178:PHE:O	2.17	0.44
3:C:77:ILE:HD12	3:C:129:ILE:HD11	1.98	0.44
1:A:93:VAL:HG11	1:A:305:ASP:HB3	1.99	0.44
1:A:353:ILE:HG22	1:A:468:PHE:HB2	2.00	0.44
1:A:443:LEU:HD22	1:A:455:MET:HE2	1.98	0.44
5:E:176:PRO:O	5:E:212:ARG:HA	2.16	0.44
10:J:7:CYS:HA	10:J:49:MET:HE3	2.00	0.44
1:A:493:GLN:HB2	2:B:1149:GLU:OE2	2.17	0.44
2:B:776:GLN:NE2	13:R:9:G:H5'	2.33	0.44
11:K:47:ARG:NH1	11:K:51:LEU:HD11	2.32	0.44
1:A:89:PRO:HD2	1:A:205:GLU:HG3	1.99	0.44
1:A:598:LEU:HB2	8:H:115:TYR:HE2	1.81	0.44
1:A:994:GLN:HA	1:A:997:LEU:HD12	2.00	0.44
2:B:705:MET:O	2:B:742:GLU:HB3	2.17	0.44
4:D:187:THR:HG22	4:D:189:ASP:H	1.83	0.44
1:A:600:PRO:HA	8:H:25:ARG:CZ	2.48	0.44
2:B:770:GLN:HG3	2:B:983:ARG:C	2.43	0.44
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.99	0.44
8:H:61:SER:HA	8:H:141:TYR:CD1	2.53	0.44
2:B:899:ILE:HD12	2:B:949:VAL:CG2	2.46	0.44
3:C:179:GLU:HG2	3:C:206:ASN:HD22	1.82	0.44
5:E:100:ILE:CG2	5:E:105:PHE:HB2	2.47	0.44
8:H:101:ALA:HB2	8:H:116:TYR:CE1	2.52	0.44
9:I:85:PHE:HD2	9:I:99:LEU:HD22	1.82	0.44
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.99	0.44
1:A:1282:VAL:CG1	1:A:1306:LEU:HD12	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:THR:HG22	2:B:27:ALA:H	1.83	0.44
2:B:428:ILE:C	2:B:430:ARG:H	2.26	0.44
1:A:242:PRO:HB2	1:A:246:VAL:HG21	2.00	0.44
2:B:181:LEU:HD11	2:B:194:GLU:HG2	1.99	0.44
2:B:555:ILE:HD11	2:B:587:HIS:CE1	2.52	0.44
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.00	0.43
1:A:333:GLU:N	1:A:333:GLU:OE1	2.51	0.43
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.99	0.43
5:E:96:PHE:CZ	5:E:100:ILE:HD11	2.53	0.43
1:A:767:GLN:HB2	1:A:799:PHE:HD1	1.83	0.43
2:B:293:PRO:HB3	9:I:11:ASN:HB3	2.00	0.43
6:F:123:LYS:NZ	6:F:127:GLU:OE2	2.51	0.43
8:H:105:GLU:HB2	8:H:113:ALA:HB3	2.00	0.43
13:R:4:G:H2'	13:R:5:A:C8	2.53	0.43
1:A:566:ILE:O	8:H:96:VAL:HB	2.16	0.43
1:A:785:PRO:HB2	2:B:703:ILE:HD12	2.00	0.43
1:A:833:GLU:OE1	1:A:1102:LYS:HE3	2.18	0.43
1:A:1004:ASN:OD1	1:A:1006:ILE:HB	2.19	0.43
1:A:1269:GLU:OE1	2:B:263:GLY:HA3	2.19	0.43
2:B:387:LEU:HD23	2:B:392:ARG:HB2	2.00	0.43
2:B:910:VAL:HA	2:B:940:PRO:HA	2.00	0.43
3:C:4:GLU:OE2	3:C:4:GLU:N	2.51	0.43
11:K:7:PHE:C	11:K:9:LEU:H	2.26	0.43
1:A:125:ALA:HA	1:A:128:ILE:HD12	2.00	0.43
1:A:302:THR:HA	1:A:305:ASP:O	2.18	0.43
1:A:305:ASP:O	1:A:308:ILE:HD11	2.18	0.43
1:A:598:LEU:HD13	8:H:124:ARG:HB2	2.00	0.43
1:A:423:ASP:CG	1:A:424:ILE:H	2.26	0.43
1:A:589:GLN:HG3	1:A:606:LEU:HD13	1.99	0.43
1:A:963:ILE:HG22	1:A:1045:VAL:HG22	2.00	0.43
1:A:1106:ASN:O	1:A:1108:ALA:N	2.52	0.43
2:B:185:THR:O	2:B:189:LEU:HD12	2.18	0.43
2:B:272:THR:OG1	2:B:279:ASP:OD2	2.37	0.43
2:B:702:LEU:HD22	2:B:737:THR:HG23	2.00	0.43
7:G:1:MET:HE3	7:G:1:MET:HB2	1.88	0.43
1:A:76:GLU:OE1	2:B:1175:LEU:HD21	2.18	0.43
1:A:1191:TRP:HB3	1:A:1260:LEU:HD13	2.00	0.43
1:A:1291:VAL:HG12	1:A:1301:GLU:HG2	2.01	0.43
1:A:1327:ILE:O	5:E:147:HIS:NE2	2.46	0.43
1:A:1442:ASP:OD1	7:G:60:ARG:HD2	2.19	0.43
2:B:390:LEU:HD13	2:B:392:ARG:HH21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:745:PRO:HB2	2:B:1047:PHE:CD2	2.53	0.43
5:E:198:ILE:HD13	5:E:212:ARG:HG3	1.99	0.43
1:A:873:MET:HG2	1:A:957:PRO:HG3	2.01	0.43
1:A:1079:MET:C	1:A:1081:LEU:N	2.77	0.43
1:A:1282:VAL:HG12	1:A:1306:LEU:HD12	2.01	0.43
4:D:202:ILE:HG21	4:D:207:LEU:HD13	2.01	0.43
5:E:55:ARG:HB3	5:E:84:ASP:OD2	2.18	0.43
8:H:18:GLY:C	8:H:20:TYR:H	2.26	0.43
9:I:83:ASN:CB	9:I:103:CYS:HA	2.49	0.43
1:A:451:HIS:HD2	1:A:454:SER:N	2.17	0.43
1:A:477:PRO:CG	1:A:521:MET:HG2	2.49	0.43
1:A:636:GLU:OE1	1:A:962:ARG:HD2	2.19	0.43
1:A:1079:MET:C	1:A:1081:LEU:H	2.27	0.43
2:B:496:ARG:O	2:B:538:ASN:OD1	2.35	0.43
2:B:794:ASN:C	2:B:795:ILE:HD12	2.43	0.43
2:B:828:ALA:HB2	2:B:1085:ILE:CG2	2.49	0.43
4:D:7:THR:HG21	4:D:32:GLU:OE2	2.18	0.43
2:B:25:ILE:HG23	2:B:29:ASP:HB2	2.00	0.43
2:B:853:SER:OG	2:B:854:LEU:N	2.52	0.43
9:I:115:LYS:HB3	9:I:115:LYS:HE2	1.79	0.43
11:K:32:VAL:HG22	11:K:74:ARG:HG3	1.99	0.43
3:C:46:ILE:HA	3:C:159:ALA:HA	2.01	0.42
1:A:121:LEU:HD23	1:A:121:LEU:HA	1.81	0.42
1:A:1116:LEU:HD11	1:A:1312:ASN:H	1.83	0.42
2:B:809:MET:C	2:B:815:ARG:HH12	2.26	0.42
2:B:1094:ARG:NH1	2:B:1098:MET:SD	2.92	0.42
7:G:98:GLY:HA3	7:G:110:VAL:O	2.19	0.42
1:A:332:LYS:HB3	1:A:333:GLU:OE1	2.19	0.42
1:A:1163:ILE:HD11	1:A:1239:ARG:NH2	2.35	0.42
1:A:1167:GLU:HA	1:A:1170:ILE:HG12	2.01	0.42
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.99	0.42
2:B:277:LYS:H	2:B:277:LYS:HG2	1.53	0.42
2:B:402:GLY:HA2	2:B:695:ALA:HB3	2.01	0.42
2:B:1072:MET:HG3	2:B:1085:ILE:HG12	2.01	0.42
4:D:183:LEU:HD23	7:G:144:ARG:NE	2.33	0.42
1:A:51:GLY:HA2	1:A:56:PRO:HB3	2.00	0.42
1:A:118:HIS:H	1:A:123:ARG:HH21	1.65	0.42
1:A:436:ILE:HG21	1:A:491:VAL:HG21	2.01	0.42
1:A:528:LEU:HD23	1:A:751:SER:HA	2.01	0.42
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.19	0.42
2:B:378:LEU:O	2:B:382:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:762:ASN:HD21	2:B:1022:THR:HG23	1.85	0.42
2:B:780:VAL:HG21	10:J:56:LEU:HD22	2.01	0.42
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.83	0.42
3:C:43:THR:HG22	3:C:44:LEU:H	1.85	0.42
3:C:46:ILE:HG23	3:C:157:CYS:HB3	2.01	0.42
5:E:15:ALA:O	5:E:19:VAL:HG23	2.19	0.42
8:H:114:VAL:HG13	8:H:130:ARG:NH2	2.34	0.42
1:A:1261:LYS:O	1:A:1261:LYS:HD3	2.20	0.42
2:B:952:VAL:HG22	2:B:966:VAL:HG22	2.02	0.42
9:I:54:GLU:OE1	9:I:118:ARG:NH2	2.50	0.42
1:A:116:ASP:CG	1:A:117:GLU:H	2.28	0.42
1:A:767:GLN:HA	1:A:799:PHE:HA	2.01	0.42
2:B:254:LEU:HD13	2:B:361:LEU:HD12	2.02	0.42
2:B:578:THR:HG23	2:B:622:LYS:C	2.45	0.42
2:B:776:GLN:HG3	2:B:1096:ARG:NH1	2.28	0.42
6:F:83:PRO:HB2	6:F:152:ILE:HD13	2.00	0.42
7:G:44:TYR:CE2	7:G:106:MET:HB2	2.55	0.42
9:I:19:ASP:HB2	9:I:24:ARG:HG2	2.01	0.42
9:I:26:LEU:HD13	9:I:35:VAL:CG1	2.49	0.42
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.55	0.42
1:A:780:VAL:HG22	2:B:699:GLU:OE1	2.19	0.42
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	2.01	0.42
2:B:394:ASP:OD1	2:B:395:GLN:N	2.53	0.42
6:F:128:LYS:NZ	6:F:151:LEU:O	2.53	0.42
7:G:18:PHE:HA	7:G:22:MET:SD	2.60	0.42
1:A:472:LEU:HD11	2:B:835:GLN:CD	2.45	0.42
1:A:1092:LYS:HA	1:A:1113:THR:HG21	2.02	0.42
2:B:384:ARG:NH1	2:B:393:LYS:HE2	2.35	0.42
2:B:570:VAL:HG23	2:B:573:GLN:HB2	2.01	0.42
2:B:1189:ILE:HD12	2:B:1190:ASP:N	2.35	0.42
4:D:71:LYS:HD2	4:D:72:ARG:HG3	2.01	0.42
1:A:173:THR:HG22	1:A:175:ARG:CZ	2.50	0.42
1:A:185:TRP:HZ3	1:A:200:ARG:HB3	1.85	0.42
1:A:303:TYR:CZ	1:A:325:ILE:HD11	2.55	0.42
1:A:674:PRO:HG3	1:A:677:ARG:HE	1.84	0.42
5:E:178:ILE:O	5:E:214:CYS:HA	2.20	0.42
1:A:674:PRO:HA	1:A:677:ARG:HB2	2.02	0.42
1:A:1066:VAL:O	1:A:1070:GLN:HG3	2.19	0.42
2:B:125:SER:HB3	2:B:169:ARG:HB3	2.00	0.42
2:B:416:LEU:HD12	2:B:466:TRP:CZ2	2.55	0.42
2:B:534:GLY:O	2:B:537:LYS:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1054:GLY:O	2:B:1058:LEU:HD12	2.20	0.42
4:D:188:ALA:HB2	4:D:208:GLU:HG3	2.01	0.42
5:E:40:GLU:HG2	5:E:41:ASP:N	2.35	0.42
5:E:69:ILE:HA	5:E:72:PHE:O	2.20	0.42
12:L:62:LYS:O	12:L:64:LEU:HD12	2.20	0.42
1:A:140:THR:HA	1:A:143:LYS:HE2	2.02	0.41
1:A:216:VAL:HA	1:A:219:PHE:CE1	2.55	0.41
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.19	0.41
7:G:142:ARG:HB2	7:G:171:ILE:HG21	2.02	0.41
1:A:344:ARG:O	2:B:1118:PRO:HD2	2.20	0.41
1:A:1434:ALA:HB1	1:A:1436:ILE:HD13	2.01	0.41
3:C:238:ILE:CD1	3:C:246:ARG:HH22	2.33	0.41
2:B:308:TRP:H	2:B:308:TRP:CD1	2.38	0.41
2:B:843:GLN:N	2:B:994:TYR:O	2.52	0.41
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.85	0.41
3:C:9:LYS:NZ	3:C:21:ILE:HD13	2.35	0.41
1:A:70:CYS:SG	1:A:80:HIS:CE1	3.14	0.41
1:A:1064:VAL:HA	1:A:1067:LEU:HB3	2.02	0.41
1:A:1359:ASP:O	1:A:1361:SER:N	2.54	0.41
2:B:220:GLY:HA2	2:B:241:ARG:HB2	2.01	0.41
2:B:283:VAL:HG21	2:B:321:GLY:HA3	2.02	0.41
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.85	0.41
1:A:42:ASP:OD1	1:A:45:GLN:HG2	2.19	0.41
1:A:567:LYS:HB2	1:A:568:PRO:HD3	2.02	0.41
1:A:752:LYS:HG2	2:B:1015:HIS:O	2.21	0.41
1:A:1097:GLY:H	1:A:1100:ARG:HB2	1.85	0.41
1:A:1189:SER:O	1:A:1241:ARG:HD3	2.19	0.41
1:A:1333:ILE:H	1:A:1333:ILE:HG13	1.73	0.41
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.54	0.41
2:B:175:ARG:HH12	2:B:189:LEU:HD21	1.84	0.41
2:B:807:ARG:H	2:B:1045:SER:HG	1.65	0.41
3:C:242:GLN:HA	3:C:245:VAL:HB	2.01	0.41
3:C:246:ARG:HA	3:C:249:ASP:HB3	2.01	0.41
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.93	0.41
2:B:294:ASP:HA	2:B:297:ILE:HB	2.02	0.41
3:C:238:ILE:HD11	3:C:246:ARG:HH22	1.86	0.41
5:E:143:ASN:OD1	5:E:145:THR:OG1	2.38	0.41
1:A:118:HIS:H	1:A:123:ARG:CZ	2.32	0.41
1:A:738:LYS:H	1:A:738:LYS:HD2	1.85	0.41
1:A:1444:MET:SD	7:G:60:ARG:HA	2.60	0.41
1:A:1453:TYR:CD1	6:F:129:LYS:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:PRO:HB2	2:B:25:ILE:H	1.71	0.41
2:B:523:CYS:HB2	2:B:750:GLY:HA3	2.03	0.41
11:K:53:ASP:HB3	11:K:56:VAL:HB	2.03	0.41
1:A:56:PRO:O	1:A:57:ARG:HB2	2.21	0.41
1:A:896:ARG:NH1	1:A:1030:ARG:HG2	2.35	0.41
2:B:276:ILE:HD12	2:B:276:ILE:HA	1.92	0.41
2:B:746:SER:H	2:B:746:SER:HG	1.61	0.41
1:A:878:ILE:HG22	1:A:955:PRO:HB2	2.03	0.41
1:A:1100:ARG:HH21	1:A:1351:GLU:CD	2.29	0.41
1:A:1341:ILE:HD13	1:A:1380:GLY:HA2	2.02	0.41
2:B:361:LEU:N	2:B:362:PRO:HD3	2.36	0.41
2:B:499:ASN:O	2:B:501:PRO:HD3	2.21	0.41
2:B:778:MET:HG3	2:B:1094:ARG:HB3	2.02	0.41
5:E:82:PHE:HD1	5:E:111:VAL:HB	1.86	0.41
5:E:147:HIS:HB3	5:E:150:VAL:HG23	2.03	0.41
6:F:97:ARG:HH12	6:F:108:PHE:HE2	1.69	0.41
6:F:128:LYS:HE3	6:F:148:VAL:O	2.21	0.41
7:G:138:THR:HG22	7:G:139:ILE:N	2.33	0.41
11:K:31:VAL:O	11:K:74:ARG:HA	2.21	0.41
12:L:57:LEU:CD2	12:L:58:LYS:H	2.28	0.41
1:A:6:TYR:O	2:B:1175:LEU:HD13	2.20	0.41
1:A:105:CYS:SG	1:A:139:TRP:HA	2.61	0.41
1:A:678:GLU:HA	1:A:681:GLU:CD	2.46	0.41
1:A:752:LYS:HE3	2:B:1019:SER:OG	2.21	0.41
1:A:1109:LYS:HD2	1:A:1333:ILE:HG21	2.03	0.41
2:B:658:ILE:O	2:B:662:MET:HG3	2.20	0.41
2:B:749:LEU:HD13	2:B:754:SER:HA	2.03	0.41
2:B:764:SER:O	2:B:768:THR:HG23	2.21	0.41
2:B:826:ALA:O	2:B:1011:ILE:HA	2.21	0.41
2:B:854:LEU:HD23	2:B:854:LEU:HA	1.96	0.41
3:C:69:LEU:HD23	3:C:169:LYS:HB3	2.02	0.41
8:H:139:ASN:OD1	8:H:139:ASN:N	2.53	0.41
1:A:230:ARG:HB3	1:A:232:GLU:OE1	2.21	0.40
1:A:737:LEU:HD22	1:A:741:ASN:ND2	2.36	0.40
2:B:104:GLU:HG3	12:L:54:ARG:NH2	2.35	0.40
2:B:1178:ASN:O	2:B:1179:GLN:HG2	2.21	0.40
3:C:169:LYS:HZ2	12:L:69:ALA:HB3	1.86	0.40
1:A:563:PRO:HD2	8:H:79:TRP:CD1	2.55	0.40
1:A:925:LEU:HD23	1:A:983:ILE:HB	2.04	0.40
3:C:241:ASP:HB3	11:K:109:TRP:CZ2	2.56	0.40
3:C:251:LEU:O	3:C:255:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:39:ASN:OD1	4:D:40:HIS:N	2.54	0.40
1:A:32:VAL:HG21	1:A:57:ARG:O	2.21	0.40
1:A:645:LEU:HD11	1:A:649:ILE:HD11	2.02	0.40
1:A:744:LYS:O	1:A:748:MET:HG2	2.20	0.40
1:A:1291:VAL:CG2	1:A:1292:PRO:HD2	2.48	0.40
1:A:1444:MET:HG3	7:G:59:GLY:O	2.22	0.40
2:B:98:THR:O	2:B:126:SER:HB3	2.22	0.40
4:D:40:HIS:HE1	7:G:73:LYS:CD	2.28	0.40
4:D:190:GLU:HA	7:G:167:TYR:CE2	2.56	0.40
5:E:23:VAL:HG12	5:E:28:TYR:HB2	2.03	0.40
12:L:55:ILE:HG13	12:L:56:LEU:N	2.21	0.40
1:A:499:ALA:HB2	6:F:118:LEU:CD1	2.52	0.40
2:B:839:MET:HE3	2:B:988:GLY:HA3	2.03	0.40
3:C:29:MET:HE2	3:C:29:MET:HB2	1.94	0.40
5:E:151:PRO:HD2	5:E:153:HIS:HE1	1.86	0.40
5:E:157:SER:H	5:E:160:GLU:HB2	1.87	0.40
6:F:136:ARG:O	6:F:143:PHE:HA	2.21	0.40
1:A:673:GLY:O	1:A:674:PRO:C	2.64	0.40
1:A:1120:LEU:HD13	1:A:1304:TRP:C	2.47	0.40
2:B:59:LEU:HD12	2:B:59:LEU:HA	1.91	0.40
9:I:37:GLU:HG3	9:I:38:ALA:N	2.36	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	1378/1733 (80%)	1202 (87%)	135 (10%)	41 (3%)	3	25
2	B	1040/1224 (85%)	920 (88%)	101 (10%)	19 (2%)	6	34
3	C	264/318 (83%)	237 (90%)	19 (7%)	8 (3%)	3	25
4	D	156/221 (71%)	137 (88%)	14 (9%)	5 (3%)	3	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	202/215 (94%)	183 (91%)	17 (8%)	2 (1%)	12	45
6	F	82/155 (53%)	76 (93%)	5 (6%)	1 (1%)	10	42
7	G	169/171 (99%)	151 (89%)	13 (8%)	5 (3%)	3	25
8	H	107/146 (73%)	87 (81%)	17 (16%)	3 (3%)	4	25
9	I	115/122 (94%)	100 (87%)	14 (12%)	1 (1%)	14	48
10	J	63/70 (90%)	56 (89%)	5 (8%)	2 (3%)	3	24
11	K	113/120 (94%)	106 (94%)	5 (4%)	2 (2%)	6	34
12	L	41/70 (59%)	22 (54%)	12 (29%)	7 (17%)	0	2
All	All	3730/4565 (82%)	3277 (88%)	357 (10%)	96 (3%)	4	27

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	MET
1	A	309	ALA
1	A	424	ILE
1	A	567	LYS
1	A	674	PRO
1	A	1361	SER
1	A	1377	THR
2	B	24	PRO
2	B	711	GLU
5	E	123	LEU
7	G	20	PRO
8	H	17	PRO
10	J	2	ILE
1	A	52	GLY
1	A	57	ARG
1	A	76	GLU
1	A	317	LYS
1	A	1078	GLN
1	A	1080	THR
1	A	1107	VAL
2	B	246	LYS
2	B	250	PHE
2	B	467	GLY
2	B	707	PRO
2	B	877	PRO
2	B	907	GLY

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Mol	Chain	Res	Type
3	C	184	ASN
3	C	218	PRO
4	D	220	LEU
7	G	63	PRO
7	G	154	VAL
9	I	47	GLU
12	L	63	ARG
1	A	335	ARG
1	A	958	VAL
1	A	1079	MET
1	A	1108	ALA
1	A	1140	HIS
1	A	1164	PRO
1	A	1171	GLN
1	A	1188	GLN
1	A	1378	GLN
1	A	1437	GLY
2	B	247	GLY
2	B	1046	PRO
2	B	1157	ALA
3	C	214	ASN
7	G	2	PHE
11	K	111	LEU
12	L	56	LEU
1	A	151	ASP
1	A	152	VAL
1	A	334	GLY
1	A	569	LYS
1	A	1084	PHE
1	A	1281	ARG
2	B	106	ASP
2	B	177	LYS
2	B	474	SER
2	B	792	MET
2	B	1017	ILE
3	C	90	ASP
3	C	227	THR
4	D	120	GLU
5	E	172	GLU
10	J	29	GLU
12	L	45	ALA
12	L	59	ALA

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Mol	Chain	Res	Type
12	L	64	LEU
1	A	54	ASN
1	A	55	ASP
1	A	223	GLY
1	A	311	GLN
1	A	1086	PHE
1	A	1362	TYR
2	B	868	MET
2	B	1165	ILE
3	C	128	ASN
6	F	75	PRO
12	L	39	SER
12	L	55	ILE
1	A	1206	ASP
4	D	198	LEU
4	D	199	ASN
8	H	62	SER
1	A	474	VAL
7	G	19	GLY
11	K	4	PRO
1	A	1360	GLY
8	H	59	ILE
1	A	600	PRO
3	C	150	GLY
4	D	42	GLY
2	B	743	ILE
1	A	310	GLY
3	C	5	GLY

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	1214/1520 (80%)	1213 (100%)	1 (0%)	88	87
2	B	919/1061 (87%)	917 (100%)	2 (0%)	87	85
3	C	234/274 (85%)	234 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	144/200 (72%)	144 (100%)	0	100	100
5	E	192/197 (98%)	192 (100%)	0	100	100
6	F	74/137 (54%)	74 (100%)	0	100	100
7	G	151/152 (99%)	151 (100%)	0	100	100
8	H	104/128 (81%)	104 (100%)	0	100	100
9	I	111/116 (96%)	111 (100%)	0	100	100
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	99/102 (97%)	99 (100%)	0	100	100
12	L	38/57 (67%)	37 (97%)	1 (3%)	40	63
All	All	3340/4009 (83%)	3336 (100%)	4 (0%)	88	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1094	VAL
2	B	651	LEU
2	B	660	LYS
12	L	51	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	GLN
1	A	358	ASN
1	A	390	GLN
1	A	439	ASN
1	A	493	GLN
1	A	515	GLN
1	A	545	GLN
1	A	589	GLN
1	A	742	ASN
1	A	854	ASN
1	A	935	GLN
1	A	965	GLN
1	A	1052	GLN
1	A	1124	HIS
1	A	1270	ASN
1	A	1354	ASN

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Mol	Chain	Res	Type
2	B	178	ASN
2	B	224	GLN
2	B	325	GLN
2	B	357	GLN
2	B	366	GLN
2	B	794	ASN
2	B	842	ASN
2	B	843	GLN
2	B	975	GLN
2	B	1117	GLN
2	B	1187	ASN
2	B	1205	GLN
3	C	79	GLN
3	C	206	ASN
4	D	23	ASN
4	D	40	HIS
4	D	132	GLN
4	D	216	ASN
5	E	32	GLN
5	E	54	GLN
5	E	61	GLN
5	E	63	ASN
5	E	114	ASN
7	G	122	ASN
7	G	153	GLN
8	H	133	ASN
9	I	12	ASN
9	I	51	ASN
9	I	89	GLN
9	I	116	ASN
10	J	53	HIS
11	K	2	ASN
11	K	29	ASN
11	K	89	ASN
11	K	92	ASN
11	K	104	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	8/9 (88%)	3 (37%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	3	C
13	R	4	G
13	R	10	G

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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, 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	1398/1733 (80%)	-0.19	16 (1%)	78 52	99, 164, 236, 345	0
2	B	1062/1224 (86%)	-0.11	14 (1%)	75 48	107, 168, 243, 327	0
3	C	266/318 (83%)	-0.28	1 (0%)	88 70	121, 166, 226, 277	0
4	D	162/221 (73%)	-0.08	3 (1%)	66 39	150, 188, 245, 298	0
5	E	208/215 (96%)	-0.26	1 (0%)	87 67	128, 203, 276, 319	0
6	F	84/155 (54%)	-0.42	0	100 100	108, 138, 185, 213	0
7	G	171/171 (100%)	-0.16	1 (0%)	85 64	128, 167, 232, 283	0
8	H	117/146 (80%)	0.12	4 (3%)	48 27	162, 205, 258, 297	0
9	I	117/122 (95%)	-0.08	3 (2%)	57 32	145, 202, 264, 332	0
10	J	65/70 (92%)	-0.23	0	100 100	134, 163, 227, 263	0
11	K	115/120 (95%)	-0.34	0	100 100	127, 166, 222, 261	0
12	L	43/70 (61%)	0.18	0	100 100	145, 191, 243, 251	0
13	R	9/9 (100%)	0.34	0	100 100	193, 224, 292, 292	0
14	T	13/13 (100%)	0.49	0	100 100	187, 213, 301, 321	0
All	All	3830/4587 (83%)	-0.16	43 (1%)	78 52	99, 171, 246, 345	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	ALA	4.5
3	C	27	LEU	4.5
1	A	57	ARG	4.1
1	A	71	GLN	3.7
4	D	187	THR	3.4
2	B	335	GLY	3.3
2	B	62	ILE	3.2
2	B	878	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1089	VAL	3.2
1	A	587	HIS	3.1
9	I	4	PHE	3.1
9	I	118	ARG	3.0
2	B	489	SER	3.0
2	B	934	LYS	2.9
2	B	64	CYS	2.9
4	D	23	ASN	2.8
1	A	1085	HIS	2.8
1	A	55	ASP	2.7
1	A	223	GLY	2.7
8	H	63	LEU	2.7
2	B	90	ILE	2.6
5	E	124	VAL	2.6
8	H	105	GLU	2.6
8	H	119	GLY	2.6
8	H	130	ARG	2.5
2	B	529	GLU	2.5
1	A	1205	LYS	2.4
2	B	476	ARG	2.4
2	B	349	ILE	2.4
2	B	651	LEU	2.4
1	A	493	GLN	2.3
1	A	1109	LYS	2.2
1	A	36	ARG	2.2
1	A	252	PHE	2.2
7	G	94	CYS	2.2
1	A	1010	ALA	2.1
4	D	25	ALA	2.1
2	B	829	CYS	2.1
1	A	1081	LEU	2.1
2	B	351	TYR	2.1
2	B	63	ILE	2.0
9	I	52	ILE	2.0
1	A	323	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates

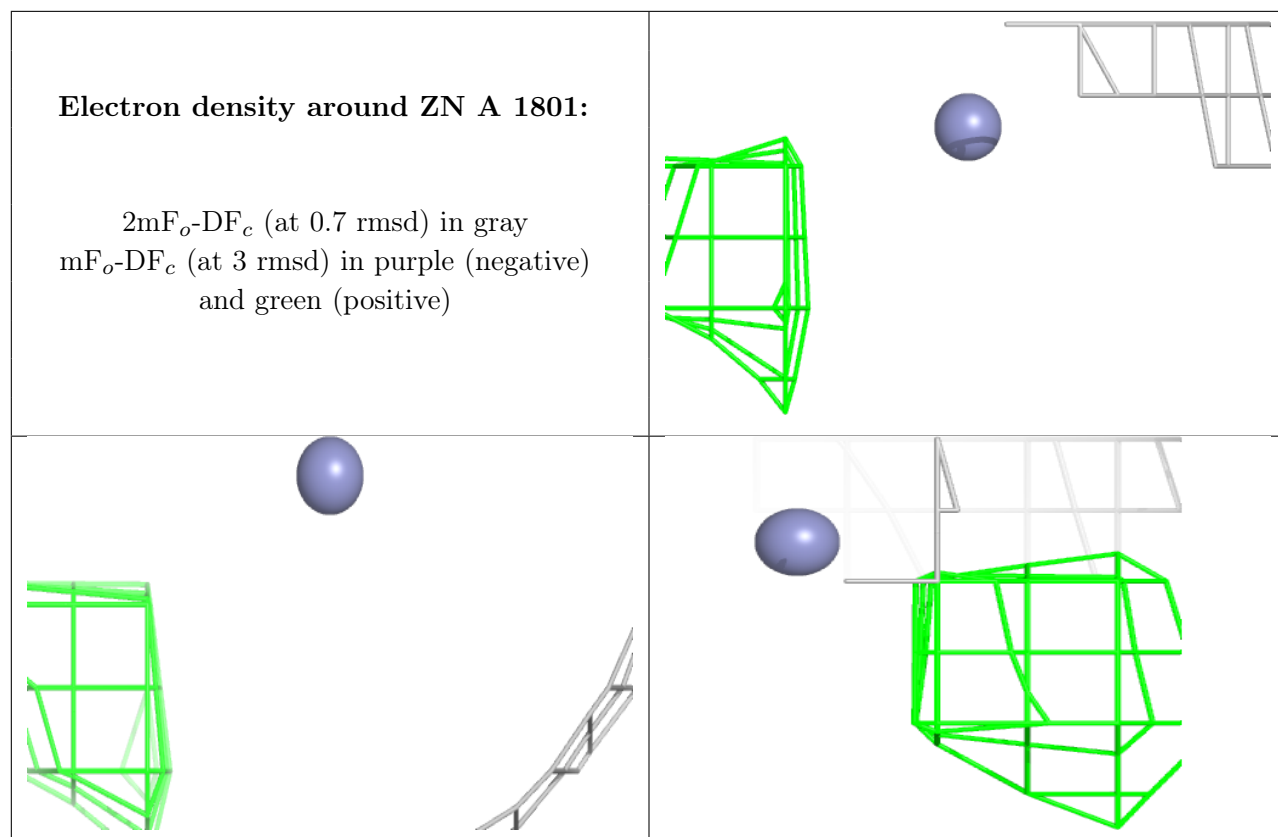
There are no oligosaccharides in this entry.

6.4 Ligands

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.

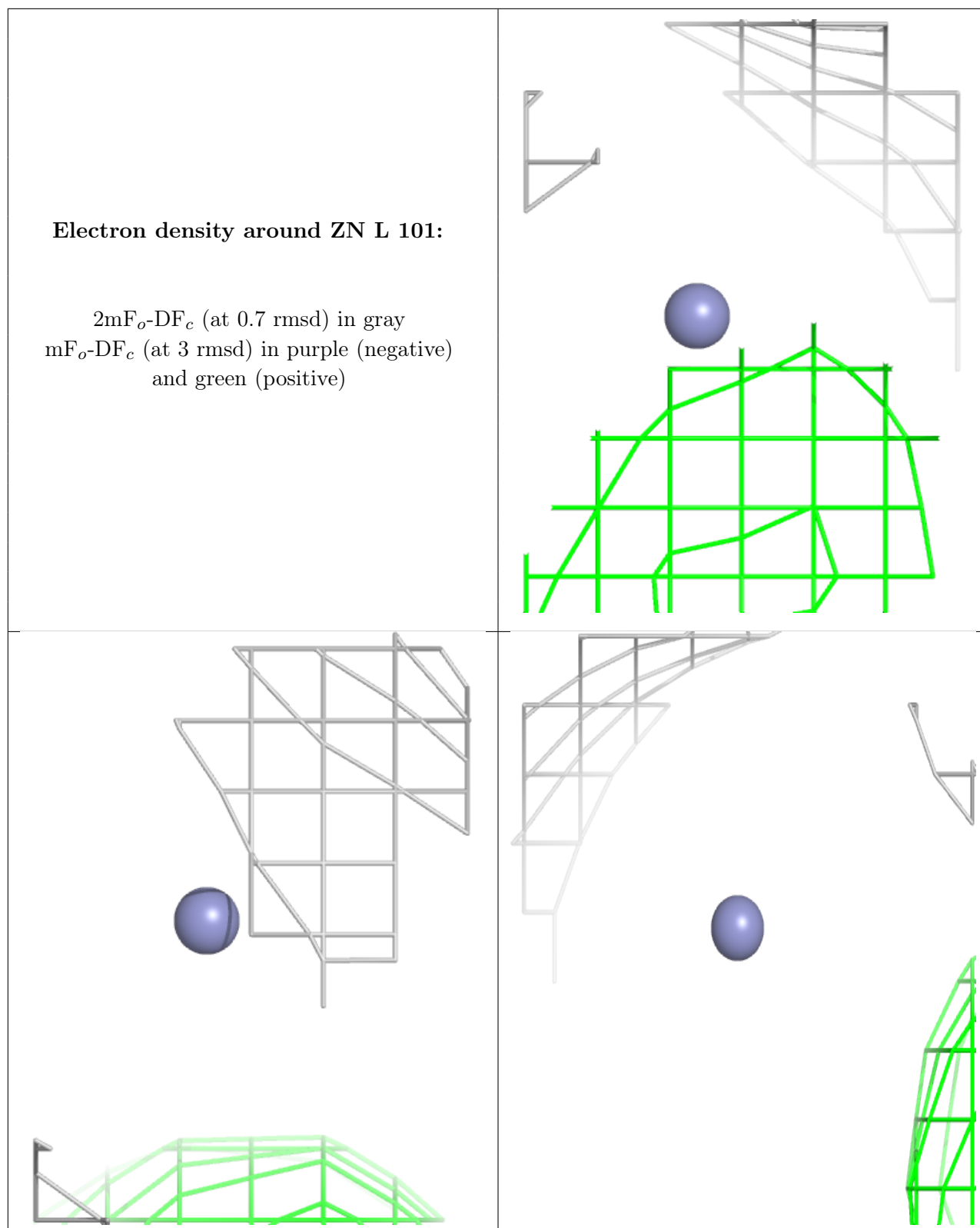
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	ZN	A	1801	1/1	0.97	0.04	190,190,190,190	0
15	ZN	L	101	1/1	0.98	0.04	207,207,207,207	0
15	ZN	B	1301	1/1	0.99	0.10	170,170,170,170	0
15	ZN	C	401	1/1	0.99	0.06	163,163,163,163	0
15	ZN	I	202	1/1	0.99	0.03	209,209,209,209	0
15	ZN	A	1802	1/1	0.99	0.06	158,158,158,158	0
15	ZN	J	101	1/1	1.00	0.04	162,162,162,162	0
15	ZN	I	201	1/1	1.00	0.03	169,169,169,169	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.



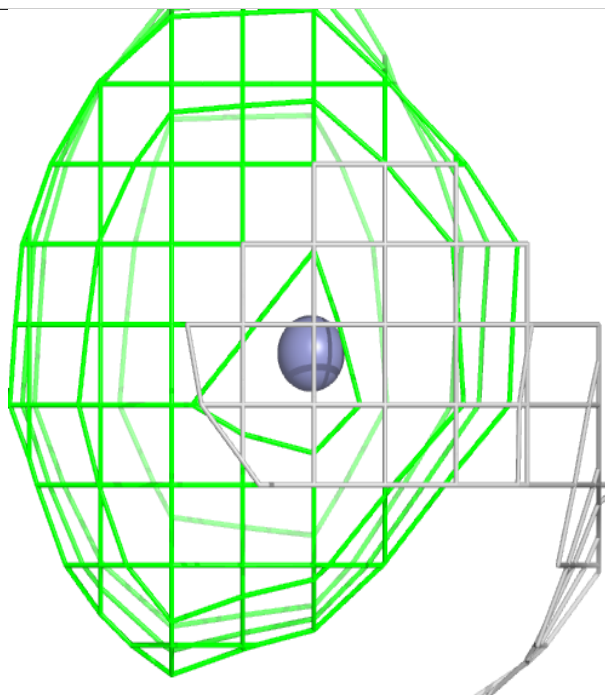
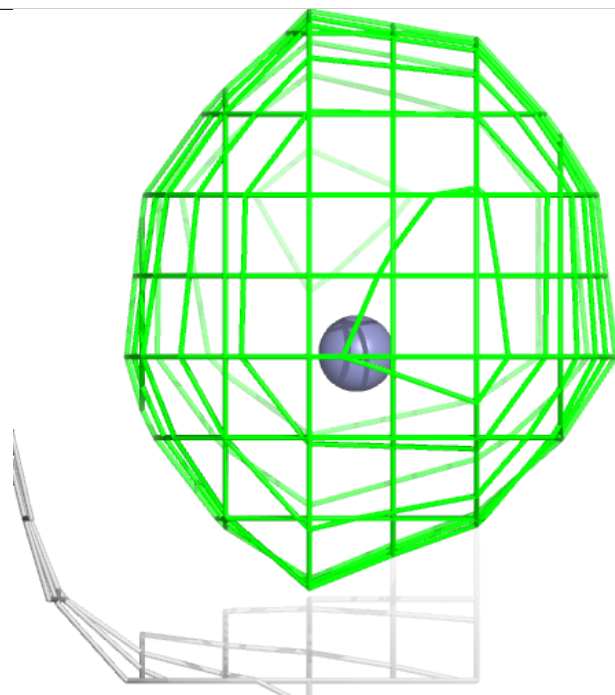
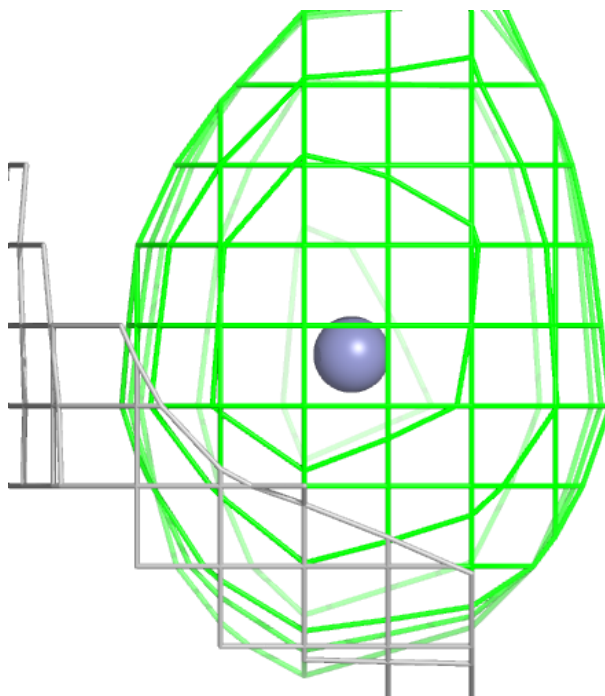
Electron density around ZN L 101:

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



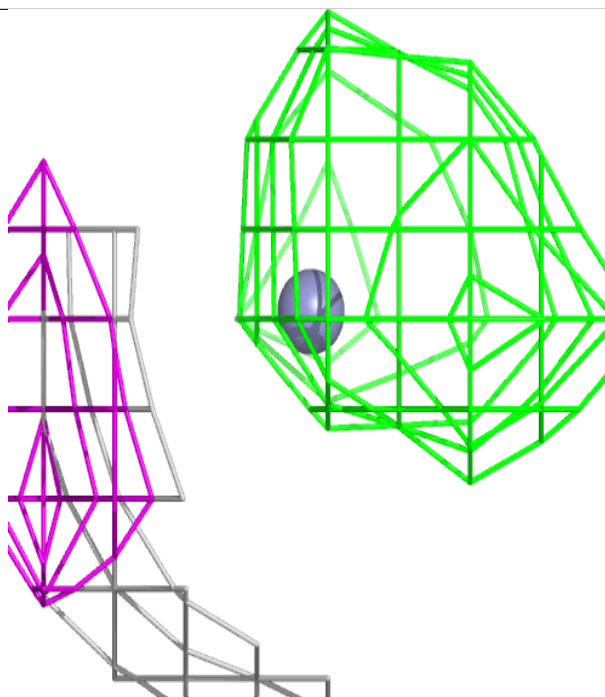
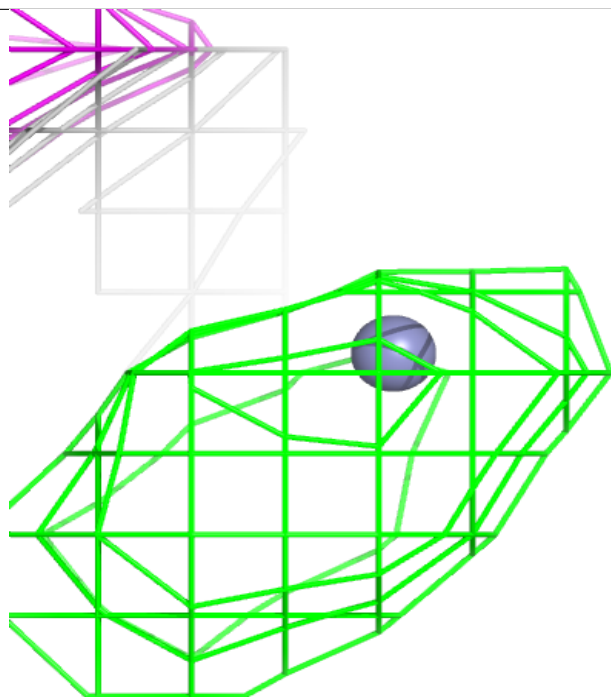
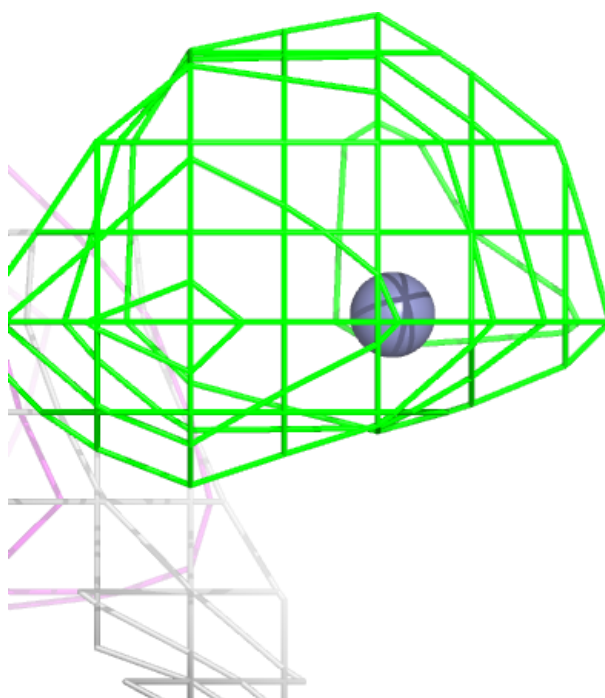
Electron density around ZN B 1301:

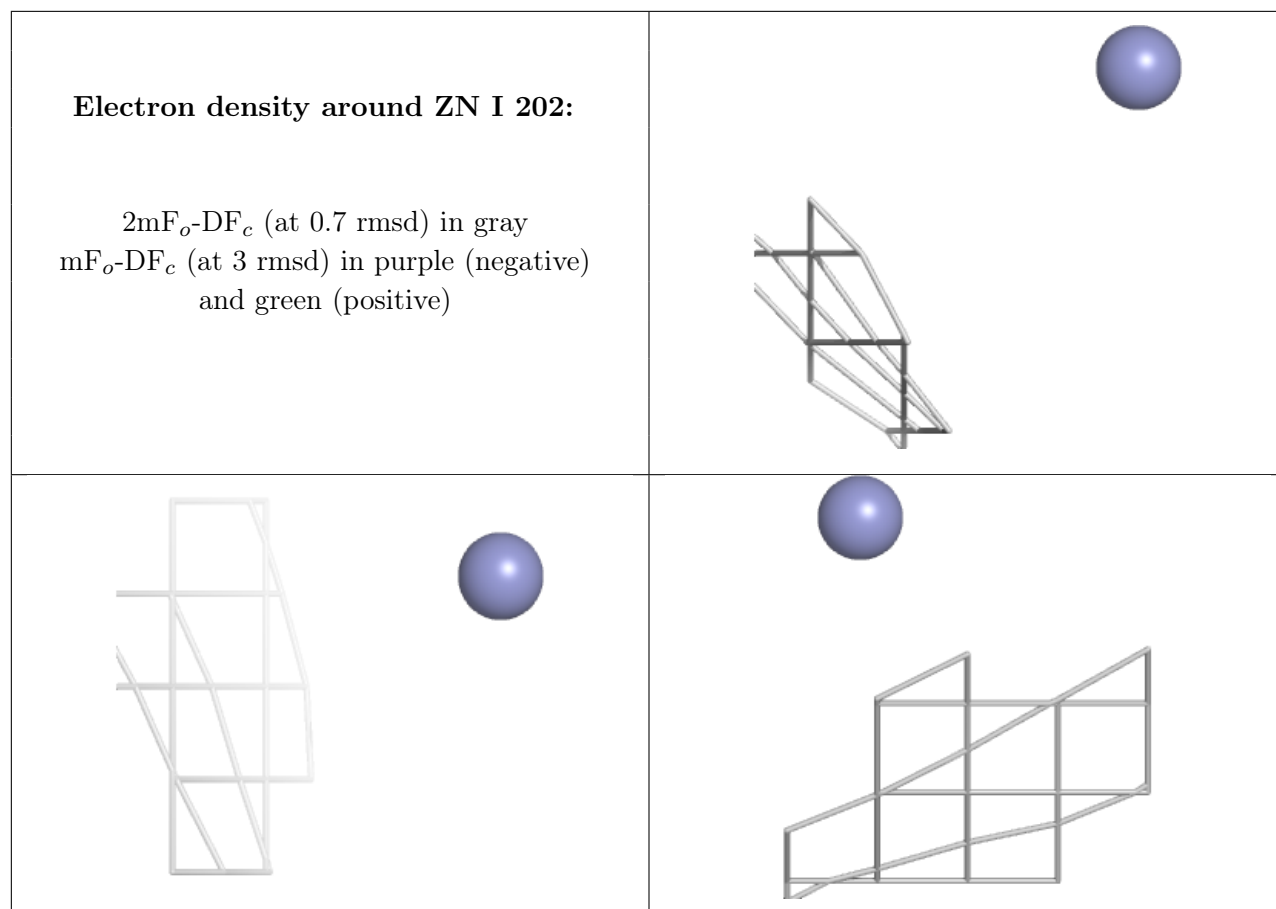
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN C 401:

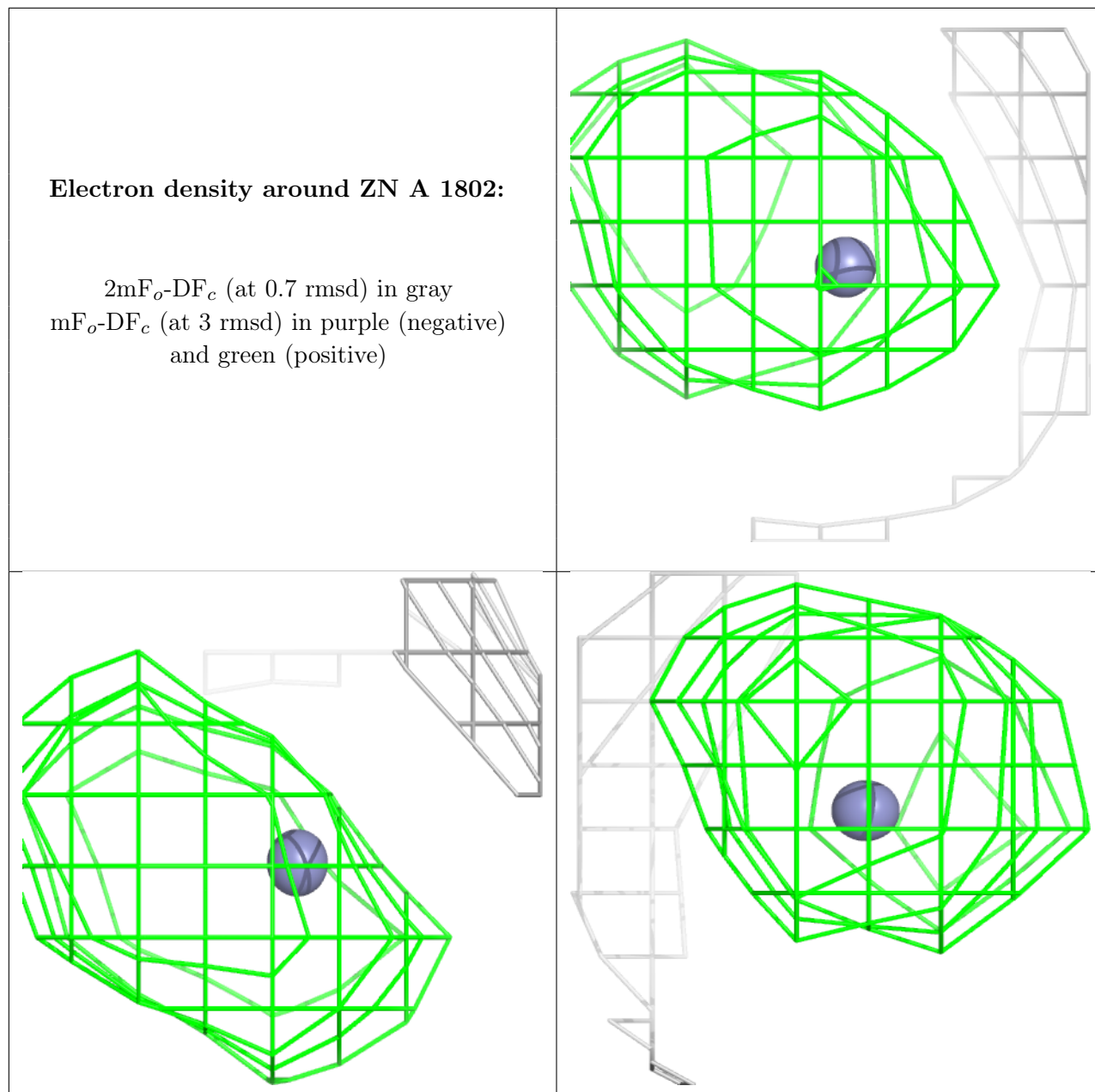
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

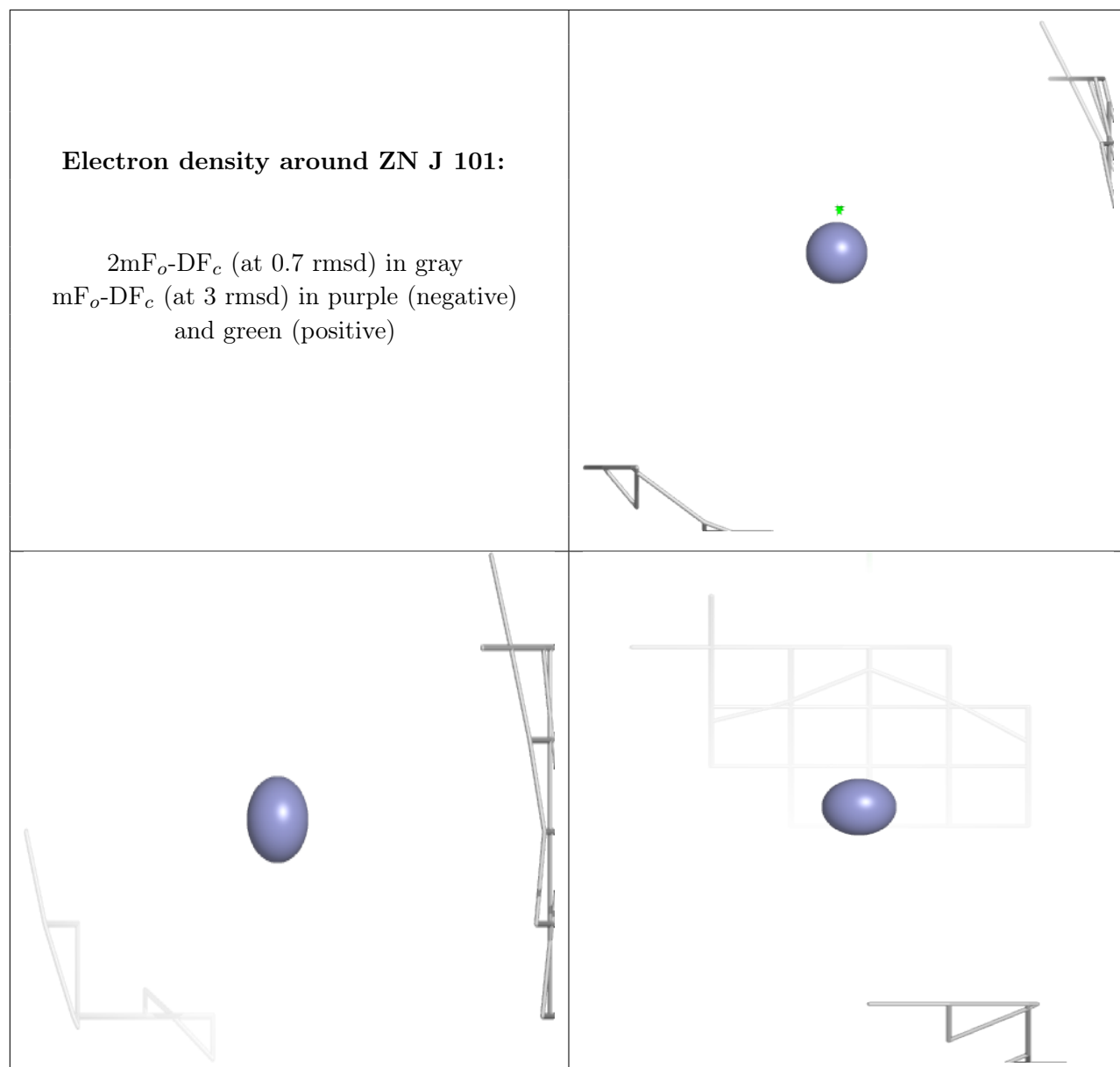


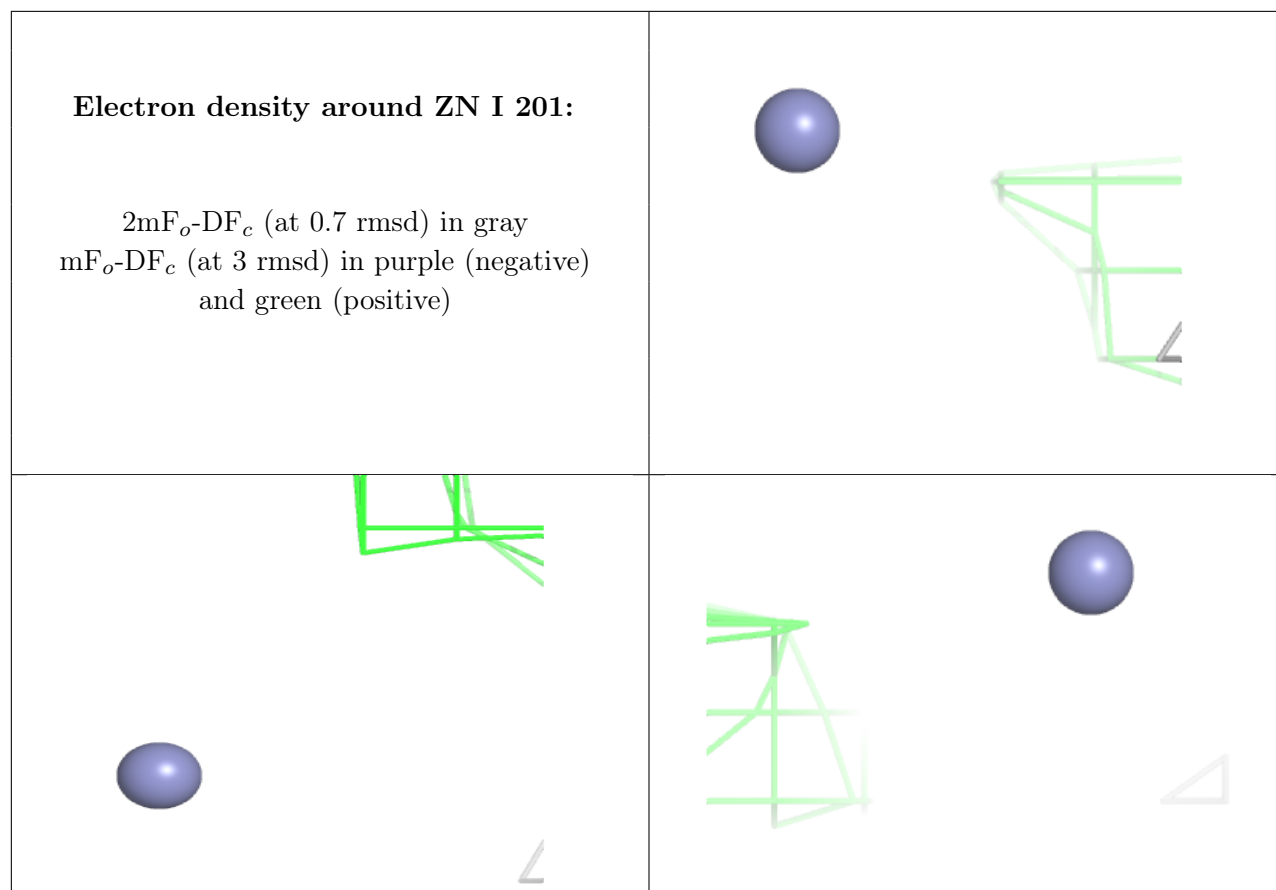


Electron density around ZN A 1802:

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







6.5 Other polymers ⓘ

There are no such residues in this entry.