



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:11 am BST

PDB ID : 6BM2  
Title : Pol II elongation complex with an abasic lesion at i-1 position  
Authors : Wang, W.; Wang, D.  
Deposited on : 2017-11-13  
Resolution : 3.40 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:

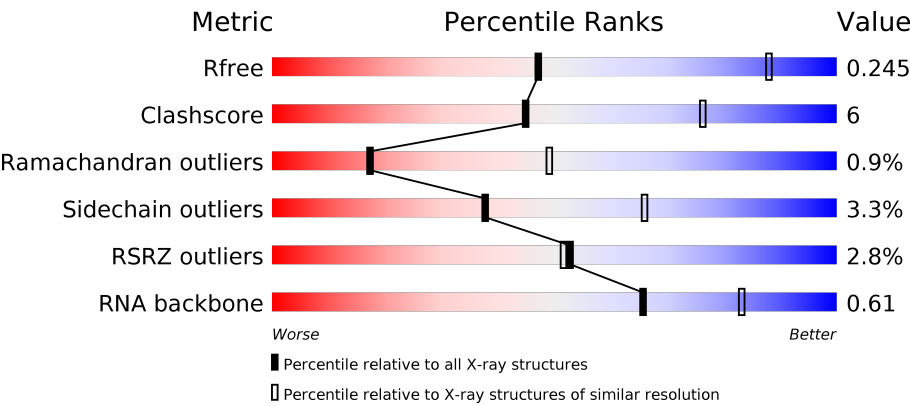
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

# 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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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 on 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	1733	<div><div>3%</div><div><div></div><div>63%</div><div>15%</div><div>•</div><div>21%</div></div></div>
2	B	1224	<div><div>•</div><div><div></div><div>71%</div><div>18%</div><div>•</div><div>10%</div></div></div>
3	C	318	<div><div></div><div><div></div><div>67%</div><div>15%</div><div>•</div><div>16%</div></div></div>
4	E	215	<div><div>8%</div><div><div></div><div>87%</div><div>12%</div><div>•</div></div></div>

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Mol	Chain	Length	Quality of chain
5	F	155	<div><div></div><div>45%9%46%</div></div>
6	H	146	<div>%<div><div></div><div>68%20%11%</div></div></div>
7	I	122	<div><div></div><div>77%16%6%</div></div>
8	J	70	<div>%<div><div></div><div>76%16%7%</div></div></div>
9	K	120	<div><div></div><div>76%19%5%</div></div>
10	L	70	<div>%<div><div></div><div>43%20%37%</div></div></div>
11	T	29	<div><div>10%</div><div><div></div><div>24%17%59%</div></div></div>
12	R	9	<div><div></div><div>56%44%</div></div>

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28244 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	1372	Total	C	N	O	S	0	0	0
			10784	6802	1887	2034	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0	0
			8726	5526	1530	1615	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 polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	213	Total	C	N	O	S	0	0	0
			1744	1107	308	318	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	130	Total	C	N	O	S	0	0	0
			1043	660	173	206	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	115	Total	C	N	O	S	0	0	0
			935	575	170	180	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	44	Total	C	N	O	S	0	0	0
			351	217	70	60	4			

- Molecule 11 is a DNA chain called DNA (5'-D(P\*CP\*AP\*(3DR)P\*CP\*TP\*CP\*TP\*TP\*GP\*AP\*TP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	T	12	Total	C	N	O	P	0	0	0
			233	111	38	72	12			

- Molecule 12 is a RNA chain called RNA (5'-R(\*AP\*UP\*CP\*AP\*AP\*GP\*AP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	R	9	Total	C	N	O	P	0	0	0
			194	88	40	58	8			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		

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

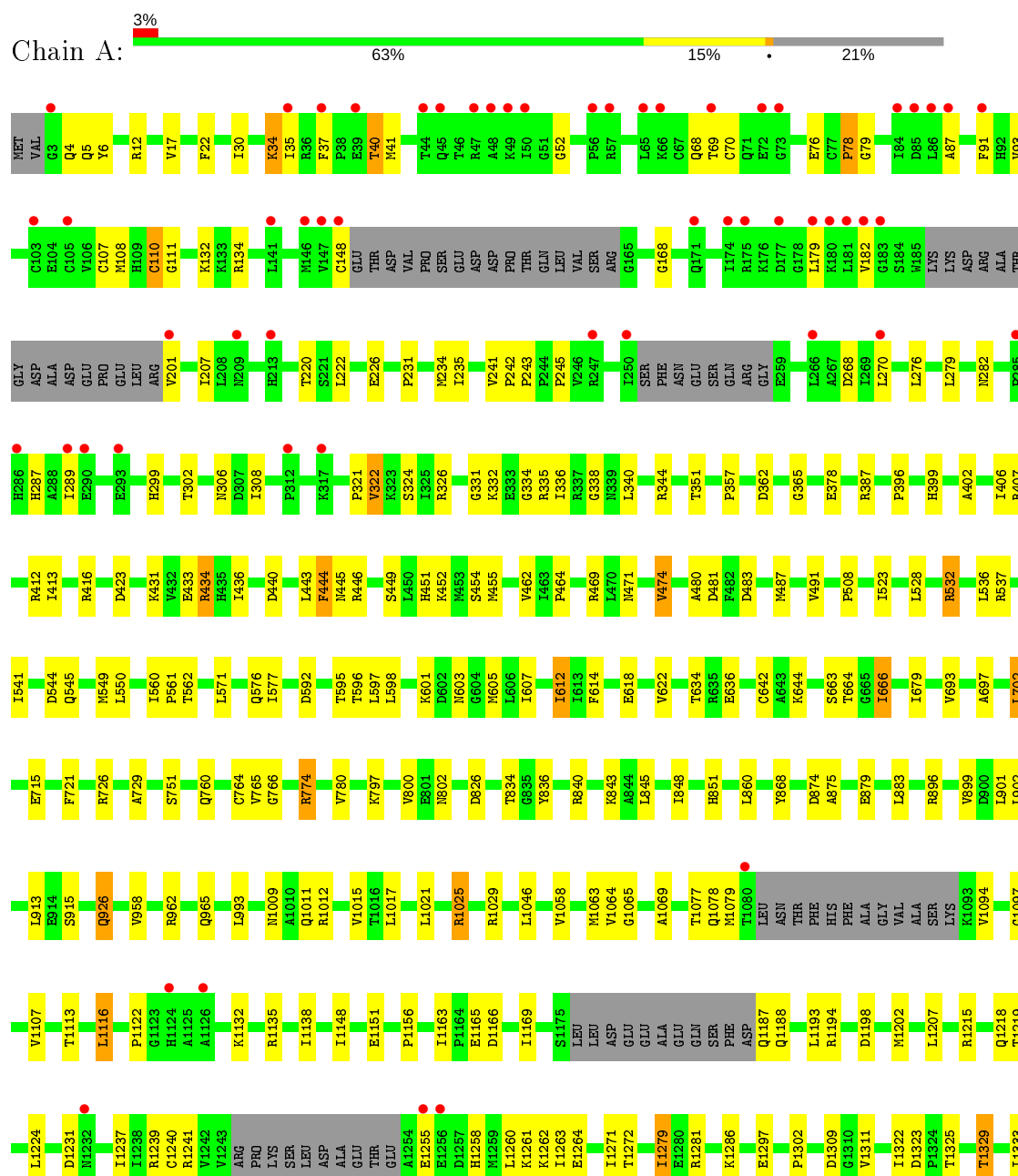
- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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

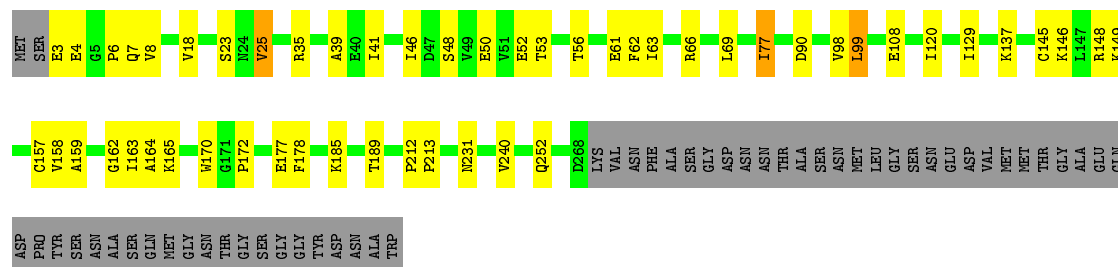




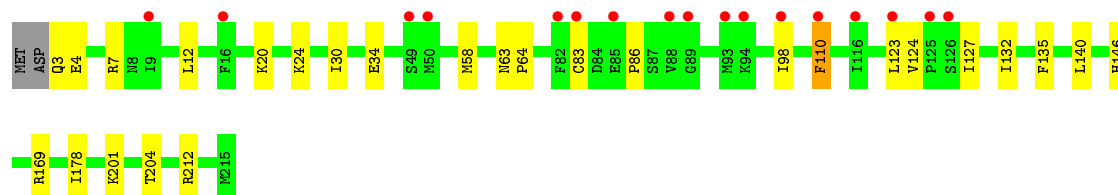
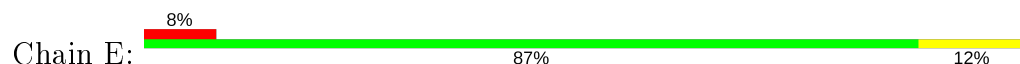




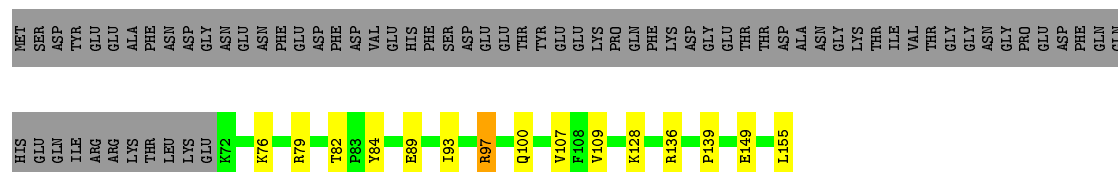
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

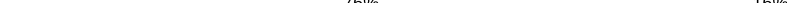


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



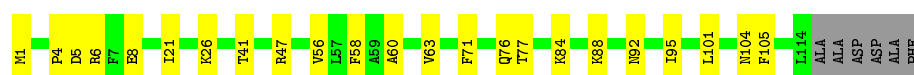
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

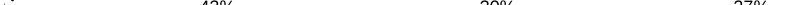
MT	T2	N12	N13	L14	F27	C32	S33	R45	I49	D65	P66	T67	L68	E74	H79	V84	F85	Q89	R92	T95	F101	L104	T111	S112	N116	LYS	ARG	THR	GLN	PRO	SER
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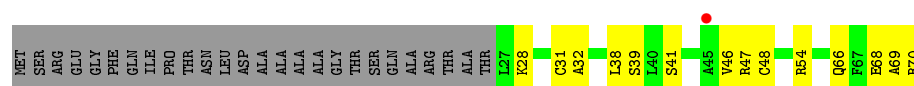
- Chain J:  76% 16% 7%



- Chain K:  76% 19% 5%



- Chain L: 



- Chain T:  10% 24% 17% 49%



- Chain R:  56% 44%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.11Å 222.27Å 193.71Å 90.00° 101.28° 90.00°	Depositor
Resolution (Å)	82.92 – 3.40 82.92 – 3.40	Depositor EDS
% Data completeness (in resolution range)	87.3 (82.92-3.40) 87.3 (82.92-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.219 , 0.244 0.221 , 0.245	Depositor DCC
$R_{free}$ test set	4079 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.6	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 36.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	28244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 3DR

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	0.21	0/10975	0.37	0/14838
2	B	0.21	0/8896	0.37	0/11996
3	C	0.20	0/2133	0.37	0/2891
4	E	0.21	0/1780	0.36	0/2395
5	F	0.20	0/691	0.38	0/933
6	H	0.21	0/1060	0.40	0/1434
7	I	0.21	0/953	0.36	0/1284
8	J	0.21	0/541	0.34	0/727
9	K	0.21	0/937	0.35	0/1265
10	L	0.20	0/353	0.35	0/468
11	T	0.48	0/246	0.87	0/374
12	R	0.15	0/218	0.63	0/339
All	All	0.21	0/28783	0.38	0/38944

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10784	0	10871	154	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8726	0	8760	135	0
3	C	2095	0	2051	34	0
4	E	1744	0	1772	12	0
5	F	679	0	701	8	0
6	H	1043	0	1015	18	0
7	I	935	0	886	13	0
8	J	532	0	542	9	0
9	K	919	0	929	17	0
10	L	351	0	375	7	0
11	T	233	0	133	6	0
12	R	194	0	99	3	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
All	All	28244	0	28134	366	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 6.

All (366) 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)
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.69	0.74
8:J:5:VAL:HG22	8:J:6:ARG:HG3	1.70	0.72
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.73	0.70
2:B:911:ILE:HD11	2:B:941:LEU:HD23	1.73	0.70
7:I:92:ARG:HB3	7:I:95:THR:HG23	1.74	0.69
2:B:1174:LYS:HB2	2:B:1179:GLN:HB2	1.74	0.69
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.73	0.69
1:A:634:THR:HG1	1:A:642:CYS:HG	1.41	0.68
3:C:66:ARG:NH2	8:J:3:VAL:O	2.26	0.68
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.75	0.68
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.74	0.68
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.74	0.68
3:C:6:PRO:HB2	9:K:101:LEU:HD23	1.76	0.67
2:B:778:MET:HE1	2:B:1094:ARG:HH11	1.59	0.67
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:ARG:NH1	2:B:324:ILE:O	2.28	0.66
2:B:642:ASP:HB3	2:B:649:LYS:HG2	1.76	0.66
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.78	0.65
2:B:1175:LEU:O	2:B:1176:ASN:ND2	2.29	0.65
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.28	0.65
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.77	0.65
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.77	0.65
1:A:40:THR:HG22	1:A:41:MET:HG3	1.78	0.64
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.80	0.64
1:A:446:ARG:NH2	12:R:9:A:O2'	2.30	0.64
1:A:134:ARG:NH1	1:A:220:THR:O	2.31	0.64
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.80	0.63
3:C:48:SER:HB3	3:C:158:VAL:HB	1.80	0.63
1:A:4:GLN:OE1	2:B:1159:ARG:NH1	2.32	0.62
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.82	0.62
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.82	0.62
1:A:1009:ASN:OD1	1:A:1012:ARG:NH2	2.32	0.62
2:B:165:VAL:HG21	2:B:448:ILE:HD12	1.82	0.61
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.33	0.61
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.83	0.61
5:F:82:THR:HG22	5:F:84:TYR:H	1.64	0.61
2:B:463:THR:HG22	11:T:27:DA:H2''	1.82	0.61
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.82	0.61
1:A:601:LYS:HB2	1:A:603:ASN:HD22	1.65	0.61
3:C:3:GLU:HG3	3:C:4:GLU:HG3	1.80	0.61
3:C:145:CYS:SG	3:C:146:LYS:N	2.73	0.61
3:C:46:ILE:HD13	3:C:159:ALA:HB2	1.83	0.61
6:H:129:TYR:O	6:H:132:LEU:N	2.35	0.60
1:A:1187:GLN:HG3	1:A:1188:GLN:HG3	1.84	0.60
1:A:469:ARG:NH2	2:B:991:GLY:O	2.35	0.59
1:A:693:VAL:HG21	1:A:721:PHE:HE2	1.66	0.59
2:B:916:THR:HG23	2:B:935:ARG:HB2	1.84	0.59
3:C:77:ILE:HG12	3:C:129:ILE:HD11	1.84	0.59
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.35	0.59
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.83	0.59
1:A:338:GLY:HA2	2:B:1129:ARG:HH21	1.68	0.58
1:A:68:GLN:O	1:A:70:CYS:N	2.34	0.58
7:I:32:CYS:SG	7:I:33:SER:N	2.76	0.58
5:F:76:LYS:O	5:F:79:ARG:NH1	2.32	0.58
2:B:28:GLU:OE1	2:B:807:ARG:NH1	2.33	0.58
1:A:1116:LEU:HD22	1:A:1329:THR:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.37	0.58
1:A:1122:PRO:HD3	1:A:1323:ASP:HB2	1.86	0.57
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.85	0.57
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.84	0.57
3:C:69:LEU:HD12	8:J:6:ARG:HD3	1.85	0.57
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.86	0.57
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.85	0.57
2:B:613:VAL:HG22	2:B:628:THR:HG23	1.87	0.57
1:A:993:LEU:HD22	1:A:1046:LEU:HG	1.87	0.57
1:A:306:ASN:ND2	1:A:321:PRO:O	2.38	0.57
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.87	0.57
2:B:103:ASN:OD1	2:B:169:ARG:NH2	2.38	0.57
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.87	0.56
1:A:1423:GLY:O	1:A:1427:ASN:ND2	2.36	0.56
6:H:89:LEU:HD13	6:H:89:LEU:H	1.70	0.56
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.39	0.56
1:A:30:ILE:HG23	2:B:1170:THR:HG23	1.88	0.56
2:B:60:GLN:NE2	2:B:64:CYS:SG	2.79	0.56
3:C:46:ILE:HD12	3:C:157:CYS:HB3	1.86	0.56
3:C:185:LYS:HG2	3:C:213:PRO:HG3	1.87	0.56
6:H:91:ASP:OD1	6:H:92:ASP:N	2.38	0.56
1:A:1148:ILE:HD13	7:I:49:ILE:HD12	1.89	0.55
1:A:34:LYS:H	1:A:34:LYS:HD3	1.72	0.55
1:A:774:ARG:HG3	1:A:797:LYS:HZ2	1.72	0.55
2:B:857:ARG:NH2	11:T:25:DC:OP1	2.40	0.55
1:A:110:CYS:SG	1:A:111:GLY:N	2.73	0.55
1:A:1239:ARG:HH22	1:A:1241:ARG:HH21	1.54	0.55
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.88	0.55
1:A:1151:GLU:OE2	7:I:45:ARG:NH1	2.40	0.54
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.89	0.54
1:A:802:ASN:OD1	2:B:729:ILE:N	2.36	0.54
8:J:36:LEU:HD11	8:J:51:LEU:HB2	1.89	0.54
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.89	0.54
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.89	0.54
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.40	0.54
1:A:562:THR:O	1:A:576:GLN:NE2	2.40	0.54
5:F:97:ARG:NH1	5:F:100:GLN:OE1	2.41	0.54
7:I:74:GLU:OE1	7:I:79:HIS:ND1	2.38	0.54
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.90	0.53
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.89	0.53
9:K:56:VAL:HG22	9:K:77:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:806:THR:HG22	2:B:808:ALA:H	1.74	0.53
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.91	0.53
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	1.90	0.53
1:A:532:ARG:HE	1:A:536:LEU:HD21	1.73	0.53
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.73	0.53
1:A:332:LYS:HE2	11:T:19:DA:H3'	1.91	0.53
6:H:137:GLN:HG3	6:H:139:ASN:H	1.73	0.53
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.43	0.53
2:B:855:PHE:HZ	2:B:857:ARG:HH11	1.57	0.52
6:H:85:GLY:HA2	6:H:86:ASP:HB3	1.91	0.52
2:B:547:VAL:N	2:B:612:GLU:OE2	2.40	0.52
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.43	0.52
1:A:1281:ARG:HG2	1:A:1309:ASP:HB2	1.91	0.52
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.41	0.52
1:A:550:LEU:HD21	1:A:561:PRO:HD2	1.90	0.52
1:A:528:LEU:HD23	1:A:751:SER:HA	1.92	0.52
2:B:877:PRO:HB2	2:B:885:MET:HE1	1.91	0.52
4:E:20:LYS:NZ	4:E:34:GLU:O	2.37	0.52
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.91	0.52
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.90	0.52
6:H:8:ASP:OD1	6:H:9:ILE:N	2.43	0.52
3:C:50:GLU:HG2	10:L:66:GLN:HG2	1.92	0.51
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.92	0.51
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.92	0.51
1:A:1286:LYS:HE2	1:A:1302:PRO:HB2	1.92	0.51
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.93	0.51
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.91	0.51
3:C:99:LEU:HB3	3:C:120:ILE:HD13	1.93	0.51
10:L:38:LEU:HD21	10:L:48:CYS:HA	1.92	0.51
12:R:7:A:H2'	12:R:8:G:C8	2.45	0.51
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.75	0.51
10:L:47:ARG:HG2	10:L:54:ARG:HG2	1.93	0.51
2:B:963:PHE:HE2	2:B:965:LYS:HE3	1.76	0.51
2:B:95:ILE:HD11	2:B:128:LEU:HB3	1.93	0.51
4:E:83:CYS:HB2	4:E:110:PHE:HE1	1.75	0.51
1:A:1325:THR:OG1	4:E:146:HIS:O	2.28	0.50
1:A:560:ILE:HB	6:H:79:TRP:H	1.75	0.50
8:J:10:CYS:SG	8:J:11:GLY:N	2.84	0.50
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.94	0.50
1:A:834:THR:HG21	1:A:1077:THR:HA	1.93	0.50
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:LYS:O	9:K:6:ARG:NH1	2.44	0.50
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.93	0.50
5:F:107:VAL:HG12	5:F:109:VAL:H	1.76	0.50
2:B:298:LEU:O	2:B:302:CYS:N	2.40	0.50
2:B:579:ARG:HA	2:B:589:VAL:HA	1.92	0.50
2:B:378:LEU:O	2:B:382:ILE:HG12	2.12	0.50
3:C:98:VAL:HG22	3:C:158:VAL:HG22	1.93	0.50
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.94	0.50
2:B:680:THR:O	2:B:683:SER:OG	2.29	0.50
1:A:182:VAL:HA	1:A:201:VAL:HA	1.94	0.49
3:C:252:GLN:HG3	9:K:95:ILE:HG23	1.92	0.49
1:A:1079:MET:HE1	1:A:1097:GLY:HA2	1.94	0.49
2:B:810:GLU:OE1	2:B:815:ARG:NH2	2.45	0.49
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.93	0.49
6:H:84:ALA:HB3	6:H:86:ASP:HB3	1.94	0.49
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.94	0.49
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.95	0.49
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.52	0.48
1:A:412:ARG:NH1	1:A:433:GLU:OE2	2.43	0.48
2:B:428:ILE:HD11	2:B:448:ILE:HG23	1.95	0.48
2:B:482:VAL:HG11	11:T:26:DG:H5"	1.94	0.48
2:B:956:THR:HG22	10:L:46:VAL:HG11	1.95	0.48
1:A:1116:LEU:HD23	1:A:1311:VAL:HA	1.95	0.48
1:A:544:ASP:OD1	1:A:545:GLN:N	2.43	0.48
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.95	0.48
2:B:522:VAL:HG11	2:B:537:LYS:HD2	1.96	0.48
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.47	0.48
2:B:620:ARG:NH2	7:I:89:GLN:OE1	2.46	0.48
1:A:1163:ILE:HG22	1:A:1165:GLU:H	1.79	0.48
2:B:298:LEU:HD22	2:B:314:LEU:HD13	1.95	0.48
9:K:21:ILE:HD13	9:K:84:LYS:HE2	1.96	0.48
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.96	0.48
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.14	0.47
3:C:163:ILE:HG22	3:C:165:LYS:H	1.79	0.47
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.96	0.47
1:A:860:LEU:HD21	1:A:1394:THR:HA	1.96	0.47
2:B:843:GLN:HB2	2:B:993:THR:HB	1.96	0.47
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.96	0.47
2:B:1017:ILE:H	2:B:1018:PRO:HD2	1.79	0.47
2:B:562:GLY:O	2:B:590:HIS:ND1	2.40	0.47
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1166:ASP:HA	1:A:1169:ILE:HD13	1.97	0.47
1:A:868:TYR:CZ	1:A:1064:VAL:HG21	2.49	0.47
1:A:1215:ARG:NH2	1:A:1218:GLN:OE1	2.47	0.47
1:A:663:SER:OG	1:A:664:THR:N	2.47	0.47
1:A:362:ASP:HB3	1:A:508:PRO:HD3	1.97	0.47
1:A:336:ILE:HA	1:A:340:LEU:HD12	1.95	0.47
3:C:7:GLN:HB2	3:C:23:SER:HB2	1.96	0.47
10:L:68:GLU:O	10:L:70:ARG:N	2.48	0.47
1:A:1194:ARG:HH21	1:A:1237:ILE:HD13	1.80	0.47
4:E:4:GLU:OE1	4:E:7:ARG:NH2	2.34	0.46
1:A:962:ARG:HA	1:A:965:GLN:HG2	1.96	0.46
2:B:1082:MET:HA	3:C:189:THR:HA	1.97	0.46
3:C:3:GLU:N	9:K:104:ASN:HD21	2.12	0.46
9:K:5:ASP:HB2	9:K:8:GLU:HG3	1.96	0.46
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.97	0.46
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.96	0.46
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.98	0.46
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.98	0.46
2:B:702:LEU:HD21	2:B:735:ALA:HB1	1.97	0.46
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.97	0.46
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.81	0.46
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.98	0.46
6:H:81:PRO:O	6:H:83:GLN:N	2.49	0.46
10:L:31:CYS:SG	10:L:32:ALA:N	2.88	0.46
1:A:108:MET:O	1:A:110:CYS:N	2.48	0.46
1:A:449:SER:HB3	2:B:1137:CYS:SG	2.56	0.46
1:A:760:GLN:HG2	1:A:765:VAL:HA	1.97	0.46
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.98	0.46
2:B:883:LEU:O	2:B:885:MET:N	2.49	0.46
1:A:148:CYS:HB2	1:A:168:GLY:HA2	1.98	0.46
1:A:595:THR:OG1	1:A:603:ASN:OD1	2.31	0.45
1:A:614:PHE:HB3	6:H:122:LEU:HD21	1.98	0.45
1:A:883:LEU:HD23	1:A:1021:LEU:HD13	1.98	0.45
3:C:52:GLU:HG2	3:C:53:THR:HG23	1.97	0.45
7:I:84:VAL:HG23	7:I:104:LEU:HD11	1.98	0.45
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.81	0.45
1:A:279:LEU:HB3	1:A:289:ILE:HG22	1.98	0.45
4:E:124:VAL:HG13	4:E:132:ILE:HB	1.99	0.45
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.98	0.45
7:I:65:ASP:HA	7:I:66:PRO:HD3	1.83	0.45
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:HB2	1:A:487:MET:HG2	1.98	0.45
2:B:326:ASP:OD1	2:B:329:THR:OG1	2.24	0.45
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.98	0.44
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.99	0.44
4:E:24:LYS:HB3	4:E:30:ILE:HB	1.99	0.44
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.99	0.44
2:B:281:PRO:HB2	2:B:284:ILE:HG12	1.99	0.44
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.98	0.44
2:B:941:LEU:HD22	2:B:942:ARG:H	1.82	0.44
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.84	0.44
2:B:610:ASN:HB3	2:B:613:VAL:HG23	2.00	0.44
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	2.00	0.44
1:A:235:ILE:H	1:A:235:ILE:HG13	1.55	0.44
1:A:242:PRO:HA	1:A:243:PRO:HD3	1.80	0.44
3:C:108:GLU:HA	3:C:149:LYS:HD3	2.00	0.44
7:I:101:PHE:HE1	7:I:112:SER:HB3	1.82	0.44
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.98	0.44
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.98	0.44
1:A:1132:LYS:HG3	1:A:1135:ARG:HH12	1.83	0.43
2:B:939:THR:HA	2:B:940:PRO:HD3	1.82	0.43
2:B:999:MET:HG3	2:B:1000:PRO:HD2	2.00	0.43
1:A:396:PRO:HG3	1:A:416:ARG:HB3	1.99	0.43
3:C:62:PHE:O	3:C:66:ARG:HG3	2.18	0.43
1:A:596:THR:C	1:A:598:LEU:H	2.21	0.43
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.33	0.43
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	2.00	0.43
5:F:82:THR:O	5:F:136:ARG:NH1	2.31	0.43
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	2.00	0.43
2:B:199:MET:N	2:B:199:MET:SD	2.82	0.43
2:B:483:LEU:HD21	2:B:491:THR:HG23	2.00	0.43
2:B:916:THR:HA	2:B:917:PRO:HD3	1.80	0.43
1:A:1333:ILE:HD13	1:A:1381:LEU:HD12	2.01	0.43
1:A:541:ILE:HD12	1:A:577:ILE:HG12	2.01	0.43
2:B:512:ARG:NH1	2:B:533:CYS:O	2.51	0.43
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.54	0.43
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.99	0.43
2:B:307:ASP:OD1	2:B:392:ARG:NH1	2.45	0.43
2:B:600:LEU:HB3	2:B:615:MET:SD	2.59	0.43
2:B:857:ARG:HH21	2:B:942:ARG:NH2	2.17	0.43
10:L:28:LYS:HA	10:L:39:SER:HA	2.00	0.43
1:A:444:PHE:HA	1:A:444:PHE:HD1	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1261:LYS:HB2	1:A:1261:LYS:HE3	1.84	0.43
2:B:861:ASP:OD1	2:B:862:GLN:N	2.50	0.43
6:H:76:THR:OG1	6:H:77:ARG:N	2.52	0.43
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	2.01	0.42
1:A:1261:LYS:O	1:A:1264:GLU:HG3	2.19	0.42
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.54	0.42
1:A:402:ALA:HA	1:A:434:ARG:HA	2.01	0.42
1:A:87:ALA:HB3	1:A:276:LEU:HD23	2.01	0.42
2:B:287:ARG:NH1	2:B:321:GLY:O	2.52	0.42
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.54	0.42
1:A:331:GLY:HA2	1:A:334:GLY:H	1.85	0.42
1:A:545:GLN:HG2	1:A:549:MET:HE3	2.01	0.42
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.55	0.42
2:B:1013:ASN:OD1	2:B:1015:HIS:ND1	2.49	0.42
2:B:771:SER:O	2:B:775:LYS:HE3	2.20	0.42
2:B:69:LEU:HB2	2:B:90:ILE:HG12	2.01	0.42
5:F:128:LYS:HD2	5:F:149:GLU:HA	2.02	0.42
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.54	0.42
2:B:1129:ARG:NH1	11:T:21:DC:OP1	2.52	0.42
1:A:78:PRO:HB2	1:A:79:GLY:H	1.62	0.42
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	2.02	0.42
1:A:1255:GLU:HB3	1:A:1258:HIS:CE1	2.55	0.42
1:A:302:THR:OG1	1:A:306:ASN:OD1	2.37	0.42
1:A:644:LYS:HA	1:A:644:LYS:HD2	1.91	0.42
4:E:63:ASN:HA	4:E:64:PRO:HD3	1.88	0.42
8:J:44:TYR:HA	8:J:47:ARG:HB3	2.01	0.42
1:A:445:ASN:HA	1:A:454:SER:O	2.20	0.42
1:A:571:LEU:HD12	6:H:46:LEU:HD11	2.01	0.42
2:B:313:MET:HE3	2:B:386:LEU:HD22	2.01	0.42
7:I:65:ASP:HB3	7:I:68:LEU:HD12	2.00	0.42
1:A:471:ASN:O	1:A:474:VAL:HG12	2.20	0.42
1:A:537:ARG:HD2	6:H:121:LEU:HD23	2.02	0.42
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.20	0.42
2:B:1106:ARG:HH11	2:B:1126:GLY:HA2	1.85	0.42
2:B:1135:ARG:NH2	2:B:1136:ASP:OD1	2.53	0.42
9:K:88:LYS:O	9:K:92:ASN:ND2	2.43	0.42
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.53	0.42
1:A:423:ASP:N	1:A:423:ASP:OD1	2.49	0.42
1:A:879:GLU:OE1	1:A:962:ARG:NH2	2.53	0.42
1:A:913:LEU:HG	1:A:915:SER:H	1.84	0.42
2:B:100:PRO:HG2	2:B:124:TYR:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:570:VAL:HB	2:B:573:GLN:HG2	2.02	0.42
6:H:6:PHE:HB3	6:H:59:ILE:HB	2.02	0.42
1:A:1260:LEU:HD12	1:A:1263:ILE:HD12	2.02	0.41
1:A:231:PRO:HA	1:A:234:MET:HG3	2.02	0.41
2:B:63:ILE:O	2:B:67:SER:OG	2.30	0.41
2:B:898:LEU:HD11	2:B:964:VAL:HG21	2.02	0.41
11:T:26:DG:H1	12:R:3:C:H42	1.67	0.41
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.20	0.41
3:C:41:ILE:HB	3:C:172:PRO:HG3	2.02	0.41
3:C:212:PRO:HA	3:C:213:PRO:HD3	1.86	0.41
6:H:14:GLU:HB3	6:H:27:GLU:HB3	2.02	0.41
1:A:107:CYS:SG	1:A:108:MET:N	2.93	0.41
1:A:1395:GLY:HA3	1:A:1426:GLU:OE2	2.19	0.41
1:A:868:TYR:HD2	1:A:1058:VAL:HG11	1.84	0.41
3:C:8:VAL:HG11	9:K:105:PHE:HD1	1.86	0.41
2:B:843:GLN:NE2	2:B:847:ASP:OD1	2.53	0.41
2:B:872:GLU:HG2	2:B:916:THR:HB	2.03	0.41
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.85	0.41
3:C:56:THR:HG21	3:C:63:ILE:HD11	2.02	0.41
4:E:135:PHE:HB3	4:E:140:LEU:HD11	2.03	0.41
6:H:133:ASN:N	6:H:133:ASN:OD1	2.54	0.41
1:A:91:PHE:HZ	1:A:207:ILE:HD12	1.85	0.41
1:A:523:ILE:HD13	1:A:622:VAL:HG22	2.03	0.41
2:B:170:LEU:HD12	2:B:171:PRO:HD2	2.02	0.41
1:A:598:LEU:O	6:H:122:LEU:HD12	2.21	0.41
1:A:1215:ARG:HD3	1:A:1272:THR:O	2.21	0.41
1:A:399:HIS:CE1	1:A:462:VAL:HG21	2.56	0.41
4:E:12:LEU:HD21	4:E:58:MET:HE1	2.02	0.41
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.49	0.41
2:B:1156:ASP:N	2:B:1156:ASP:OD1	2.52	0.41
2:B:128:LEU:HD21	2:B:170:LEU:HB2	2.03	0.41
2:B:487:THR:OG1	2:B:777:ALA:O	2.39	0.41
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.03	0.41
2:B:778:MET:HE1	2:B:1094:ARG:NH1	2.31	0.41
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.56	0.41
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.56	0.41
1:A:843:LYS:HA	1:A:843:LYS:HD3	1.94	0.41
2:B:364:ILE:HG13	2:B:365:THR:OG1	2.21	0.41
2:B:496:ARG:NH1	2:B:539:LEU:O	2.54	0.41
7:I:14:LEU:HD13	7:I:27:PHE:HB3	2.03	0.41
1:A:445:ASN:HD22	1:A:455:MET:HG2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:ILE:HG12	1:A:612:ILE:HA	2.03	0.40
1:A:851:HIS:CG	5:F:139:PRO:HG3	2.56	0.40
2:B:122:LEU:HD22	2:B:958:GLN:HB2	2.03	0.40
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.21	0.40
8:J:36:LEU:HD13	8:J:47:ARG:HG3	2.04	0.40
9:K:47:ARG:HH11	9:K:47:ARG:HB3	1.85	0.40
9:K:63:VAL:HG22	9:K:71:PHE:HB3	2.03	0.40
1:A:1021:LEU:HD11	1:A:1025:ARG:NH1	2.36	0.40
1:A:874:ASP:HB2	1:A:1058:VAL:HA	2.04	0.40
1:A:1373:ASP:HA	1:A:1376:THR:HG22	2.03	0.40
1:A:577:ILE:H	1:A:577:ILE:HG13	1.71	0.40
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.54	0.40
2:B:651:LEU:HD11	2:B:707:PRO:HB3	2.02	0.40
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.20	0.40
2:B:118:ARG:NH2	2:B:194:GLU:OE2	2.52	0.40
4:E:201:LYS:HA	4:E:201:LYS:HD3	1.95	0.40
2:B:63:ILE:HD12	2:B:95:ILE:HB	2.03	0.40
1:A:464:PRO:HB2	9:K:4:PRO:HD3	2.04	0.40
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.56	0.40
1:A:848:ILE:HB	1:A:1065:GLY:HA3	2.02	0.40
2:B:762:ASN:OD1	2:B:984:HIS:HD2	2.05	0.40
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	2.04	0.40
9:K:47:ARG:HD2	9:K:60:ALA:HA	2.03	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	1358/1733 (78%)	1238 (91%)	106 (8%)	14 (1%)	15 46
2	B	1077/1224 (88%)	1001 (93%)	67 (6%)	9 (1%)	19 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	264/318 (83%)	243 (92%)	19 (7%)	2 (1%)	19	51
4	E	211/215 (98%)	201 (95%)	9 (4%)	1 (0%)	29	61
5	F	82/155 (53%)	79 (96%)	3 (4%)	0	100	100
6	H	124/146 (85%)	107 (86%)	15 (12%)	2 (2%)	9	34
7	I	113/122 (93%)	100 (88%)	13 (12%)	0	100	100
8	J	63/70 (90%)	58 (92%)	5 (8%)	0	100	100
9	K	112/120 (93%)	108 (96%)	3 (3%)	1 (1%)	17	49
10	L	42/70 (60%)	34 (81%)	6 (14%)	2 (5%)	2	15
All	All	3446/4173 (83%)	3169 (92%)	246 (7%)	31 (1%)	17	49

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
1	A	322	VAL
1	A	110	CYS
1	A	1437	GLY
2	B	468	GLU
2	B	1046	PRO
4	E	86	PRO
2	B	337	ARG
2	B	884	ARG
2	B	1017	ILE
3	C	90	ASP
3	C	148	ARG
10	L	69	ALA
1	A	40	THR
1	A	282	ASN
2	B	277	LYS
2	B	1108	ARG
9	K	26	LYS
10	L	41	SER
1	A	226	GLU
1	A	958	VAL
1	A	1156	PRO
1	A	1279	ILE
6	H	82	PRO
1	A	69	THR
1	A	592	ASP

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Mol	Chain	Res	Type
1	A	597	LEU
2	B	260	GLY
6	H	18	GLY
2	B	824	ILE
1	A	1107	VAL

### 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	1196/1520 (79%)	1147 (96%)	49 (4%)	30	59
2	B	952/1061 (90%)	922 (97%)	30 (3%)	39	67
3	C	234/274 (85%)	228 (97%)	6 (3%)	46	72
4	E	195/197 (99%)	188 (96%)	7 (4%)	35	63
5	F	74/137 (54%)	71 (96%)	3 (4%)	30	59
6	H	114/128 (89%)	112 (98%)	2 (2%)	59	79
7	I	109/116 (94%)	107 (98%)	2 (2%)	59	79
8	J	60/65 (92%)	59 (98%)	1 (2%)	60	80
9	K	99/102 (97%)	98 (99%)	1 (1%)	76	88
10	L	39/57 (68%)	39 (100%)	0	100	100
All	All	3072/3657 (84%)	2971 (97%)	101 (3%)	38	66

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	12	ARG
1	A	22	PHE
1	A	34	LYS
1	A	93	VAL
1	A	132	LYS
1	A	179	LEU
1	A	222	LEU

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Mol	Chain	Res	Type
1	A	270	LEU
1	A	287	HIS
1	A	308	ILE
1	A	322	VAL
1	A	326	ARG
1	A	335	ARG
1	A	351	THR
1	A	434	ARG
1	A	443	LEU
1	A	444	PHE
1	A	451	HIS
1	A	452	LYS
1	A	474	VAL
1	A	481	ASP
1	A	532	ARG
1	A	605	MET
1	A	612	ILE
1	A	618	GLU
1	A	666	ILE
1	A	702	LEU
1	A	764	CYS
1	A	774	ARG
1	A	780	VAL
1	A	826	ASP
1	A	896	ARG
1	A	926	GLN
1	A	1017	LEU
1	A	1025	ARG
1	A	1078	GLN
1	A	1116	LEU
1	A	1207	LEU
1	A	1231	ASP
1	A	1262	LYS
1	A	1297	GLU
1	A	1322	ILE
1	A	1329	THR
1	A	1334	ASP
1	A	1374	VAL
1	A	1377	THR
1	A	1400	CYS
1	A	1407	GLU
2	B	46	GLN

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Mol	Chain	Res	Type
2	B	90	ILE
2	B	109	THR
2	B	134	LYS
2	B	319	GLU
2	B	364	ILE
2	B	365	THR
2	B	396	ASP
2	B	483	LEU
2	B	547	VAL
2	B	549	THR
2	B	570	VAL
2	B	628	THR
2	B	737	THR
2	B	797	TYR
2	B	825	VAL
2	B	839	MET
2	B	868	MET
2	B	916	THR
2	B	931	TYR
2	B	983	ARG
2	B	1007	VAL
2	B	1051	THR
2	B	1099	VAL
2	B	1147	LEU
2	B	1159	ARG
2	B	1176	ASN
2	B	1188	LYS
2	B	1194	ILE
2	B	1202	LEU
3	C	18	VAL
3	C	25	VAL
3	C	77	ILE
3	C	99	LEU
3	C	137	LYS
3	C	240	VAL
4	E	3	GLN
4	E	98	ILE
4	E	110	PHE
4	E	123	LEU
4	E	127	ILE
4	E	169	ARG
4	E	204	THR

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Mol	Chain	Res	Type
5	F	93	ILE
5	F	97	ARG
5	F	155	LEU
6	H	89	LEU
6	H	124	ARG
7	I	14	LEU
7	I	111	THR
8	J	5	VAL
9	K	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	742	ASN
2	B	762	ASN
2	B	984	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	R	8/9 (88%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
11	3DR	T	20	11	8,11,12	1.46	1 (12%)	9,14,17	1.06	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	3DR	T	20	11	-	1/3/15/16	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	20	3DR	O4'-C4'	-2.66	1.40	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	20	3DR	O4'-C4'-C3'	2.27	107.06	103.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	T	20	3DR	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	1372/1733 (79%)	0.14	57 (4%) 36 35	13, 57, 149, 257	0
2	B	1097/1224 (89%)	-0.06	16 (1%) 73 72	11, 45, 111, 194	0
3	C	266/318 (83%)	-0.23	0 100 100	18, 46, 89, 158	0
4	E	213/215 (99%)	0.42	17 (7%) 12 13	31, 82, 157, 206	0
5	F	84/155 (54%)	-0.15	0 100 100	27, 60, 104, 162	0
6	H	130/146 (89%)	0.09	2 (1%) 73 72	35, 80, 141, 196	0
7	I	115/122 (94%)	-0.04	0 100 100	24, 59, 99, 112	0
8	J	65/70 (92%)	-0.42	1 (1%) 73 72	19, 35, 72, 146	0
9	K	114/120 (95%)	-0.17	0 100 100	22, 51, 86, 115	0
10	L	44/70 (62%)	0.20	1 (2%) 60 59	25, 89, 158, 208	0
11	T	11/29 (37%)	1.07	3 (27%) 0 0	107, 128, 181, 183	0
12	R	9/9 (100%)	0.77	0 100 100	82, 102, 140, 147	0
All	All	3520/4211 (83%)	0.04	97 (2%) 53 51	11, 54, 138, 257	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	THR	7.3
4	E	93	MET	6.0
1	A	183	GLY	5.5
1	A	69	THR	5.4
1	A	45	GLN	4.8
1	A	182	VAL	4.8
2	B	474	SER	4.8
10	L	45	ALA	4.7
1	A	49	LYS	4.7
1	A	147	VAL	4.3
2	B	643	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	868	MET	4.0
1	A	1126	ALA	4.0
1	A	250	ILE	3.9
4	E	125	PRO	3.8
1	A	73	GLY	3.8
1	A	174	ILE	3.7
1	A	177	ASP	3.6
4	E	126	SER	3.5
1	A	286	HIS	3.5
4	E	123	LEU	3.4
11	T	19	DA	3.3
1	A	289	ILE	3.3
4	E	110	PHE	3.3
1	A	65	LEU	3.3
4	E	98	ILE	3.2
1	A	209	ASN	3.1
1	A	312	PRO	3.1
1	A	105	CYS	3.1
2	B	1183	LYS	3.0
1	A	141	LEU	3.0
1	A	1256	GLU	3.0
2	B	929	THR	3.0
2	B	1189	ILE	3.0
1	A	180	LYS	2.9
1	A	47	ARG	2.9
1	A	91	PHE	2.8
4	E	83	CYS	2.8
4	E	85	GLU	2.8
6	H	139	ASN	2.8
1	A	84	ILE	2.8
4	E	9	ILE	2.8
1	A	293	GLU	2.8
2	B	432	MET	2.8
2	B	647	GLY	2.7
1	A	285	PRO	2.7
1	A	317	LYS	2.7
1	A	171	GLN	2.7
2	B	867	GLY	2.6
1	A	86	LEU	2.6
1	A	270	LEU	2.6
1	A	181	LEU	2.6
1	A	148	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	146	MET	2.6
8	J	65	PRO	2.5
1	A	85	ASP	2.5
1	A	1232	ASN	2.5
1	A	56	PRO	2.5
2	B	472	ALA	2.5
2	B	869	SER	2.5
2	B	275	TYR	2.4
4	E	116	ILE	2.4
1	A	179	LEU	2.4
1	A	87	ALA	2.4
1	A	175	ARG	2.4
1	A	290	GLU	2.4
1	A	1255	GLU	2.4
4	E	49	SER	2.3
4	E	82	PHE	2.3
2	B	476	ARG	2.3
1	A	103	CYS	2.3
1	A	1124	HIS	2.3
1	A	213	HIS	2.3
2	B	262	GLU	2.3
1	A	66	LYS	2.2
1	A	72	GLU	2.2
1	A	50	ILE	2.2
4	E	16	PHE	2.2
11	T	18	DC	2.2
1	A	35	ILE	2.2
1	A	201	VAL	2.2
1	A	247	ARG	2.2
1	A	37	PHE	2.2
6	H	86	ASP	2.2
4	E	88	VAL	2.1
11	T	29	DG	2.1
4	E	50	MET	2.1
1	A	1080	THR	2.1
2	B	263	GLY	2.1
1	A	57	ARG	2.1
2	B	865	LYS	2.1
4	E	94	LYS	2.0
1	A	39	GLU	2.0
1	A	48	ALA	2.0
1	A	266	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	3	GLY	2.0
4	E	89	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
11	3DR	T	20	11/12	0.85	0.27	136,143,151,154	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
13	ZN	A	1801	1/1	0.90	0.07	132,132,132,132	0
13	ZN	A	1802	1/1	0.94	0.10	82,82,82,82	0
13	ZN	I	202	1/1	0.98	0.12	28,28,28,28	0
13	ZN	B	1301	1/1	0.98	0.07	79,79,79,79	0
14	MG	A	1803	1/1	0.98	0.31	10,10,10,10	0
13	ZN	I	201	1/1	0.99	0.12	43,43,43,43	0
13	ZN	C	401	1/1	0.99	0.12	36,36,36,36	0
13	ZN	L	101	1/1	0.99	0.07	83,83,83,83	0
13	ZN	J	101	1/1	0.99	0.13	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.