



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:17 PM GMT

PDB ID : 4BXX
Title : Structures of RNA polymerase II complexes with Bye1, a chromatin- binding PHF3 DIDO homologue
Authors : Kinkelin, K.; Wozniak, G.G.; Rothbart, S.B.; Lidschreiber, M.; Strahl, B.D.; Cramer, P.
Deposited on : 2013-07-16
Resolution : 3.28 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

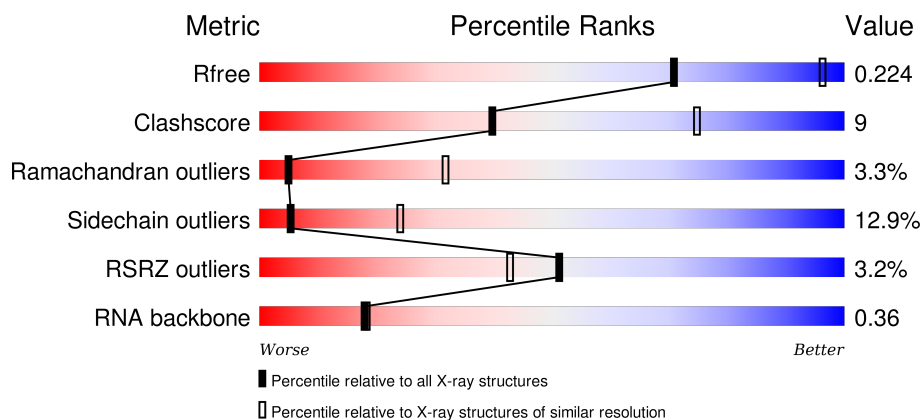
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1756 (3.36-3.20)
Clashscore	102246	1941 (3.36-3.20)
Ramachandran outliers	100387	1905 (3.36-3.20)
Sidechain outliers	100360	1903 (3.36-3.20)
RSRZ outliers	91569	1764 (3.36-3.20)
RNA backbone	2183	1022 (3.80-2.76)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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> <div>2%</div> <div>57%</div> <div>21%</div> <div>•</div> <div>18%</div> </div> </div>
2	B	1224	<div> <div>2%</div> <div>63%</div> <div>24%</div> <div>•</div> <div>10%</div> </div>
3	C	318	<div> <div>59%</div> <div>20%</div> <div>•</div> <div>16%</div> </div>
4	D	221	<div> <div>59%</div> <div>18%</div> <div>•</div> <div>20%</div> </div>

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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	N	14	
14	P	11	
15	T	27	
16	X	146	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 32756 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	1429	Total	C	N	O	S	0	0	0
			11249	7087	1964	2136	62			

- 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
			8720	5526	1523	1617	54			

- 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	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

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
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

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 I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called 5'-D(*GP*AP*GP*GP*TP*AP*AP*GP*CP*TP*AP*

GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	10	Total	C	N	O	P	0	0	0
			209	99	42	58	10			

- Molecule 14 is a RNA chain called 5'-D(*CP*CP*CP*CP*CP*CP*CP*CP*CP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	11	Total	C	N	O	P	0	0	0
			220	99	33	77	11			

- Molecule 15 is a DNA chain called 5'-D(*AP*GP*CP*TP*AP*GP*CP*TP*TP*AP*CP*CP*TP*GP *GP*TP*GP* BRUP*TP*GP*CP*TP*CP*TP*AP*AP*DC)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	14	Total	Br	C	N	O	P	0	0
			287	1	136	49	87	14		

- Molecule 16 is a protein called TRANSCRIPTION FACTOR BYE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	X	120	Total	C	N	O	S	0	0	0
			986	634	164	185	3			

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

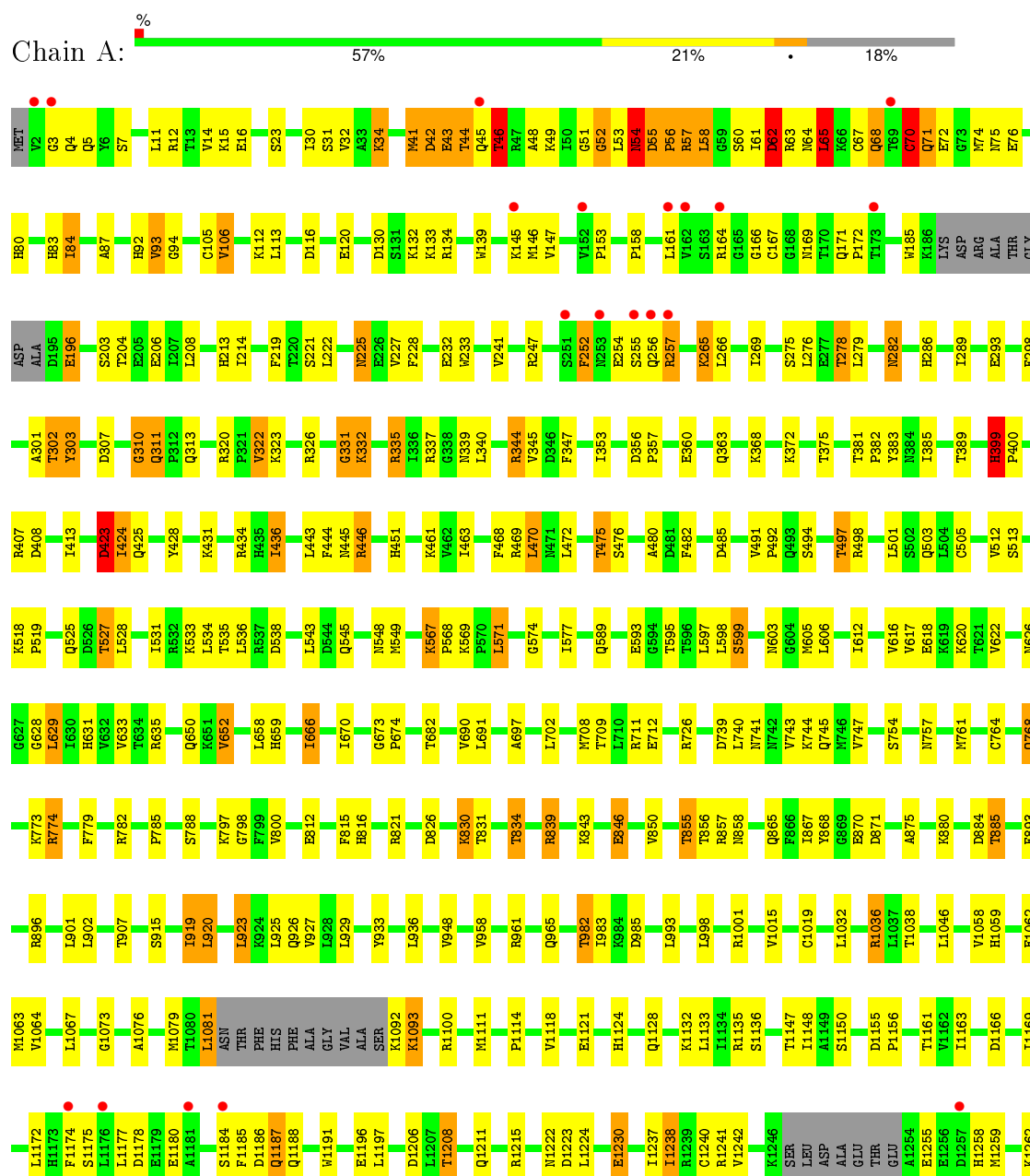
- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

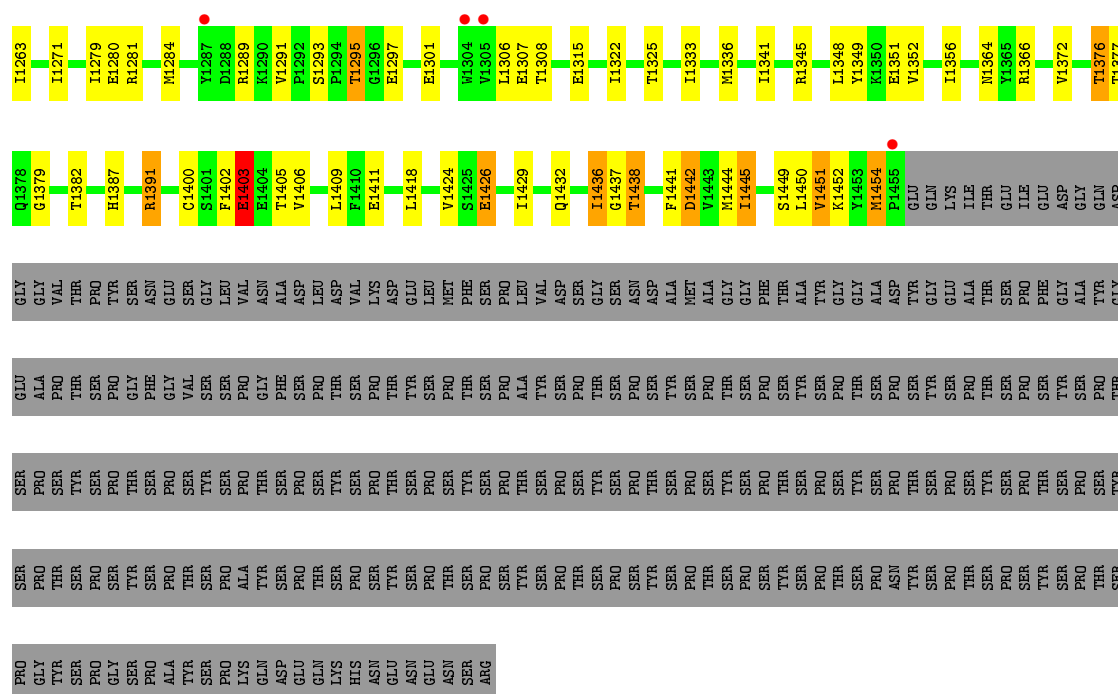
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

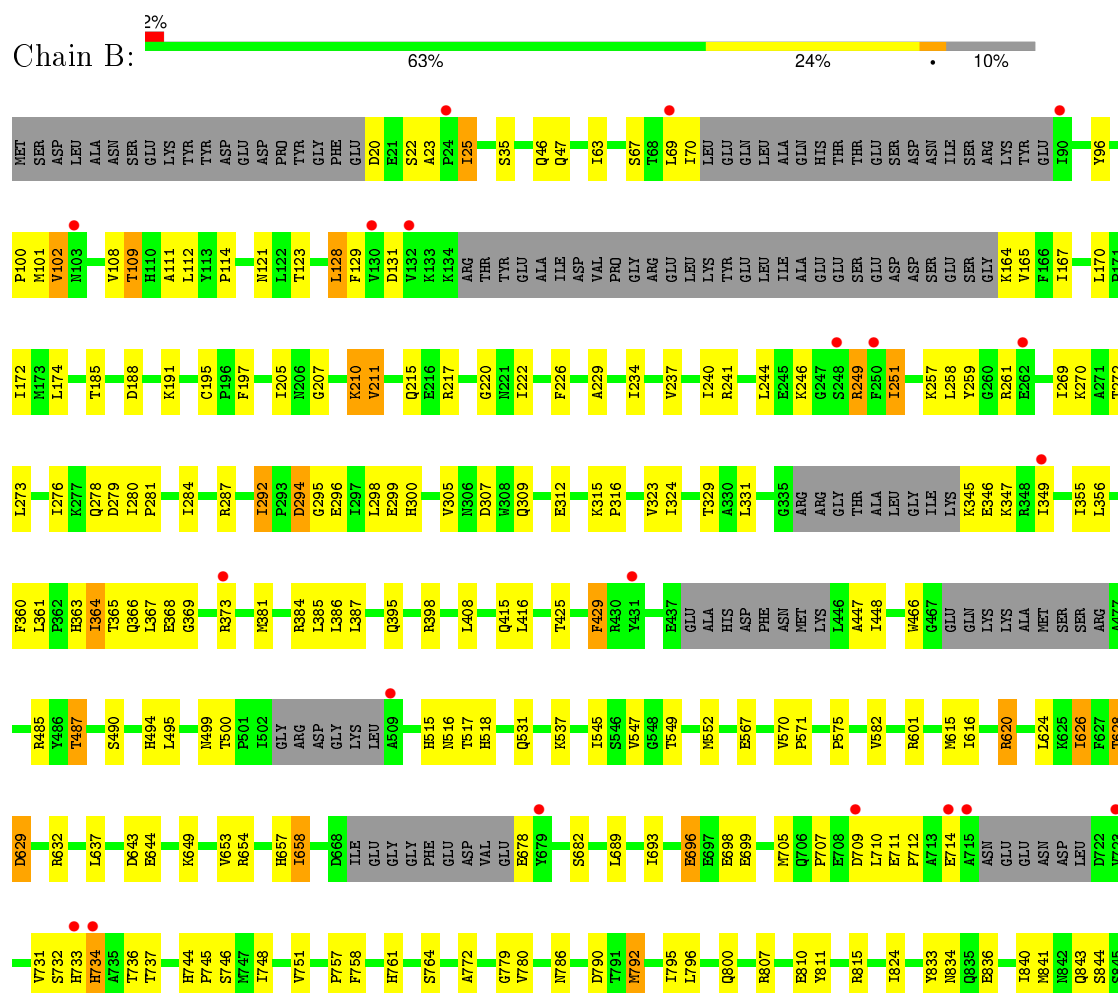
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

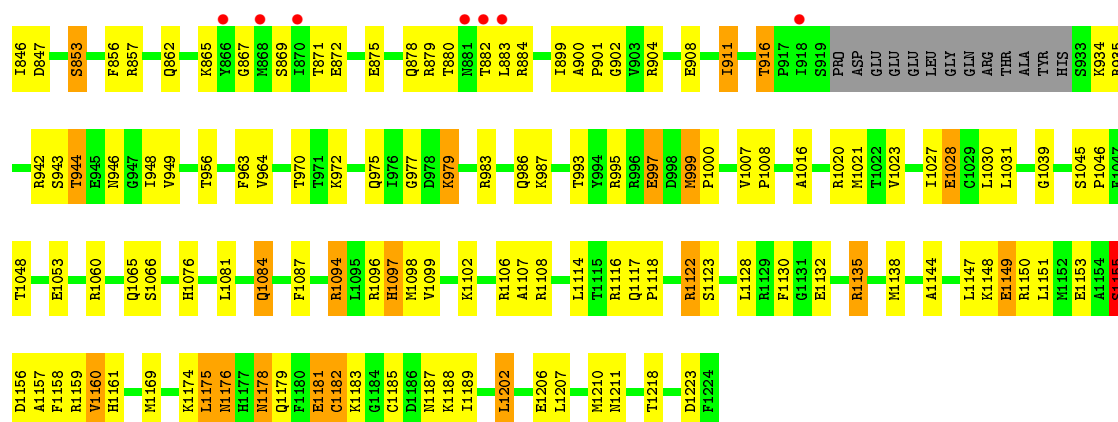
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1



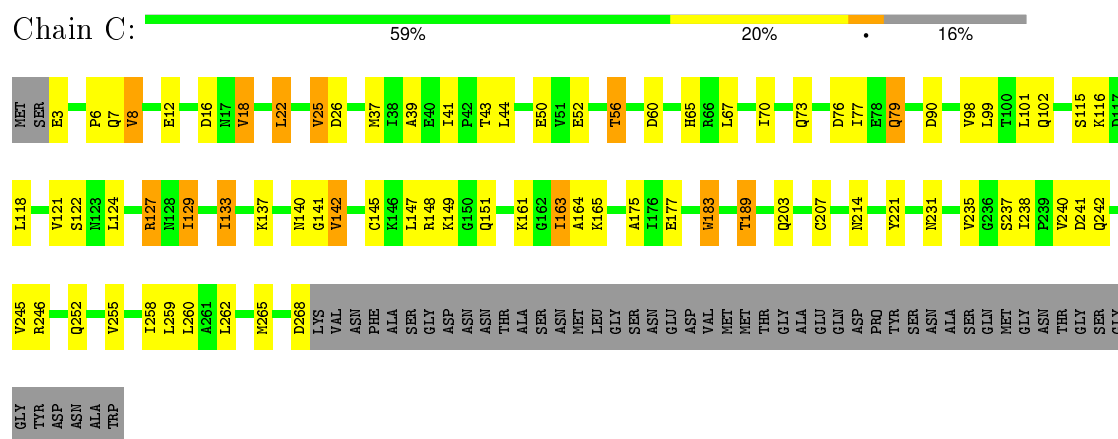


• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

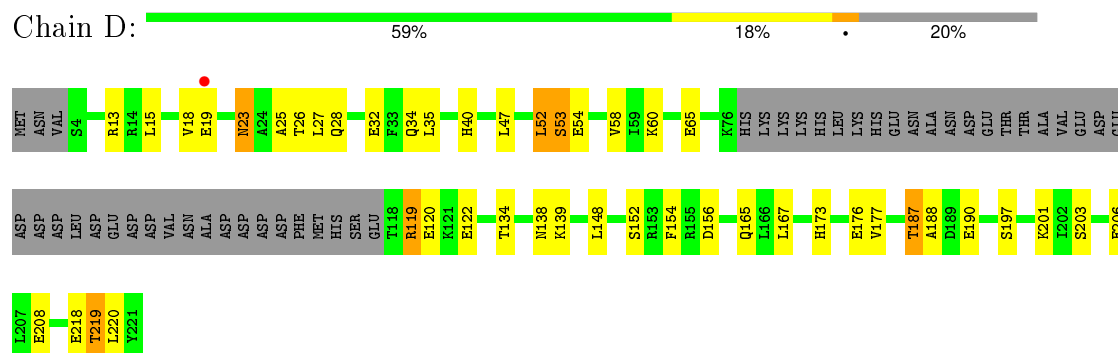




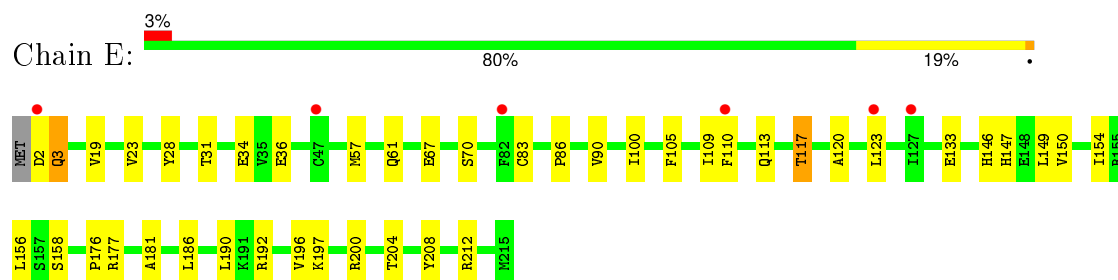
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3



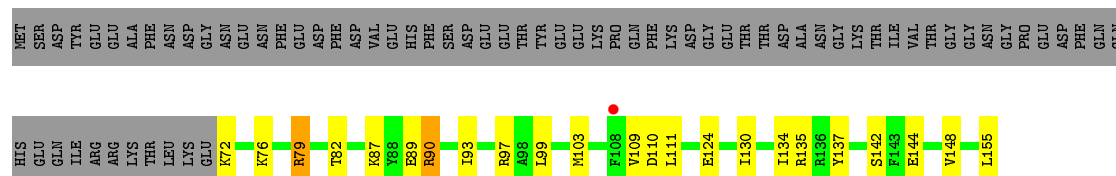
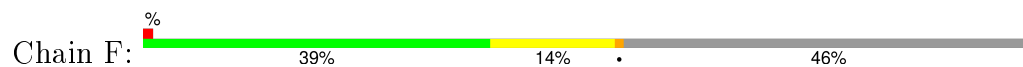
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4



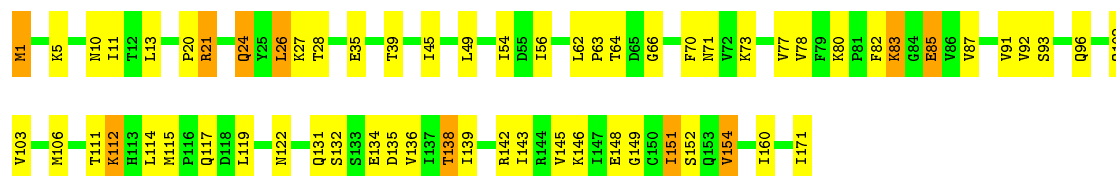
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



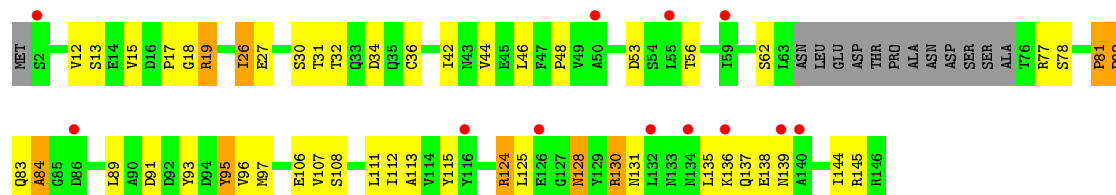
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2



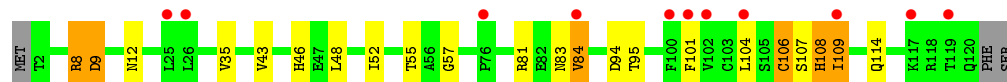
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7



• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3



• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

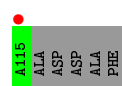


• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

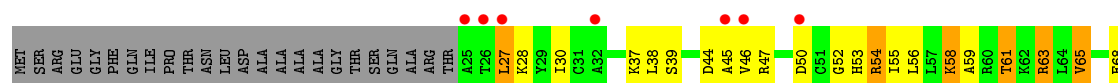
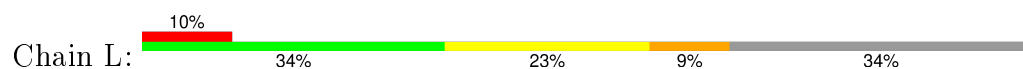


• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

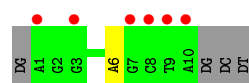
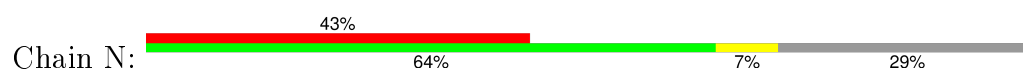




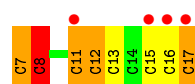
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



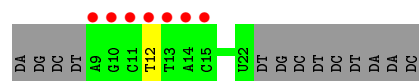
- Molecule 13: 5'-D(*GP*AP*GP*GP*TP*AP*AP*GP*CP*TP*AP*GP*CP*TP)-3'



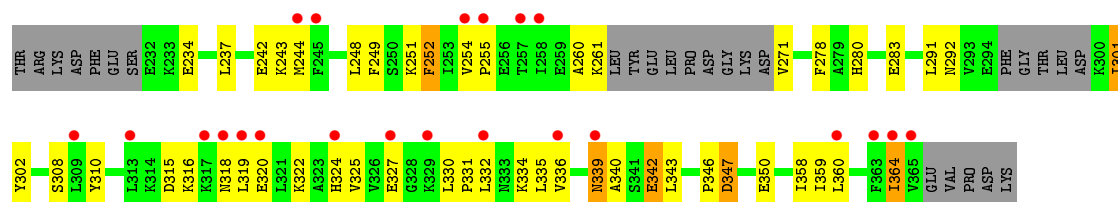
- Molecule 14: 5'-D(*CP*CP*CP*CP*CP*CP*CP*CP*CP*CP)-3'



- Molecule 15: 5'-D(*AP*GP*CP*TP*AP*GP*CP*TP*TP*AP*CP*CP*TP*GP *GP*TP*GP*BRUP*TP*GP*CP*TP*CP*TP*AP*AP*DC)-3'



- Molecule 16: TRANSCRIPTION FACTOR BYE1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.92Å 392.67Å 281.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 3.28 49.08 – 3.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.08-3.28) 100.0 (49.08-3.28)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.180 , 0.208 0.200 , 0.224	Depositor DCC
R_{free} test set	3698 reflections (2.02%)	DCC
Wilson B-factor (Å ²)	98.3	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 100.9	EDS
Estimated twinning fraction	0.012 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.018 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 187168 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32756	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ZN, BRU

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	0.54	0/11450	0.82	10/15483 (0.1%)
2	B	0.51	0/8889	0.77	3/11987 (0.0%)
3	C	0.50	0/2133	0.79	1/2891 (0.0%)
4	D	0.53	0/1365	0.84	2/1837 (0.1%)
5	E	0.45	0/1788	0.67	0/2406
6	F	0.60	0/691	0.78	0/933
7	G	0.53	0/1368	0.82	1/1844 (0.1%)
8	H	0.49	0/1086	0.76	0/1470
9	I	0.45	0/989	0.72	0/1331
10	J	0.54	0/541	0.82	0/727
11	K	0.48	0/938	0.70	0/1267
12	L	0.56	0/365	0.90	0/485
13	N	0.99	0/235	0.89	0/361
14	P	1.59	5/241 (2.1%)	1.04	0/370
15	T	1.27	0/298	0.99	0/458
16	X	0.50	0/999	0.75	0/1336
All	All	0.55	5/33376 (0.0%)	0.79	17/45186 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	17	C	C1'-N1	5.93	1.57	1.48
14	P	15	C	C1'-N1	5.59	1.57	1.48
14	P	11	C	C3'-O3'	5.20	1.49	1.42
14	P	8	C	C1'-N1	5.16	1.56	1.48
14	P	7	C	C1'-N1	5.16	1.56	1.48

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	GLY	C-N-CA	8.18	142.14	121.70
4	D	25	ALA	C-N-CA	7.72	141.00	121.70
1	A	56	PRO	C-N-CA	6.95	139.07	121.70
1	A	399	HIS	N-CA-CB	6.93	123.07	110.60
1	A	54	ASN	C-N-CA	6.55	138.09	121.70
1	A	43	GLU	C-N-CA	6.18	137.15	121.70
2	B	628	THR	C-N-CA	6.10	136.96	121.70
2	B	1130	PHE	N-CA-C	-5.88	95.12	111.00
1	A	55	ASP	N-CA-CB	5.85	121.12	110.60
1	A	1403	GLU	C-N-CA	-5.64	107.61	121.70
1	A	331	GLY	N-CA-C	5.47	126.79	113.10
3	C	183	TRP	N-CA-C	-5.45	96.28	111.00
1	A	310	GLY	C-N-CA	5.31	134.97	121.70
4	D	26	THR	N-CA-C	-5.23	96.89	111.00
1	A	451	HIS	CB-CA-C	-5.21	99.97	110.40
2	B	1155	SER	C-N-CA	5.18	134.65	121.70
7	G	154	VAL	C-N-CA	5.06	134.36	121.70

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	11249	0	11312	256	0
2	B	8720	0	8744	151	0
3	C	2095	0	2051	40	0
4	D	1356	0	1319	20	0
5	E	1752	0	1776	21	0
6	F	679	0	701	19	0
7	G	1340	0	1357	40	0
8	H	1068	0	1040	31	0
9	I	971	0	927	13	0
10	J	532	0	542	13	0
11	K	920	0	929	20	0
12	L	363	0	386	10	0
13	N	209	0	113	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	P	220	0	122	2	0
15	T	287	0	157	1	0
16	X	986	0	1009	18	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	32756	0	32485	571	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 9.

All (571) 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:867:ILE:CD1	1:A:867:ILE:CG1	1.81	1.55
1:A:53:LEU:HD23	1:A:54:ASN:H	1.06	1.10
1:A:567:LYS:HB3	8:H:96:VAL:H	1.21	1.03
1:A:855:THR:HG21	1:A:857:ARG:HE	1.22	1.02
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.39	1.01
4:D:53:SER:HB3	4:D:152:SER:HB2	1.45	0.95
1:A:567:LYS:HD2	1:A:568:PRO:HD3	1.47	0.94
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.15	0.92
2:B:705:MET:H	2:B:710:LEU:HD12	1.35	0.90
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.53	0.89
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.56	0.88
1:A:53:LEU:HD23	1:A:54:ASN:N	1.89	0.86
8:H:95:TYR:HE1	8:H:97:MET:HG3	1.40	0.86
1:A:567:LYS:HB3	8:H:96:VAL:N	1.92	0.84
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.59	0.83
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.44	0.82
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.60	0.81
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.61	0.81
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.63	0.81
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.62	0.80
1:A:567:LYS:CD	1:A:568:PRO:HD3	2.12	0.79
2:B:654:ARG:H	2:B:657:HIS:HD2	1.30	0.78
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ASP:HB3	1:A:64:ASN:HD22	1.47	0.77
10:J:48:ARG:HE	10:J:49:MET:HE2	1.48	0.77
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.65	0.77
3:C:142:VAL:H	10:J:16:ASP:HB3	1.50	0.76
16:X:248:LEU:O	16:X:252:PHE:HB3	1.85	0.76
16:X:316:LYS:HG2	16:X:320:GLU:HB3	1.68	0.76
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.68	0.75
1:A:53:LEU:CD2	1:A:54:ASN:H	1.96	0.75
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.67	0.75
7:G:26:LEU:HD13	7:G:56:ILE:HD11	1.69	0.75
4:D:53:SER:HB3	4:D:152:SER:CB	2.18	0.73
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.71	0.72
1:A:43:GLU:HB2	1:A:46:THR:HB	1.69	0.72
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.72	0.72
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.71	0.72
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.72	0.72
1:A:265:LYS:HG2	1:A:303:TYR:HB2	1.71	0.72
1:A:61:ILE:HG22	1:A:62:ASP:H	1.53	0.71
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.72	0.71
8:H:95:TYR:CE1	8:H:97:MET:HG3	2.25	0.71
2:B:800:GLN:HB3	10:J:52:THR:HG23	1.71	0.71
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.26	0.71
1:A:347:PHE:H	2:B:1107:ALA:HA	1.57	0.70
2:B:744:HIS:HD2	2:B:746:SER:H	1.36	0.70
10:J:48:ARG:O	10:J:52:THR:HG22	1.91	0.69
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.74	0.69
1:A:34:LYS:HZ1	1:A:57:ARG:HH12	1.40	0.69
7:G:1:MET:CE	7:G:80:LYS:O	2.40	0.69
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.28	0.69
1:A:754:SER:H	1:A:757:ASN:HD22	1.41	0.68
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.23	0.68
1:A:626:ASN:O	1:A:631:HIS:HD2	1.76	0.68
1:A:41:MET:HB2	1:A:49:LYS:HA	1.74	0.68
1:A:535:THR:HG21	1:A:617:VAL:H	1.58	0.68
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	1.94	0.68
1:A:255:SER:H	2:B:935:ARG:HH22	1.42	0.68
1:A:741:ASN:HD22	1:A:744:LYS:H	1.42	0.68
1:A:907:THR:HG21	1:A:920:LEU:HD12	1.76	0.67
2:B:900:ALA:HB3	12:L:61:THR:HG23	1.75	0.67
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.77	0.67
1:A:52:GLY:H	1:A:56:PRO:HB3	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.77	0.66
1:A:626:ASN:O	1:A:631:HIS:CD2	2.49	0.66
2:B:872:GLU:HG2	2:B:916:THR:HG23	1.78	0.65
1:A:534:LEU:O	1:A:574:GLY:HA3	1.97	0.65
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.79	0.64
2:B:408:LEU:HD21	2:B:545:ILE:HD13	1.77	0.64
2:B:853:SER:HB3	2:B:1094:ARG:HH11	1.63	0.64
6:F:76:LYS:HA	6:F:79:ARG:CD	2.28	0.64
1:A:527:THR:HG21	1:A:650:GLN:HA	1.80	0.64
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.94	0.63
1:A:203:SER:OG	1:A:206:GLU:HB2	1.98	0.63
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.63	0.63
16:X:322:LYS:HD2	16:X:346:PRO:HD3	1.80	0.63
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.63	0.63
12:L:61:THR:HB	12:L:63:ARG:HG3	1.81	0.63
7:G:138:THR:HG22	7:G:139:ILE:H	1.63	0.62
1:A:503:GLN:NE2	6:F:90:ARG:HH21	1.97	0.62
7:G:151:ILE:HD11	7:G:160:ILE:HD11	1.81	0.62
7:G:21:ARG:NH1	7:G:24:GLN:H	1.98	0.62
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.82	0.62
6:F:99:LEU:O	6:F:103:MET:HG2	2.00	0.62
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.81	0.62
1:A:52:GLY:N	1:A:56:PRO:HB3	2.14	0.61
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.82	0.61
1:A:1451:VAL:O	1:A:1454:MET:HG3	2.00	0.61
16:X:339:ASN:HA	16:X:343:LEU:HD11	1.83	0.61
1:A:75:ASN:HA	2:B:1116:ARG:HH12	1.63	0.61
4:D:187:THR:HB	4:D:190:GLU:H	1.65	0.61
1:A:658:LEU:HD23	1:A:659:HIS:CE1	2.35	0.61
7:G:1:MET:HE3	7:G:80:LYS:O	2.01	0.60
1:A:1148:ILE:HD12	1:A:1196:GLU:HG2	1.83	0.60
1:A:528:LEU:O	1:A:531:ILE:HG22	2.01	0.60
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.47	0.60
2:B:47:GLN:HE21	2:B:408:LEU:HD12	1.66	0.60
1:A:901:LEU:HA	1:A:907:THR:HG23	1.83	0.60
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.82	0.60
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.83	0.60
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.84	0.60
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.32	0.60
8:H:91:ASP:C	8:H:93:TYR:H	2.05	0.60
1:A:497:THR:HG21	2:B:1149:GLU:OE2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ASP:C	1:A:44:THR:H	2.05	0.59
1:A:1128:GLN:HE21	1:A:1132:LYS:HE2	1.67	0.59
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.68	0.59
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.17	0.59
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.65	0.59
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.85	0.59
2:B:363:HIS:O	2:B:364:ILE:HB	2.02	0.59
2:B:234:ILE:HG21	2:B:237:VAL:HG23	1.84	0.59
5:E:147:HIS:CD2	5:E:149:LEU:H	2.20	0.59
7:G:112:LYS:HE2	7:G:112:LYS:O	2.02	0.59
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.02	0.59
1:A:57:ARG:O	1:A:68:GLN:HG2	2.02	0.59
1:A:492:PRO:HB2	1:A:497:THR:HG23	1.84	0.59
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.84	0.59
2:B:637:LEU:HD12	2:B:693:ILE:HD13	1.83	0.59
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.84	0.59
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.67	0.58
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.86	0.58
4:D:119:ARG:HH21	4:D:120:GLU:HB2	1.67	0.58
2:B:902:GLY:O	12:L:65:VAL:HG11	2.04	0.58
1:A:55:ASP:HA	1:A:58:LEU:H	1.68	0.58
1:A:1333:ILE:H	1:A:1333:ILE:HD12	1.68	0.58
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.86	0.58
2:B:862:GLN:HG3	2:B:963:PHE:HD1	1.68	0.58
12:L:28:LYS:HB2	12:L:39:SER:HA	1.84	0.58
7:G:83:LYS:HD2	7:G:149:GLY:HA2	1.86	0.58
1:A:1230:GLU:OE1	16:X:308:SER:HA	2.04	0.57
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.86	0.57
1:A:933:TYR:HA	1:A:936:LEU:HD12	1.85	0.57
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.85	0.57
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.87	0.57
1:A:709:THR:HG23	9:I:94:ASP:HA	1.87	0.57
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.86	0.57
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.51	0.57
1:A:1185:PHE:C	1:A:1187:GLN:H	2.07	0.56
2:B:20:ASP:HB2	2:B:23:ALA:HB2	1.87	0.56
1:A:92:HIS:HD2	1:A:94:GLY:H	1.52	0.56
1:A:34:LYS:HZ2	1:A:57:ARG:NH2	2.02	0.56
1:A:34:LYS:HZ2	1:A:57:ARG:HH22	1.51	0.56
7:G:1:MET:HE1	7:G:80:LYS:O	2.05	0.56
2:B:276:ILE:HD11	2:B:355:ILE:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.87	0.56
1:A:265:LYS:CG	1:A:303:TYR:HB2	2.36	0.56
1:A:535:THR:HG21	1:A:616:VAL:HA	1.86	0.56
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.85	0.56
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.87	0.56
1:A:55:ASP:N	1:A:56:PRO:HD3	2.21	0.56
12:L:27:LEU:HD13	12:L:37:LYS:HG2	1.88	0.56
7:G:10:ASN:ND2	7:G:71:ASN:HD22	2.03	0.56
1:A:1377:THR:HG22	5:E:176:PRO:HB3	1.87	0.56
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.88	0.56
6:F:93:ILE:CD1	6:F:134:ILE:HD11	2.26	0.56
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.06	0.55
8:H:15:VAL:HG22	8:H:26:ILE:HG13	1.88	0.55
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.05	0.55
1:A:1177:LEU:HD21	16:X:237:LEU:HA	1.88	0.55
1:A:353:ILE:HD12	1:A:482:PHE:HD1	1.70	0.55
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.41	0.55
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.89	0.55
2:B:244:LEU:HD21	2:B:366:GLN:HE22	1.71	0.55
1:A:1184:SER:C	1:A:1186:ASP:H	2.08	0.55
1:A:567:LYS:CB	8:H:96:VAL:H	2.06	0.55
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.35	0.55
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.87	0.55
1:A:855:THR:CG2	1:A:857:ARG:HE	2.08	0.55
3:C:98:VAL:H	3:C:122:SER:HB3	1.71	0.55
1:A:885:THR:HG22	1:A:893:PHE:HE2	1.71	0.54
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.90	0.54
2:B:620:ARG:HG3	9:I:57:GLY:HA3	1.89	0.54
2:B:323:VAL:HG23	2:B:324:ILE:HD12	1.89	0.54
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.89	0.54
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.90	0.54
1:A:65:LEU:HD23	1:A:71:GLN:HB2	1.89	0.54
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.90	0.54
2:B:705:MET:N	2:B:710:LEU:HD12	2.14	0.54
1:A:743:VAL:O	1:A:747:VAL:HG23	2.08	0.54
1:A:709:THR:HB	1:A:712:GLU:H	1.73	0.54
3:C:252:GLN:HG2	11:K:95:ILE:HG23	1.90	0.54
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.89	0.54
1:A:252:PHE:HD2	1:A:256:GLN:HB3	1.73	0.54
1:A:708:MET:HG2	1:A:712:GLU:HB3	1.89	0.54
2:B:1158:PHE:CE2	2:B:1160:VAL:HG13	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:47:ARG:HG3	12:L:54:ARG:HG3	1.89	0.54
1:A:1387:HIS:O	1:A:1391:ARG:HG2	2.07	0.53
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.90	0.53
1:A:571:LEU:HD22	8:H:46:LEU:HD11	1.89	0.53
2:B:654:ARG:H	2:B:657:HIS:CD2	2.19	0.53
2:B:732:SER:HB2	2:B:734:HIS:CE1	2.44	0.53
1:A:219:PHE:HA	1:A:222:LEU:HD12	1.90	0.53
1:A:761:MET:HG3	2:B:1021:MET:HG2	1.91	0.53
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.90	0.53
1:A:494:SER:H	1:A:497:THR:HG22	1.73	0.53
2:B:35:SER:HA	2:B:811:TYR:HE1	1.73	0.53
2:B:882:THR:HG22	2:B:884:ARG:H	1.74	0.53
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.35	0.53
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.90	0.53
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.74	0.53
1:A:298:PHE:O	1:A:302:THR:HB	2.08	0.53
4:D:52:LEU:HB3	4:D:148:LEU:CD2	2.39	0.53
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.89	0.53
4:D:32:GLU:O	7:G:5:LYS:HE2	2.08	0.53
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.91	0.53
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.90	0.53
16:X:234:GLU:HA	16:X:237:LEU:HD12	1.91	0.52
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.90	0.52
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.91	0.52
2:B:899:ILE:HD12	2:B:911:ILE:HA	1.90	0.52
4:D:167:LEU:HB3	4:D:177:VAL:HG13	1.90	0.52
2:B:705:MET:H	2:B:710:LEU:CD1	2.16	0.52
1:A:134:ARG:HD2	1:A:221:SER:O	2.09	0.52
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.90	0.52
12:L:27:LEU:HB3	12:L:37:LYS:HD3	1.90	0.52
1:A:856:THR:HB	1:A:865:GLN:HB2	1.92	0.52
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.91	0.52
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.95	0.52
1:A:535:THR:CG2	1:A:616:VAL:HA	2.40	0.52
2:B:234:ILE:HG12	2:B:257:LYS:HB3	1.91	0.52
1:A:55:ASP:O	1:A:55:ASP:OD2	2.28	0.51
1:A:923:LEU:O	1:A:927:VAL:HG23	2.11	0.51
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.91	0.51
1:A:709:THR:HG22	1:A:711:ARG:H	1.75	0.51
5:E:147:HIS:HD2	5:E:149:LEU:H	1.55	0.51
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:42:ILE:HG23	8:H:95:TYR:HE2	1.76	0.51
2:B:373:ARG:HH21	2:B:567:GLU:HG2	1.75	0.51
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.76	0.51
1:A:106:VAL:HG21	1:A:214:ILE:HG12	1.92	0.51
7:G:142:ARG:HB3	7:G:171:ILE:HD12	1.91	0.51
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.41	0.51
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.51	0.51
3:C:76:ASP:O	3:C:79:GLN:HG2	2.11	0.51
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.92	0.50
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.46	0.50
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.92	0.50
7:G:21:ARG:HD3	7:G:24:GLN:HB2	1.92	0.50
5:E:109:ILE:HG12	5:E:133:GLU:HB2	1.92	0.50
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.52	0.50
11:K:65:HIS:CD2	11:K:67:PHE:H	2.29	0.50
8:H:135:LEU:C	8:H:137:GLN:H	2.14	0.50
5:E:117:THR:HB	5:E:120:ALA:H	1.75	0.50
2:B:582:VAL:HG22	2:B:626:ILE:HD12	1.94	0.50
6:F:103:MET:HE2	7:G:66:GLY:H	1.77	0.50
1:A:353:ILE:HD12	1:A:482:PHE:CD1	2.46	0.50
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.93	0.50
1:A:62:ASP:HB3	1:A:64:ASN:ND2	2.23	0.50
3:C:18:VAL:O	3:C:231:ASN:HA	2.11	0.50
5:E:19:VAL:O	5:E:23:VAL:HG23	2.12	0.50
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.60	0.50
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.92	0.50
1:A:982:THR:HB	1:A:985:ASP:H	1.77	0.50
4:D:219:THR:HG23	4:D:220:LEU:H	1.76	0.50
2:B:114:PRO:HB3	2:B:174:LEU:HD21	1.93	0.50
1:A:1208:THR:HB	1:A:1211:GLN:H	1.77	0.50
1:A:41:MET:CB	1:A:49:LYS:HA	2.42	0.49
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.12	0.49
8:H:89:LEU:C	8:H:91:ASP:H	2.16	0.49
1:A:41:MET:O	1:A:42:ASP:C	2.50	0.49
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.94	0.49
4:D:40:HIS:CG	7:G:73:LYS:HZ1	2.30	0.49
2:B:1188:LYS:H	2:B:1189:ILE:HD12	1.77	0.49
3:C:255:VAL:HG21	11:K:94:ILE:HG21	1.94	0.49
1:A:816:HIS:HE2	2:B:764:SER:H	1.59	0.49
16:X:360:LEU:O	16:X:364:ILE:HB	2.13	0.49
1:A:629:LEU:O	1:A:633:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:ND2	1:A:228:PHE:H	2.10	0.49
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.47	0.49
7:G:91:VAL:CG2	7:G:143:ILE:HD12	2.43	0.49
1:A:1079:MET:HB3	1:A:1081:LEU:HD21	1.93	0.49
2:B:487:THR:HG22	2:B:490:SER:H	1.77	0.49
2:B:1096:ARG:O	2:B:1097:HIS:CG	2.66	0.49
2:B:295:GLY:H	2:B:298:LEU:HB2	1.78	0.49
2:B:515:HIS:H	2:B:518:HIS:CD2	2.31	0.49
1:A:1279:ILE:HG13	1:A:1308:THR:HG21	1.94	0.49
1:A:548:ASN:HD21	11:K:47:ARG:HE	1.60	0.49
3:C:148:ARG:HB3	3:C:151:GLN:HG3	1.95	0.49
8:H:82:PRO:C	8:H:84:ALA:H	2.15	0.48
1:A:535:THR:HG21	1:A:617:VAL:N	2.27	0.48
2:B:792:MET:HA	2:B:856:PHE:O	2.13	0.48
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.78	0.48
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.39	0.48
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.53	0.48
2:B:882:THR:HG1	2:B:935:ARG:N	2.12	0.48
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.97	0.48
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.95	0.48
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.96	0.48
16:X:249:PHE:HA	16:X:252:PHE:HD1	1.79	0.48
5:E:83:CYS:HB2	5:E:110:PHE:CZ	2.49	0.48
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.96	0.48
2:B:299:GLU:HG2	2:B:571:PRO:HG2	1.95	0.48
2:B:128:LEU:HD21	2:B:170:LEU:HB2	1.96	0.48
1:A:43:GLU:CD	1:A:48:ALA:HB3	2.34	0.48
2:B:515:HIS:CD2	2:B:517:THR:H	2.32	0.48
14:P:12:C:H5'	14:P:13:C:H5'	1.96	0.48
16:X:255:PRO:HG3	16:X:316:LYS:HD3	1.96	0.48
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.96	0.48
1:A:549:MET:HG2	1:A:652:VAL:HG22	1.96	0.48
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.78	0.48
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.96	0.48
1:A:494:SER:O	1:A:498:ARG:HG2	2.14	0.47
3:C:124:LEU:HD22	3:C:129:ILE:HG22	1.96	0.47
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.14	0.47
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.96	0.47
2:B:1158:PHE:HE2	2:B:1160:VAL:HG13	1.79	0.47
16:X:242:GLU:HB2	16:X:283:GLU:HG3	1.95	0.47
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:HIS:HE1	2:B:1210:MET:O	1.97	0.47
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.97	0.47
2:B:1023:VAL:HG12	2:B:1027:ILE:HD11	1.95	0.47
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.96	0.47
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.97	0.47
5:E:156:LEU:HD11	5:E:197:LYS:HB2	1.96	0.47
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.50	0.47
2:B:847:ASP:O	3:C:65:HIS:HE1	1.97	0.47
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.96	0.47
1:A:34:LYS:HZ1	1:A:57:ARG:NH1	2.09	0.47
7:G:112:LYS:HE3	7:G:119:LEU:O	2.15	0.47
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.97	0.47
1:A:225:ASN:HD22	1:A:227:VAL:H	1.62	0.47
1:A:1150:SER:H	9:I:46:HIS:HB3	1.79	0.47
7:G:87:VAL:HB	7:G:103:VAL:HG11	1.97	0.47
2:B:516:ASN:HD22	2:B:516:ASN:H	1.63	0.47
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.97	0.47
1:A:492:PRO:CB	1:A:497:THR:HG23	2.45	0.47
1:A:225:ASN:ND2	1:A:227:VAL:H	2.13	0.47
7:G:132:SER:HB3	7:G:135:ASP:H	1.79	0.47
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.28	0.46
2:B:841:MET:O	2:B:993:THR:HA	2.16	0.46
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.96	0.46
1:A:1454:MET:HG2	7:G:20:PRO:HB3	1.97	0.46
5:E:31:THR:HG23	5:E:34:GLU:H	1.80	0.46
2:B:70:ILE:HD13	2:B:429:PHE:HZ	1.78	0.46
1:A:925:LEU:HD22	1:A:983:ILE:HB	1.96	0.46
1:A:1449:SER:HA	1:A:1452:LYS:HG2	1.96	0.46
2:B:882:THR:HB	2:B:934:LYS:C	2.36	0.46
1:A:658:LEU:HD21	2:B:1076:HIS:CD2	2.50	0.46
1:A:1191:TRP:HZ3	9:I:43:VAL:HG21	1.80	0.46
1:A:482:PHE:CD2	2:B:836:GLU:HB2	2.51	0.46
7:G:91:VAL:HG23	7:G:143:ILE:HD12	1.97	0.46
7:G:82:PHE:O	7:G:85:GLU:HB2	2.14	0.46
7:G:1:MET:C	7:G:1:MET:SD	2.94	0.46
7:G:112:LYS:HA	7:G:115:MET:HE3	1.97	0.46
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.98	0.46
4:D:23:ASN:HA	4:D:28:GLN:O	2.16	0.46
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.48	0.46
1:A:1426:GLU:HG2	1:A:1426:GLU:H	1.42	0.46
16:X:325:VAL:HG12	16:X:330:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:219:THR:HG23	4:D:220:LEU:N	2.31	0.45
8:H:42:ILE:HG23	8:H:95:TYR:CE2	2.51	0.45
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.52	0.45
3:C:133:ILE:HD13	3:C:237:SER:HA	1.98	0.45
3:C:258:ILE:HD12	3:C:258:ILE:N	2.32	0.45
11:K:7:PHE:HB2	11:K:11:LEU:HD22	1.98	0.45
3:C:37:MET:HA	3:C:41:ILE:HD12	1.98	0.45
1:A:785:PRO:HG3	2:B:698:GLU:HG2	1.98	0.45
2:B:259:TYR:HE2	2:B:270:LYS:HB2	1.80	0.45
2:B:745:PRO:O	2:B:748:ILE:HG12	2.16	0.45
2:B:101:MET:HG2	2:B:111:ALA:HA	1.99	0.45
1:A:839:ARG:HH21	1:A:843:LYS:HE2	1.81	0.45
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.46	0.45
3:C:22:LEU:HD11	11:K:101:LEU:HD21	1.98	0.45
4:D:54:GLU:O	4:D:58:VAL:HG23	2.16	0.45
2:B:1176:ASN:H	2:B:1178:ASN:H	1.62	0.45
7:G:131:GLN:HG2	7:G:136:VAL:HG22	1.99	0.45
1:A:961:ARG:O	1:A:965:GLN:HG3	2.16	0.45
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.97	0.45
1:A:1032:LEU:O	1:A:1036:ARG:HD3	2.17	0.45
6:F:109:VAL:HG21	6:F:124:GLU:HA	1.97	0.45
7:G:122:ASN:HD22	7:G:131:GLN:HE22	1.64	0.45
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.51	0.45
1:A:423:ASP:HB3	1:A:424:ILE:H	1.65	0.45
16:X:331:PRO:HB2	16:X:334:LYS:HB2	1.99	0.45
1:A:55:ASP:C	1:A:57:ARG:H	2.18	0.45
1:A:70:CYS:O	1:A:72:GLU:HG2	2.17	0.45
3:C:79:GLN:HG3	3:C:127:ARG:HD2	1.99	0.45
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.99	0.45
11:K:63:VAL:HG12	11:K:71:PHE:HB3	1.98	0.45
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.99	0.45
8:H:95:TYR:HE1	8:H:97:MET:CG	2.20	0.45
1:A:56:PRO:CD	1:A:58:LEU:HG	2.47	0.44
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	2.00	0.44
3:C:115:SER:HB3	3:C:142:VAL:HB	1.99	0.44
1:A:275:SER:O	1:A:279:LEU:HG	2.17	0.44
2:B:1084:GLN:OE1	3:C:189:THR:HG22	2.17	0.44
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.53	0.44
5:E:61:GLN:HG3	5:E:105:PHE:CE1	2.52	0.44
16:X:249:PHE:HA	16:X:252:PHE:CD1	2.53	0.44
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:154:PHE:HA	4:D:219:THR:HB	1.97	0.44
1:A:344:ARG:HB3	2:B:1118:PRO:HB2	1.98	0.44
2:B:246:LYS:HA	2:B:249:ARG:HH21	1.81	0.44
2:B:188:ASP:HA	2:B:191:LYS:HD2	2.00	0.44
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.99	0.44
1:A:800:VAL:HA	1:A:812:GLU:HG2	1.99	0.44
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.99	0.44
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.83	0.44
1:A:1444:MET:HE3	6:F:135:ARG:HB2	1.99	0.44
3:C:6:PRO:HB3	3:C:25:VAL:HG13	2.00	0.44
3:C:258:ILE:HD11	11:K:42:LEU:HD21	1.99	0.44
2:B:979:LYS:HE3	2:B:987:LYS:HD2	1.99	0.44
2:B:901:PRO:HD3	12:L:58:LYS:HB3	2.00	0.44
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.00	0.44
2:B:237:VAL:HG22	2:B:257:LYS:HG2	2.00	0.44
1:A:982:THR:H	1:A:985:ASP:HB2	1.83	0.44
2:B:904:ARG:HG3	2:B:948:ILE:HG13	1.98	0.44
9:I:8:ARG:O	9:I:9:ASP:CB	2.66	0.44
6:F:89:GLU:O	6:F:93:ILE:HD12	2.18	0.44
1:A:492:PRO:HG3	1:A:501:LEU:HD12	2.00	0.44
1:A:929:LEU:CD2	1:A:983:ILE:HG21	2.47	0.44
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.58	0.44
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	1.99	0.44
1:A:116:ASP:OD2	1:A:164:ARG:HD2	2.18	0.44
3:C:43:THR:HG22	3:C:44:LEU:H	1.82	0.44
4:D:40:HIS:CG	7:G:73:LYS:NZ	2.86	0.44
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.99	0.44
2:B:977:GLY:HA3	2:B:1099:VAL:HB	2.00	0.44
2:B:865:LYS:HE2	2:B:869:SER:HA	1.99	0.44
1:A:567:LYS:CB	8:H:95:TYR:HA	2.46	0.43
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.18	0.43
5:E:154:ILE:O	5:E:196:VAL:HA	2.18	0.43
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.99	0.43
2:B:234:ILE:CG2	2:B:237:VAL:HG23	2.47	0.43
7:G:10:ASN:HD21	7:G:71:ASN:HD22	1.65	0.43
1:A:153:PRO:HA	1:A:161:LEU:HA	2.00	0.43
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.99	0.43
1:A:337:ARG:HD3	1:A:839:ARG:NH2	2.32	0.43
2:B:345:LYS:C	2:B:347:LYS:H	2.21	0.43
2:B:649:LYS:HD3	2:B:736:THR:O	2.18	0.43
2:B:220:GLY:HA2	2:B:241:ARG:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:6:DA:H61	15:T:12:DT:H3	1.66	0.43
2:B:294:ASP:H	9:I:12:ASN:HD22	1.66	0.43
1:A:84:ILE:HG22	1:A:241:VAL:CG2	2.48	0.43
2:B:1016:ALA:O	2:B:1020:ARG:HG3	2.18	0.43
11:K:65:HIS:HD2	11:K:67:PHE:H	1.66	0.43
1:A:332:LYS:H	1:A:337:ARG:HB2	1.82	0.43
1:A:475:THR:HG21	2:B:836:GLU:OE2	2.18	0.43
5:E:61:GLN:HG3	5:E:105:PHE:HE1	1.84	0.43
1:A:779:PHE:CE2	1:A:785:PRO:HD3	2.53	0.43
7:G:92:VAL:CG2	7:G:102:GLN:HB2	2.49	0.43
8:H:125:LEU:HG	8:H:130:ARG:NH2	2.34	0.43
1:A:67:CYS:C	1:A:68:GLN:HG3	2.38	0.43
1:A:915:SER:O	1:A:919:ILE:HB	2.19	0.43
1:A:49:LYS:NZ	1:A:60:SER:HA	2.34	0.43
3:C:258:ILE:CD1	11:K:42:LEU:HD21	2.49	0.43
2:B:309:GLN:HG3	9:I:52:ILE:HD11	2.00	0.43
16:X:347:ASP:O	16:X:350:GLU:HB2	2.19	0.43
10:J:14:VAL:HG13	10:J:50:ILE:HD11	2.01	0.43
1:A:1059:HIS:HE1	6:F:155:LEU:HD21	1.84	0.43
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.83	0.43
3:C:163:ILE:HD12	3:C:165:LYS:HB2	2.00	0.43
2:B:211:VAL:HG21	2:B:494:HIS:CE1	2.53	0.43
8:H:113:ALA:HA	8:H:125:LEU:O	2.19	0.42
4:D:138:ASN:ND2	7:G:35:GLU:HG2	2.34	0.42
8:H:95:TYR:HB3	8:H:144:ILE:HB	2.01	0.42
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.34	0.42
5:E:100:ILE:HG23	5:E:105:PHE:HB2	2.01	0.42
2:B:69:LEU:HD21	2:B:425:THR:HG22	2.02	0.42
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.54	0.42
1:A:774:ARG:HG3	1:A:797:LYS:HD3	2.01	0.42
2:B:757:PRO:HG2	2:B:1028:GLU:HG3	2.02	0.42
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.55	0.42
2:B:101:MET:HB3	2:B:109:THR:HG22	2.02	0.42
2:B:999:MET:HG3	2:B:1000:PRO:HD2	2.00	0.42
8:H:30:SER:HB3	8:H:36:CYS:HB3	2.00	0.42
1:A:34:LYS:NZ	1:A:57:ARG:NH1	2.67	0.42
2:B:515:HIS:CD2	2:B:516:ASN:N	2.88	0.42
1:A:512:VAL:HA	1:A:519:PRO:HA	2.01	0.42
1:A:605:MET:HE1	1:A:612:ILE:HG23	2.01	0.42
2:B:1185:CYS:C	2:B:1187:ASN:H	2.22	0.42
7:G:146:LYS:HD3	7:G:148:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:PHE:CE2	1:A:470:LEU:HD22	2.51	0.42
1:A:697:ALA:HB2	1:A:702:LEU:HD13	2.02	0.42
1:A:1092:LYS:HD3	1:A:1093:LYS:HE3	2.01	0.42
2:B:47:GLN:NE2	2:B:408:LEU:HD12	2.34	0.42
2:B:315:LYS:N	2:B:316:PRO:HD2	2.34	0.42
1:A:382:PRO:HA	1:A:428:TYR:CE1	2.55	0.42
1:A:739:ASP:H	8:H:19:ARG:NH1	2.17	0.42
2:B:972:LYS:HD2	2:B:1098:MET:HE2	2.00	0.42
3:C:262:LEU:HA	3:C:262:LEU:HD23	1.90	0.42
2:B:100:PRO:HG3	2:B:172:ILE:HD13	2.02	0.42
1:A:741:ASN:ND2	1:A:743:VAL:HB	2.34	0.42
8:H:12:VAL:HG13	8:H:26:ILE:HG23	2.01	0.42
3:C:44:LEU:HB2	3:C:77:ILE:HD13	2.02	0.42
12:L:28:LYS:H	12:L:39:SER:HA	1.84	0.42
2:B:515:HIS:HD2	2:B:517:THR:H	1.67	0.42
2:B:1181:GLU:HG3	2:B:1182:CYS:N	2.34	0.42
8:H:44:VAL:HG13	8:H:48:PRO:HA	2.01	0.42
16:X:244:MET:HG2	16:X:310:TYR:CE2	2.55	0.42
9:I:8:ARG:O	9:I:9:ASP:HB2	2.20	0.42
2:B:757:PRO:HG3	2:B:983:ARG:CZ	2.50	0.42
1:A:830:LYS:O	1:A:834:THR:HB	2.20	0.42
2:B:296:GLU:O	2:B:300:HIS:CD2	2.73	0.42
3:C:56:THR:HG23	3:C:147:LEU:HD23	2.02	0.42
16:X:318:ASN:HB3	16:X:346:PRO:HD2	2.02	0.41
1:A:1147:THR:HB	9:I:48:LEU:HD22	2.02	0.41
5:E:181:ALA:HA	5:E:186:LEU:HD21	2.02	0.41
1:A:463:ILE:HD13	1:A:469:ARG:HD2	2.02	0.41
1:A:673:GLY:N	1:A:674:PRO:HD2	2.35	0.41
1:A:1379:GLY:HA2	5:E:177:ARG:O	2.20	0.41
1:A:567:LYS:HZ1	8:H:46:LEU:HB2	1.86	0.41
7:G:21:ARG:HH11	7:G:24:GLN:H	1.68	0.41
1:A:595:THR:HG23	1:A:599:SER:HB3	2.01	0.41
2:B:1081:LEU:O	3:C:189:THR:HG23	2.20	0.41
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.56	0.41
1:A:32:VAL:HG21	1:A:80:HIS:HB2	2.01	0.41
1:A:31:SER:OG	1:A:83:HIS:HD2	2.03	0.41
2:B:123:THR:HG23	2:B:205:ILE:HA	2.02	0.41
2:B:294:ASP:H	9:I:12:ASN:ND2	2.17	0.41
2:B:165:VAL:HG11	2:B:448:ILE:HD13	2.02	0.41
1:A:1442:ASP:HB2	6:F:137:TYR:HE2	1.86	0.41
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1284:MET:HA	1:A:1306:LEU:HD23	2.02	0.41
1:A:254:GLU:HB3	2:B:935:ARG:NH2	2.35	0.41
1:A:92:HIS:HD2	1:A:94:GLY:N	2.18	0.41
11:K:8:GLU:O	11:K:37:LYS:HD3	2.19	0.41
14:P:7:C:H2'	14:P:8:C:C6	2.55	0.41
9:I:84:VAL:HB	9:I:104:LEU:HD21	2.03	0.41
7:G:62:LEU:HA	7:G:63:PRO:HD3	1.84	0.41
1:A:105:CYS:SG	1:A:139:TRP:HA	2.61	0.41
9:I:101:PHE:O	9:I:109:ILE:HA	2.21	0.41
4:D:27:LEU:HD11	4:D:176:GLU:OE2	2.20	0.41
2:B:258:LEU:HB2	2:B:385:LEU:HD21	2.02	0.41
1:A:278:THR:O	1:A:282:ASN:HB2	2.20	0.41
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	2.03	0.41
1:A:42:ASP:HB3	1:A:45:GLN:H	1.86	0.41
3:C:101:LEU:HB2	3:C:118:LEU:HD23	2.03	0.41
2:B:696:GLU:O	2:B:699:GLU:HB2	2.20	0.41
3:C:241:ASP:O	3:C:245:VAL:HG23	2.21	0.41
5:E:23:VAL:HG12	5:E:28:TYR:HB2	2.02	0.41
7:G:143:ILE:HG22	7:G:145:VAL:HG23	2.03	0.41
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.21	0.41
2:B:1114:LEU:HG	2:B:1202:LEU:HD11	2.01	0.41
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	2.02	0.41
1:A:535:THR:HB	1:A:616:VAL:HG13	2.03	0.41
1:A:494:SER:HB3	1:A:497:THR:HB	2.03	0.41
10:J:36:LEU:HD13	10:J:47:ARG:HB3	2.02	0.41
2:B:35:SER:HA	2:B:811:TYR:CE1	2.54	0.41
1:A:1352:VAL:O	1:A:1356:ILE:HD12	2.20	0.41
11:K:59:ALA:HA	11:K:74:ARG:O	2.20	0.41
1:A:92:HIS:CD2	1:A:94:GLY:H	2.37	0.41
2:B:324:ILE:HG23	2:B:329:THR:HB	2.03	0.41
3:C:8:VAL:HG13	3:C:22:LEU:HD12	2.02	0.41
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.55	0.41
1:A:266:LEU:HA	1:A:269:ILE:HD12	2.03	0.41
1:A:1445:ILE:CD1	7:G:70:PHE:CZ	3.04	0.41
2:B:210:LYS:HD2	2:B:210:LYS:HA	1.94	0.41
2:B:734:HIS:CD2	2:B:734:HIS:H	2.39	0.40
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.86	0.40
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.56	0.40
2:B:346:GLU:H	2:B:349:ILE:HD12	1.86	0.40
2:B:944:THR:HB	2:B:1122:ARG:HH21	1.86	0.40
1:A:1402:PHE:CD2	1:A:1403:GLU:HG3	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:810:GLU:HG3	2:B:815:ARG:HH12	1.86	0.40
8:H:56:THR:HB	8:H:145:ARG:HG2	2.03	0.40
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.37	0.40
5:E:86:PRO:HA	5:E:113:GLN:HB2	2.02	0.40
6:F:72:LYS:HD2	6:F:142:SER:HB3	2.03	0.40
16:X:342:GLU:H	16:X:342:GLU:HG3	1.61	0.40
12:L:47:ARG:NH2	12:L:54:ARG:HE	2.20	0.40
3:C:73:GLN:O	3:C:129:ILE:HA	2.21	0.40
4:D:173:HIS:CD2	4:D:201:LYS:HZ1	2.40	0.40
8:H:115:TYR:CE2	8:H:124:ARG:HG3	2.57	0.40
1:A:1258:HIS:O	1:A:1262:LYS:HG3	2.22	0.40
7:G:92:VAL:HG21	7:G:102:GLN:HB2	2.03	0.40
1:A:1121:GLU:HB3	1:A:1124:HIS:HD2	1.86	0.40
1:A:589:GLN:HG2	1:A:606:LEU:HD13	2.03	0.40
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	2.04	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	1419/1733 (82%)	1259 (89%)	111 (8%)	49 (4%)	4	30
2	B	1075/1224 (88%)	962 (90%)	78 (7%)	35 (3%)	5	32
3	C	264/318 (83%)	242 (92%)	15 (6%)	7 (3%)	6	37
4	D	173/221 (78%)	151 (87%)	17 (10%)	5 (3%)	6	35
5	E	212/215 (99%)	201 (95%)	9 (4%)	2 (1%)	21	63
6	F	82/155 (53%)	75 (92%)	7 (8%)	0	100	100
7	G	169/171 (99%)	153 (90%)	15 (9%)	1 (1%)	30	71
8	H	129/146 (88%)	100 (78%)	16 (12%)	13 (10%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	117/122 (96%)	99 (85%)	16 (14%)	2 (2%)	11	50
10	J	63/70 (90%)	54 (86%)	5 (8%)	4 (6%)	2	14
11	K	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
12	L	44/70 (63%)	27 (61%)	11 (25%)	6 (14%)	0	2
16	X	114/146 (78%)	99 (87%)	9 (8%)	6 (5%)	2	18
All	All	3974/4711 (84%)	3530 (89%)	314 (8%)	130 (3%)	5	32

All (130) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	44	THR
1	A	54	ASN
1	A	57	ARG
1	A	70	CYS
1	A	74	MET
1	A	76	GLU
1	A	169	ASN
1	A	257	ARG
1	A	536	LEU
1	A	567	LYS
1	A	597	LEU
1	A	628	GLY
1	A	1175	SER
1	A	1403	GLU
2	B	367	LEU
2	B	629	ASP
2	B	731	VAL
2	B	751	VAL
2	B	772	ALA
2	B	879	ARG
2	B	1046	PRO
2	B	1097	HIS
2	B	1176	ASN
2	B	1181	GLU
2	B	1223	ASP
3	C	161	LYS
4	D	15	LEU
8	H	78	SER
8	H	139	ASN

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Mol	Chain	Res	Type
16	X	315	ASP
16	X	339	ASN
1	A	58	LEU
1	A	65	LEU
1	A	166	GLY
1	A	525	GLN
1	A	846	GLU
1	A	1180	GLU
1	A	1271	ILE
1	A	1405	THR
1	A	1437	GLY
2	B	108	VAL
2	B	447	ALA
2	B	867	GLY
2	B	880	THR
2	B	1066	SER
2	B	1175	LEU
3	C	141	GLY
4	D	13	ARG
4	D	18	VAL
4	D	53	SER
8	H	18	GLY
8	H	81	PRO
8	H	82	PRO
9	I	9	ASP
10	J	6	ARG
12	L	50	ASP
12	L	53	HIS
12	L	56	LEU
16	X	260	ALA
16	X	340	ALA
1	A	42	ASP
1	A	167	CYS
1	A	286	HIS
1	A	311	GLN
1	A	399	HIS
1	A	423	ASP
1	A	543	LEU
1	A	593	GLU
1	A	1255	GLU
2	B	67	SER
2	B	229	ALA

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Mol	Chain	Res	Type
2	B	364	ILE
2	B	643	ASP
2	B	711	GLU
2	B	712	PRO
2	B	1157	ALA
7	G	154	VAL
8	H	83	GLN
8	H	108	SER
9	I	95	THR
12	L	45	ALA
1	A	62	ASP
1	A	332	LYS
1	A	1206	ASP
2	B	307	ASP
2	B	792	MET
2	B	943	SER
3	C	90	ASP
3	C	142	VAL
3	C	149	LYS
4	D	19	GLU
5	E	36	GLU
8	H	84	ALA
8	H	128	ASN
10	J	64	ASN
12	L	59	ALA
1	A	46	THR
1	A	310	GLY
1	A	322	VAL
1	A	424	ILE
1	A	599	SER
1	A	958	VAL
1	A	1188	GLN
2	B	251	ILE
2	B	305	VAL
2	B	368	GLU
2	B	883	LEU
3	C	175	ALA
5	E	3	GLN
8	H	17	PRO
10	J	2	ILE
1	A	5	GLN
2	B	707	PRO

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Mol	Chain	Res	Type
2	B	1108	ARG
2	B	1155	SER
3	C	214	ASN
8	H	19	ARG
8	H	131	ASN
8	H	136	LYS
10	J	3	VAL
16	X	302	TYR
1	A	52	GLY
12	L	52	GLY
1	A	331	GLY
1	A	1156	PRO
2	B	369	GLY
16	X	301	ILE
1	A	158	PRO
1	A	196	GLU

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	1251/1520 (82%)	1084 (87%)	167 (13%)	5	22
2	B	952/1061 (90%)	835 (88%)	117 (12%)	6	26
3	C	234/274 (85%)	204 (87%)	30 (13%)	5	24
4	D	140/200 (70%)	123 (88%)	17 (12%)	6	27
5	E	196/197 (100%)	183 (93%)	13 (7%)	21	60
6	F	74/137 (54%)	68 (92%)	6 (8%)	15	49
7	G	152/152 (100%)	130 (86%)	22 (14%)	4	19
8	H	117/128 (91%)	99 (85%)	18 (15%)	3	16
9	I	113/116 (97%)	102 (90%)	11 (10%)	10	38
10	J	60/65 (92%)	50 (83%)	10 (17%)	3	13
11	K	99/102 (97%)	88 (89%)	11 (11%)	8	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	40/57 (70%)	28 (70%)	12 (30%)	0	1
16	X	110/136 (81%)	88 (80%)	22 (20%)	1	7
All	All	3538/4145 (85%)	3082 (87%)	456 (13%)	5	24

All (456) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	15	LYS
1	A	30	ILE
1	A	34	LYS
1	A	41	MET
1	A	46	THR
1	A	62	ASP
1	A	63	ARG
1	A	65	LEU
1	A	68	GLN
1	A	70	CYS
1	A	71	GLN
1	A	84	ILE
1	A	93	VAL
1	A	106	VAL
1	A	112	LYS
1	A	113	LEU
1	A	120	GLU
1	A	132	LYS
1	A	145	LYS
1	A	146	MET
1	A	147	VAL
1	A	171	GLN
1	A	196	GLU
1	A	204	THR
1	A	208	LEU
1	A	213	HIS
1	A	225	ASN
1	A	232	GLU
1	A	252	PHE
1	A	257	ARG
1	A	265	LYS
1	A	278	THR
1	A	282	ASN

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Mol	Chain	Res	Type
1	A	289	ILE
1	A	293	GLU
1	A	302	THR
1	A	303	TYR
1	A	307	ASP
1	A	311	GLN
1	A	313	GLN
1	A	320	ARG
1	A	322	VAL
1	A	323	LYS
1	A	335	ARG
1	A	344	ARG
1	A	372	LYS
1	A	375	THR
1	A	381	THR
1	A	383	TYR
1	A	385	ILE
1	A	389	THR
1	A	408	ASP
1	A	423	ASP
1	A	425	GLN
1	A	431	LYS
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	446	ARG
1	A	461	LYS
1	A	470	LEU
1	A	472	LEU
1	A	475	THR
1	A	476	SER
1	A	485	ASP
1	A	497	THR
1	A	505	CYS
1	A	513	SER
1	A	518	LYS
1	A	527	THR
1	A	538	ASP
1	A	545	GLN
1	A	571	LEU
1	A	577	ILE

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Mol	Chain	Res	Type
1	A	598	LEU
1	A	618	GLU
1	A	620	LYS
1	A	622	VAL
1	A	629	LEU
1	A	635	ARG
1	A	652	VAL
1	A	666	ILE
1	A	670	ILE
1	A	682	THR
1	A	690	VAL
1	A	691	LEU
1	A	726	ARG
1	A	740	LEU
1	A	764	CYS
1	A	768	GLN
1	A	773	LYS
1	A	774	ARG
1	A	782	ARG
1	A	788	SER
1	A	821	ARG
1	A	826	ASP
1	A	830	LYS
1	A	831	THR
1	A	834	THR
1	A	839	ARG
1	A	855	THR
1	A	858	ASN
1	A	880	LYS
1	A	884	ASP
1	A	885	THR
1	A	896	ARG
1	A	919	ILE
1	A	920	LEU
1	A	923	LEU
1	A	948	VAL
1	A	982	THR
1	A	998	LEU
1	A	1001	ARG
1	A	1036	ARG
1	A	1038	THR
1	A	1062	GLU

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Mol	Chain	Res	Type
1	A	1064	VAL
1	A	1067	LEU
1	A	1081	LEU
1	A	1093	LYS
1	A	1133	LEU
1	A	1135	ARG
1	A	1136	SER
1	A	1172	LEU
1	A	1174	PHE
1	A	1178	ASP
1	A	1187	GLN
1	A	1208	THR
1	A	1215	ARG
1	A	1222	ASN
1	A	1223	ASP
1	A	1230	GLU
1	A	1237	ILE
1	A	1238	ILE
1	A	1242	VAL
1	A	1263	ILE
1	A	1280	GLU
1	A	1281	ARG
1	A	1289	ARG
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1301	GLU
1	A	1307	GLU
1	A	1315	GLU
1	A	1322	ILE
1	A	1325	THR
1	A	1336	MET
1	A	1341	ILE
1	A	1364	ASN
1	A	1376	THR
1	A	1382	THR
1	A	1391	ARG
1	A	1400	CYS
1	A	1403	GLU
1	A	1411	GLU
1	A	1424	VAL
1	A	1426	GLU

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Mol	Chain	Res	Type
1	A	1436	ILE
1	A	1438	THR
1	A	1442	ASP
1	A	1445	ILE
1	A	1450	LEU
1	A	1451	VAL
1	A	1454	MET
2	B	22	SER
2	B	25	ILE
2	B	46	GLN
2	B	63	ILE
2	B	102	VAL
2	B	109	THR
2	B	128	LEU
2	B	167	ILE
2	B	185	THR
2	B	210	LYS
2	B	211	VAL
2	B	217	ARG
2	B	222	ILE
2	B	240	ILE
2	B	249	ARG
2	B	251	ILE
2	B	261	ARG
2	B	272	THR
2	B	278	GLN
2	B	279	ASP
2	B	292	ILE
2	B	294	ASP
2	B	312	GLU
2	B	331	LEU
2	B	361	LEU
2	B	365	THR
2	B	381	MET
2	B	384	ARG
2	B	387	LEU
2	B	398	ARG
2	B	415	GLN
2	B	416	LEU
2	B	429	PHE
2	B	466	TRP
2	B	485	ARG

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Mol	Chain	Res	Type
2	B	487	THR
2	B	495	LEU
2	B	500	THR
2	B	531	GLN
2	B	537	LYS
2	B	547	VAL
2	B	549	THR
2	B	552	MET
2	B	570	VAL
2	B	575	PRO
2	B	601	ARG
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	624	LEU
2	B	626	ILE
2	B	628	THR
2	B	644	GLU
2	B	658	ILE
2	B	678	GLU
2	B	682	SER
2	B	696	GLU
2	B	709	ASP
2	B	714	GLU
2	B	734	HIS
2	B	737	THR
2	B	780	VAL
2	B	786	ASN
2	B	790	ASP
2	B	795	ILE
2	B	844	SER
2	B	853	SER
2	B	857	ARG
2	B	871	THR
2	B	875	GLU
2	B	878	GLN
2	B	908	GLU
2	B	911	ILE
2	B	916	THR
2	B	942	ARG
2	B	944	THR
2	B	946	ASN

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Mol	Chain	Res	Type
2	B	956	THR
2	B	964	VAL
2	B	970	THR
2	B	975	GLN
2	B	979	LYS
2	B	986	GLN
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1028	GLU
2	B	1048	THR
2	B	1053	GLU
2	B	1060	ARG
2	B	1065	GLN
2	B	1084	GLN
2	B	1094	ARG
2	B	1102	LYS
2	B	1106	ARG
2	B	1122	ARG
2	B	1123	SER
2	B	1128	LEU
2	B	1135	ARG
2	B	1138	MET
2	B	1147	LEU
2	B	1148	LYS
2	B	1149	GLU
2	B	1150	ARG
2	B	1151	LEU
2	B	1153	GLU
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1169	MET
2	B	1175	LEU
2	B	1178	ASN
2	B	1179	GLN
2	B	1182	CYS
2	B	1183	LYS
2	B	1202	LEU
2	B	1211	ASN
3	C	3	GLU
3	C	7	GLN

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Mol	Chain	Res	Type
3	C	8	VAL
3	C	12	GLU
3	C	16	ASP
3	C	18	VAL
3	C	22	LEU
3	C	25	VAL
3	C	26	ASP
3	C	50	GLU
3	C	52	GLU
3	C	56	THR
3	C	60	ASP
3	C	79	GLN
3	C	102	GLN
3	C	121	VAL
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	137	LYS
3	C	145	CYS
3	C	163	ILE
3	C	189	THR
3	C	203	GLN
3	C	235	VAL
3	C	238	ILE
3	C	240	VAL
3	C	260	LEU
3	C	265	MET
3	C	268	ASP
4	D	23	ASN
4	D	34	GLN
4	D	35	LEU
4	D	47	LEU
4	D	52	LEU
4	D	60	LYS
4	D	65	GLU
4	D	119	ARG
4	D	122	GLU
4	D	134	THR
4	D	139	LYS
4	D	156	ASP
4	D	165	GLN
4	D	187	THR

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Mol	Chain	Res	Type
4	D	197	SER
4	D	218	GLU
4	D	219	THR
5	E	2	ASP
5	E	3	GLN
5	E	57	MET
5	E	67	GLU
5	E	70	SER
5	E	117	THR
5	E	123	LEU
5	E	146	HIS
5	E	158	SER
5	E	190	LEU
5	E	192	ARG
5	E	200	ARG
5	E	204	THR
6	F	79	ARG
6	F	82	THR
6	F	87	LYS
6	F	90	ARG
6	F	110	ASP
6	F	111	LEU
7	G	1	MET
7	G	11	ILE
7	G	13	LEU
7	G	21	ARG
7	G	24	GLN
7	G	26	LEU
7	G	28	THR
7	G	39	THR
7	G	64	THR
7	G	83	LYS
7	G	85	GLU
7	G	93	SER
7	G	96	GLN
7	G	106	MET
7	G	111	THR
7	G	112	LYS
7	G	114	LEU
7	G	117	GLN
7	G	134	GLU
7	G	138	THR

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Mol	Chain	Res	Type
7	G	151	ILE
7	G	152	SER
8	H	13	SER
8	H	26	ILE
8	H	27	GLU
8	H	31	THR
8	H	32	THR
8	H	34	ASP
8	H	53	ASP
8	H	62	SER
8	H	77	ARG
8	H	95	TYR
8	H	106	GLU
8	H	107	VAL
8	H	111	LEU
8	H	112	ILE
8	H	124	ARG
8	H	128	ASN
8	H	130	ARG
8	H	138	GLU
9	I	8	ARG
9	I	35	VAL
9	I	55	THR
9	I	81	ARG
9	I	83	ASN
9	I	84	VAL
9	I	106	CYS
9	I	107	SER
9	I	108	HIS
9	I	109	ILE
9	I	114	GLN
10	J	2	ILE
10	J	3	VAL
10	J	7	CYS
10	J	12	LYS
10	J	14	VAL
10	J	22	LEU
10	J	30	LEU
10	J	48	ARG
10	J	52	THR
10	J	56	LEU
11	K	11	LEU

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Mol	Chain	Res	Type
11	K	18	LYS
11	K	20	LYS
11	K	25	THR
11	K	29	ASN
11	K	31	VAL
11	K	37	LYS
11	K	47	ARG
11	K	101	LEU
11	K	107	THR
11	K	113	THR
12	L	27	LEU
12	L	30	ILE
12	L	38	LEU
12	L	44	ASP
12	L	46	VAL
12	L	54	ARG
12	L	55	ILE
12	L	58	LYS
12	L	61	THR
12	L	63	ARG
12	L	65	VAL
12	L	68	GLU
16	X	243	LYS
16	X	251	LYS
16	X	252	PHE
16	X	254	VAL
16	X	261	LYS
16	X	271	VAL
16	X	278	PHE
16	X	280	HIS
16	X	291	LEU
16	X	292	ASN
16	X	301	ILE
16	X	319	LEU
16	X	324	HIS
16	X	327	GLU
16	X	332	LEU
16	X	335	LEU
16	X	336	VAL
16	X	342	GLU
16	X	347	ASP
16	X	358	ILE

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Mol	Chain	Res	Type
16	X	359	ILE
16	X	364	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	75	ASN
1	A	83	HIS
1	A	92	HIS
1	A	225	ASN
1	A	299	HIS
1	A	313	GLN
1	A	339	ASN
1	A	435	HIS
1	A	503	GLN
1	A	545	GLN
1	A	548	ASN
1	A	631	HIS
1	A	660	ASN
1	A	736	ASN
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	1124	HIS
1	A	1128	GLN
1	A	1140	HIS
1	A	1188	GLN
1	A	1258	HIS
1	A	1270	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	47	GLN
2	B	121	ASN
2	B	215	GLN
2	B	255	GLN
2	B	300	HIS

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Mol	Chain	Res	Type
2	B	325	GLN
2	B	366	GLN
2	B	383	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	657	HIS
2	B	734	HIS
2	B	744	HIS
2	B	957	ASN
2	B	975	GLN
2	B	1015	HIS
2	B	1065	GLN
2	B	1117	GLN
2	B	1161	HIS
2	B	1176	ASN
2	B	1177	HIS
3	C	65	HIS
3	C	73	GLN
3	C	102	GLN
3	C	112	ASN
3	C	242	GLN
4	D	23	ASN
4	D	28	GLN
4	D	37	GLN
4	D	143	ASN
4	D	150	ASN
5	E	147	HIS
7	G	10	ASN
7	G	14	HIS
7	G	126	ASN
7	G	131	GLN
8	H	133	ASN
9	I	12	ASN
9	I	89	GLN
10	J	53	HIS
11	K	29	ASN
11	K	65	HIS
12	L	53	HIS
12	L	66	GLN
16	X	312	ASN
16	X	345	ASN

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Mol	Chain	Res	Type
16	X	362	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	10/11 (90%)	5 (50%)	2 (20%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	8	C
14	P	11	C
14	P	12	C
14	P	16	C
14	P	17	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	11	C
14	P	16	C

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
15	BRU	T	22	15	13,21,22	2.67	1 (7%)	16,30,33	2.28	3 (18%)

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
15	BRU	T	22	15	-	0/3/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	C4-C5	9.41	1.50	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C5-C4-N3	-4.42	119.28	124.00
15	T	22	BRU	O4'-C1'-N1	2.60	112.21	107.72
15	T	22	BRU	C4-N3-C2	7.25	121.52	115.25

There are no chirality outliers.

There are no torsion outliers.

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, 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	1429/1733 (82%)	0.02	24 (1%) 73 65	59, 101, 164, 229	0
2	B	1097/1224 (89%)	0.15	27 (2%) 61 52	59, 114, 175, 208	0
3	C	266/318 (83%)	-0.13	0 100 100	77, 101, 141, 173	0
4	D	177/221 (80%)	-0.05	1 (0%) 90 87	80, 111, 165, 179	0
5	E	214/215 (99%)	0.09	6 (2%) 56 48	76, 135, 181, 211	0
6	F	84/155 (54%)	-0.22	1 (1%) 81 74	63, 83, 110, 134	0
7	G	171/171 (100%)	0.06	0 100 100	73, 100, 139, 166	0
8	H	133/146 (91%)	0.63	12 (9%) 12 8	112, 148, 183, 209	0
9	I	119/122 (97%)	0.38	11 (9%) 11 8	116, 148, 186, 203	0
10	J	65/70 (92%)	-0.10	0 100 100	82, 101, 138, 146	0
11	K	115/120 (95%)	0.03	2 (1%) 73 65	70, 103, 141, 155	0
12	L	46/70 (65%)	0.93	7 (15%) 3 2	86, 180, 196, 201	0
13	N	10/14 (71%)	2.32	6 (60%) 0 0	239, 248, 270, 275	0
14	P	11/11 (100%)	2.30	4 (36%) 0 0	204, 214, 222, 224	0
15	T	13/27 (48%)	2.01	7 (53%) 0 0	165, 186, 260, 263	0
16	X	120/146 (82%)	0.98	22 (18%) 2 1	172, 203, 219, 229	0
All	All	4070/4763 (85%)	0.13	130 (3%) 51 43	59, 110, 188, 275	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	115	ALA	7.9
12	L	25	ALA	7.9
14	P	16	C	6.8
12	L	26	THR	6.1
1	A	69	THR	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	1455	PRO	5.6
16	X	324	HIS	5.3
2	B	250	PHE	5.1
2	B	709	ASP	4.5
14	P	17	C	4.5
15	T	9	DA	4.4
13	N	8	DC	4.2
8	H	139	ASN	4.2
12	L	27	LEU	4.1
15	T	10	DG	4.0
16	X	257	THR	4.0
1	A	253	ASN	3.9
16	X	317	LYS	3.9
1	A	256	GLN	3.8
1	A	2	VAL	3.7
5	E	123	LEU	3.7
5	E	82	PHE	3.6
1	A	1257	ASP	3.6
1	A	1174	PHE	3.6
11	K	114	LEU	3.5
15	T	13	DT	3.5
16	X	320	GLU	3.5
9	I	119	THR	3.4
2	B	733	HIS	3.4
2	B	883	LEU	3.4
16	X	313	LEU	3.4
2	B	132	VAL	3.3
2	B	918	ILE	3.3
12	L	50	ASP	3.3
16	X	364	ILE	3.3
8	H	132	LEU	3.3
16	X	318	ASN	3.3
9	I	84	VAL	3.2
1	A	161	LEU	3.2
15	T	14	DA	3.2
1	A	257	ARG	3.1
13	N	9	DT	3.1
15	T	11	DC	3.1
12	L	45	ALA	3.0
16	X	258	ILE	3.0
2	B	734	HIS	3.0
16	X	245	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	173	THR	3.0
16	X	363	PHE	3.0
16	X	339	ASN	2.9
16	X	365	VAL	2.9
1	A	255	SER	2.9
2	B	509	ALA	2.9
5	E	110	PHE	2.9
2	B	870	ILE	2.9
8	H	134	ASN	2.8
16	X	327	GLU	2.8
16	X	244	MET	2.8
16	X	254	VAL	2.8
2	B	130	VAL	2.8
9	I	25	LEU	2.7
16	X	255	PRO	2.7
2	B	723	VAL	2.7
2	B	69	LEU	2.7
2	B	248	SER	2.7
16	X	319	LEU	2.7
2	B	679	TYR	2.7
13	N	7	DG	2.6
6	F	108	PHE	2.6
12	L	46	VAL	2.6
8	H	140	ALA	2.6
2	B	868	MET	2.6
1	A	251	SER	2.6
1	A	1184	SER	2.5
12	L	32	ALA	2.5
14	P	15	C	2.5
2	B	103	ASN	2.5
15	T	12	DT	2.5
2	B	262	GLU	2.5
8	H	55	LEU	2.5
9	I	102	VAL	2.5
13	N	10	DA	2.5
16	X	360	LEU	2.4
8	H	86	ASP	2.4
8	H	59	ILE	2.4
9	I	100	PHE	2.4
1	A	164	ARG	2.3
4	D	19	GLU	2.3
2	B	715	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	431	TYR	2.3
2	B	373	ARG	2.3
16	X	309	LEU	2.3
8	H	2	SER	2.3
16	X	336	VAL	2.3
1	A	162	VAL	2.3
2	B	882	THR	2.3
2	B	881	ASN	2.3
1	A	1304	TRP	2.3
9	I	76	PRO	2.3
15	T	15	DC	2.3
2	B	24	PRO	2.3
14	P	11	C	2.3
1	A	1181	ALA	2.2
13	N	3	DG	2.3
16	X	329	LYS	2.2
2	B	90	ILE	2.2
5	E	127	ILE	2.2
1	A	1287	TYR	2.2
2	B	866	TYR	2.2
8	H	50	ALA	2.2
1	A	145	LYS	2.2
2	B	349	ILE	2.2
13	N	1	DA	2.2
8	H	136	LYS	2.1
1	A	45	GLN	2.1
8	H	126	GLU	2.1
9	I	117	LYS	2.1
5	E	2	ASP	2.1
1	A	3	GLY	2.1
16	X	332	LEU	2.1
9	I	109	ILE	2.1
1	A	1176	LEU	2.1
8	H	116	TYR	2.1
9	I	26	LEU	2.1
1	A	1305	VAL	2.1
9	I	101	PHE	2.0
9	I	104	LEU	2.0
5	E	47	CYS	2.0
2	B	714	GLU	2.0
1	A	152	VAL	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
15	BRU	T	22	20/21	0.64	0.32	-	191,208,212,215	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
17	ZN	B	2225	1/1	0.99	0.22	0.89	83,83,83,83	0
17	ZN	I	1121	1/1	0.99	0.15	-0.06	124,124,124,124	0
17	ZN	J	1066	1/1	0.99	0.23	-0.54	90,90,90,90	0
17	ZN	A	2457	1/1	1.00	0.17	-0.83	79,79,79,79	0
17	ZN	C	1269	1/1	1.00	0.12	-0.88	81,81,81,81	0
17	ZN	A	2456	1/1	0.99	0.06	-1.78	141,141,141,141	0
18	MG	A	2458	1/1	0.92	0.10	-1.82	77,77,77,77	0
17	ZN	I	1122	1/1	0.97	0.03	-1.95	196,196,196,196	0
17	ZN	L	1071	1/1	0.98	0.06	-2.50	207,207,207,207	0

6.5 Other polymers [i](#)

There are no such residues in this entry.