



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:10 AM UTC

PDB ID : 6FF4 / pdb_00006ff4
EMDB ID : EMD-4255
Title : human Bact spliceosome core structure
Authors : Haselbach, D.; Komarov, I.; Agafonov, D.; Hartmuth, K.; Graf, B.; Kastner, B.; Luehrmann, R.; Stark, H.
Deposited on : 2018-01-03
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

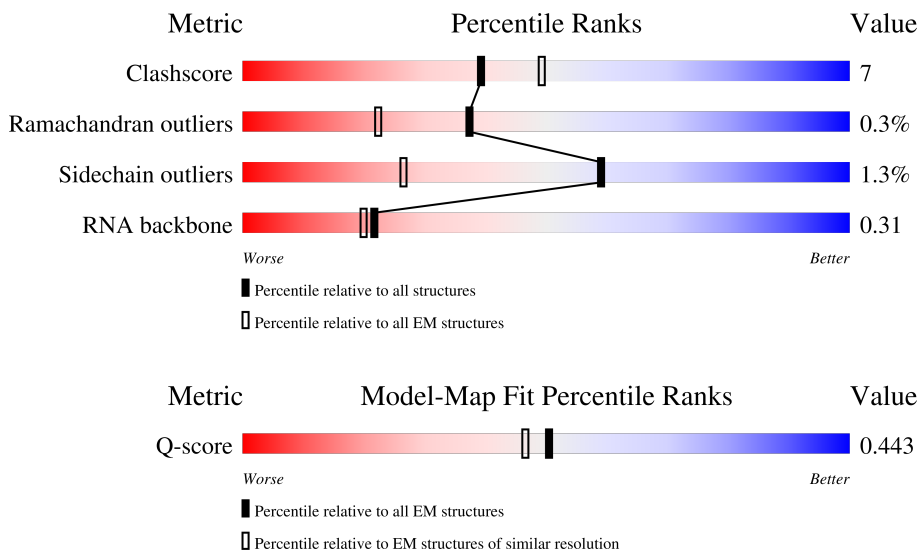
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

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.




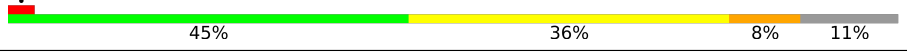

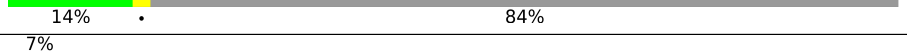
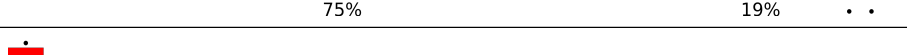
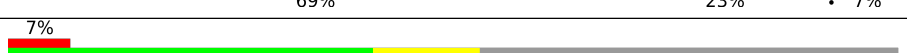
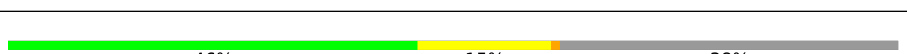
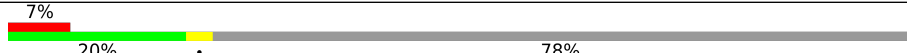


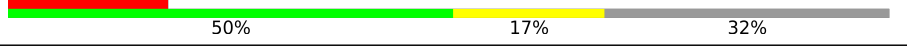


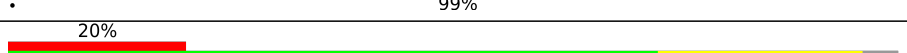




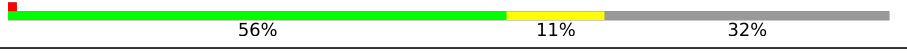



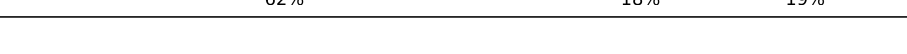


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	322	
2	2	188	
3	3	619	

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Mol	Chain	Length	Quality of chain
4	5	116	
5	6	107	
6	7	464	
7	8	895	
8	A	2335	
9	B	972	
10	C	536	
11	D	514	
12	E	579	
13	L	802	
14	O	848	
15	P	420	
16	Q	144	
17	R	229	
18	S	2752	
19	V	166	
20	Y	904	
21	Z	478	
22	s	472	
23	t	343	
24	u	1304	
25	v	1217	
26	x	86	
27	y	110	
28	z	125	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	IHP	A	3001	-	-	X	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 72392 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA-binding motif protein, X-linked 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	122	981	623	168	187	3	0	0

- Molecule 2 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	60	1262	565	207	430	60	0	0

- Molecule 3 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	118	981	609	185	182	5	0	0

- Molecule 4 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	5	70	1470	659	243	498	70	0	0

- Molecule 5 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	6	95	2035	910	377	653	95	0	0

- Molecule 6 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	93	733	444	145	140	4	0	0

- Molecule 7 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	8	144	1211	776	219	210	6	0	0

- Molecule 8 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	A	2238	18569	11953	3245	3290	81	0	0

- Molecule 9 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	B	902	7137	4566	1187	1349	35	0	0

- Molecule 10 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C	286	2287	1427	419	429	12	0	0

- Molecule 11 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	D	320	2517	1588	457	464	8	0	0

- Molecule 12 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	E	130	1054	664	175	211	4	0	0

- Molecule 13 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	L	103	858	548	157	149	4	0	0

- Molecule 14 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	253	Total	C	N	O	S	0	0
			2235	1433	399	397	6		

- Molecule 15 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	286	Total	C	N	O	S	0	0
			2305	1447	411	427	20		

- Molecule 16 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	138	Total	C	N	O	S	0	0
			1153	728	212	203	10		

- Molecule 17 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	102	Total	C	N	O	S	0	0
			869	532	169	166	2		

- Molecule 18 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	34	Total	C	N	O	S	0	0
			261	158	56	46	1		

- Molecule 19 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	159	Total	C	N	O	S	0	0
			1236	787	215	227	7		

- Molecule 20 is a protein called Serine/arginine repetitive matrix protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	95	Total	C	N	O	S	0	0
			762	494	121	142	5		

- Molecule 21 is a RNA chain called pre mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	Z	48	1013	454	173	338	48	0	0

- Molecule 22 is a protein called Peptidyl-prolyl cis-trans isomerase CWC27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	s	175	1377	869	240	263	5	0	0

- Molecule 23 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	t	172	1415	880	257	267	11	0	0

- Molecule 24 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	u	881	7013	4496	1201	1274	42	0	0

- Molecule 25 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	v	1189	9315	5908	1586	1776	45	0	0

- Molecule 26 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	x	79	656	415	115	120	6	0	0

- Molecule 27 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	y	100	766	473	135	145	13	0	0

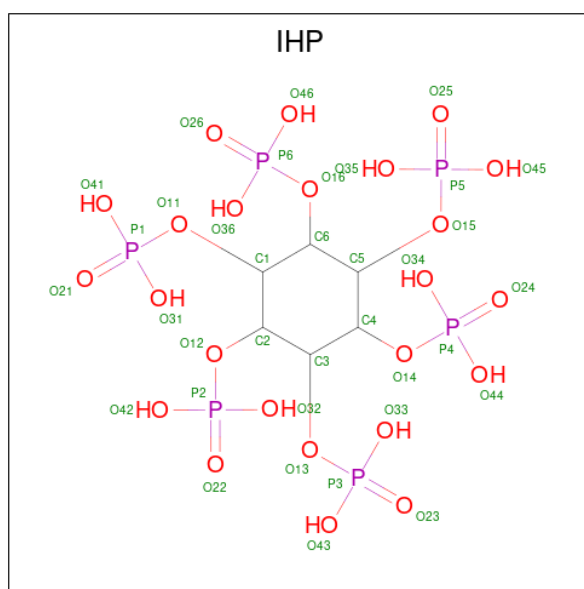
- Molecule 28 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	z	101	839	538	146	151	4	0	0

- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

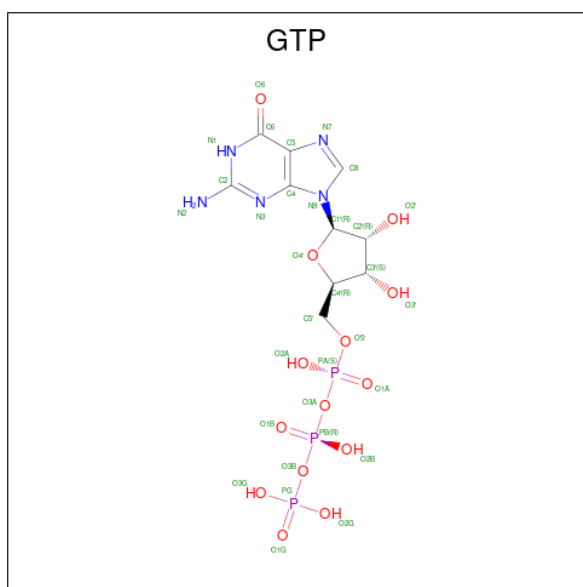
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
29	6	4	4	4	0

- Molecule 30 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
30	A	1	36	6	24	6	0

- Molecule 31 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



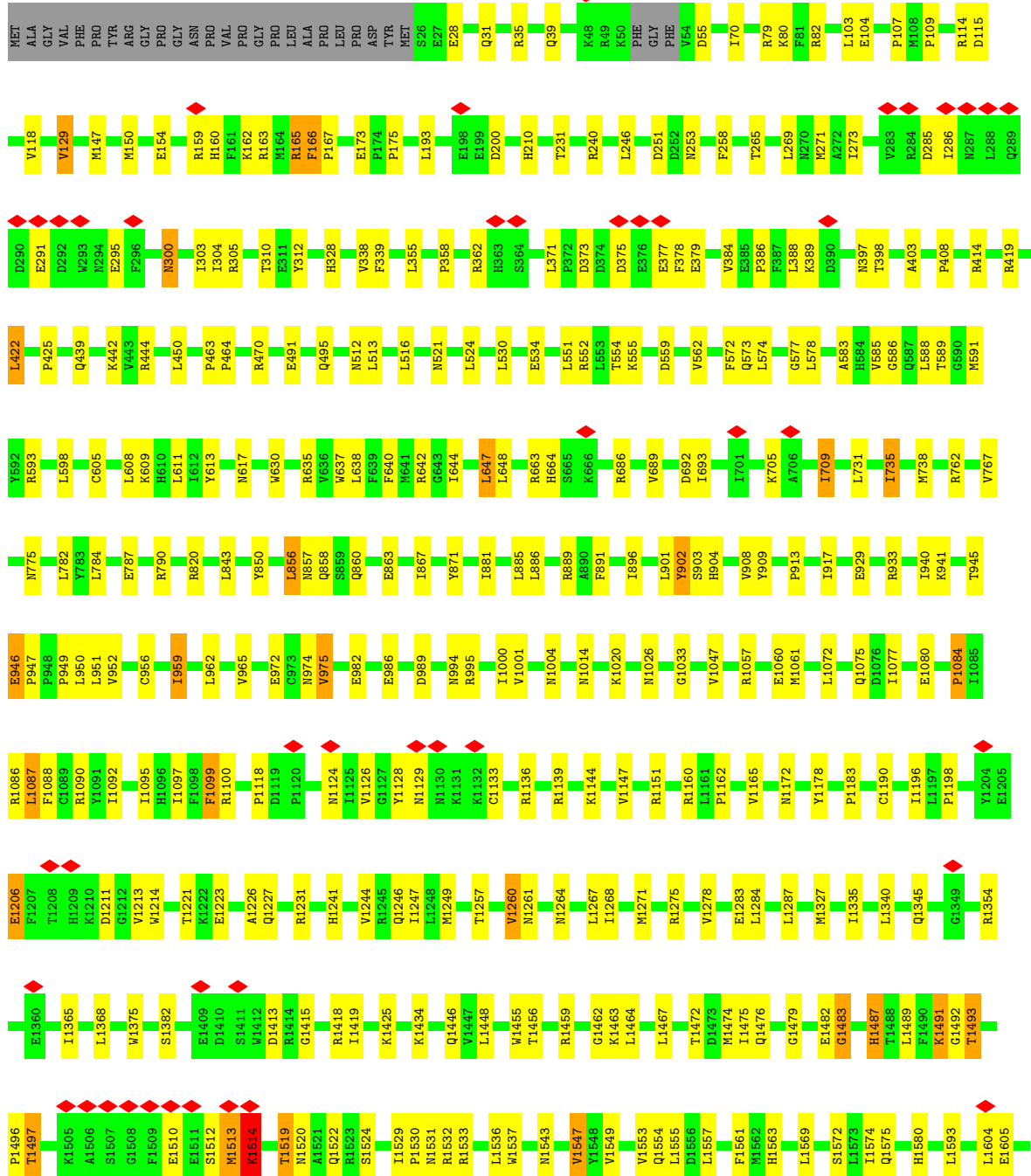
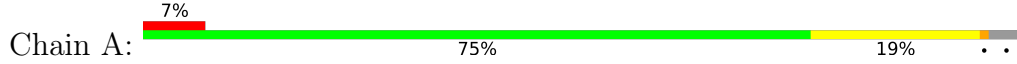
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
31	B	1	32	10	5	14	3	0

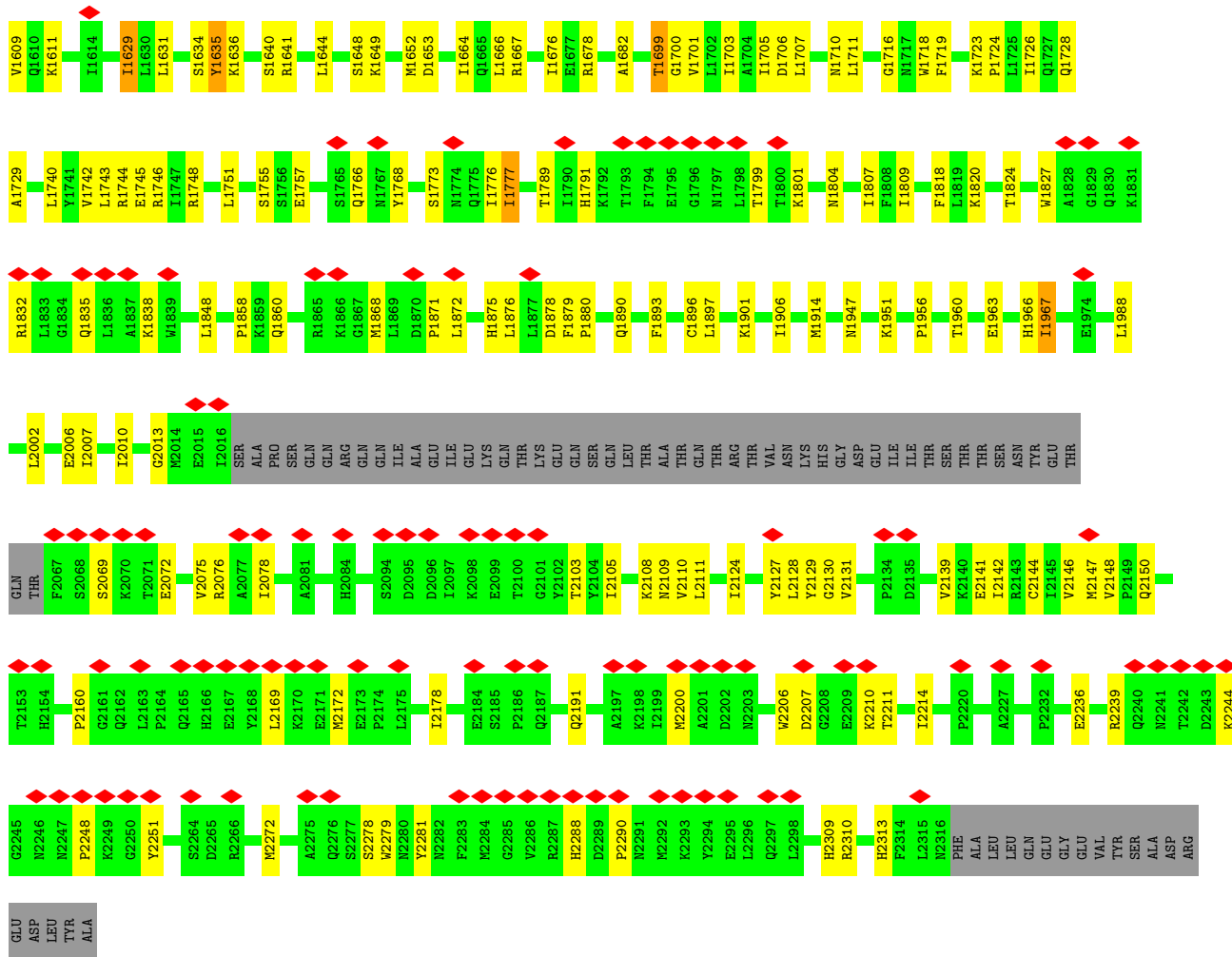
- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
32	P	3	3	3	0
32	Q	3	3	3	0
32	t	1	1	1	0
32	y	3	3	3	0

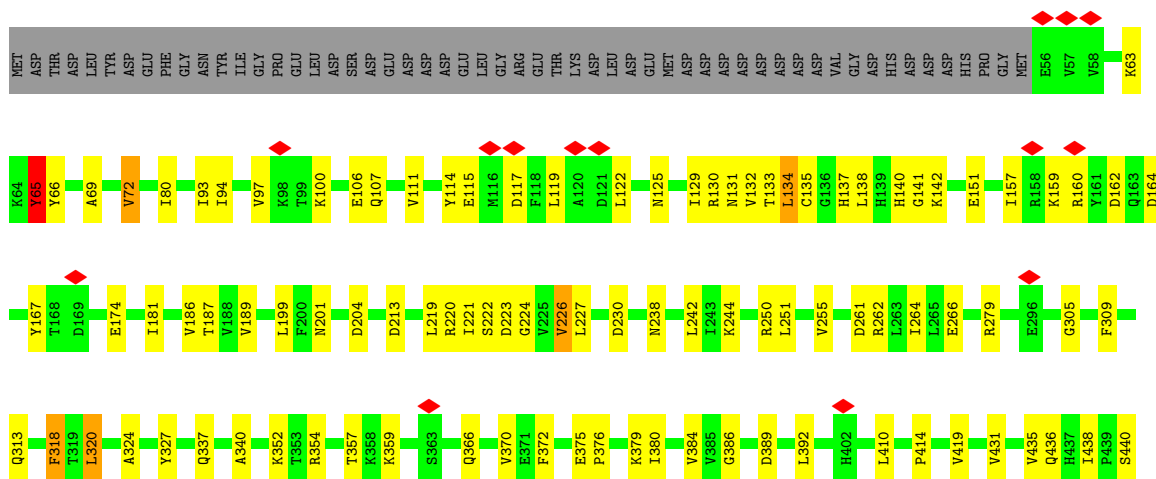
LEU	GLN	GLY	VAL	GLY	VAL	GLY	VAL	ALA	LEU	PRO	PRO	GLY	GLY	GLY	ASP	ASP	MET	MET	THR	GLN	LYS	LYS	GLY	GLY	GLY	HIS	VAL	ARG	ARG	GLY	GLN	GLN	ALA	ALA	GLN	GLN	VAL	VAL	GLY	GLY	GLY	ASP	PHE	PHE	ASP	MET	VAL	ALA	ALA	GLY	HIS	ALA	ALA	LYS	LYS	GLN	GLN	GLN	LYS	LYS	ARG	LYS	ALA	GLN	PRO
GLN	ASP	SER	ARG	ARG	GLY	GLY	SER	LYS	LYS	TYR	PRO	GLY	GLY	GLY	PRO	PRO	LEU	ALA	ALA	PRO	LEU	PRO	ASP	TYR	MET	MET	S26	E27	E28	Q31	R35	Q39	T231	R240	L246	D251	D252	N253	F258	I70	R79	K80	F81	R82	L103	E104	F107	M108	P109	R114	D115														

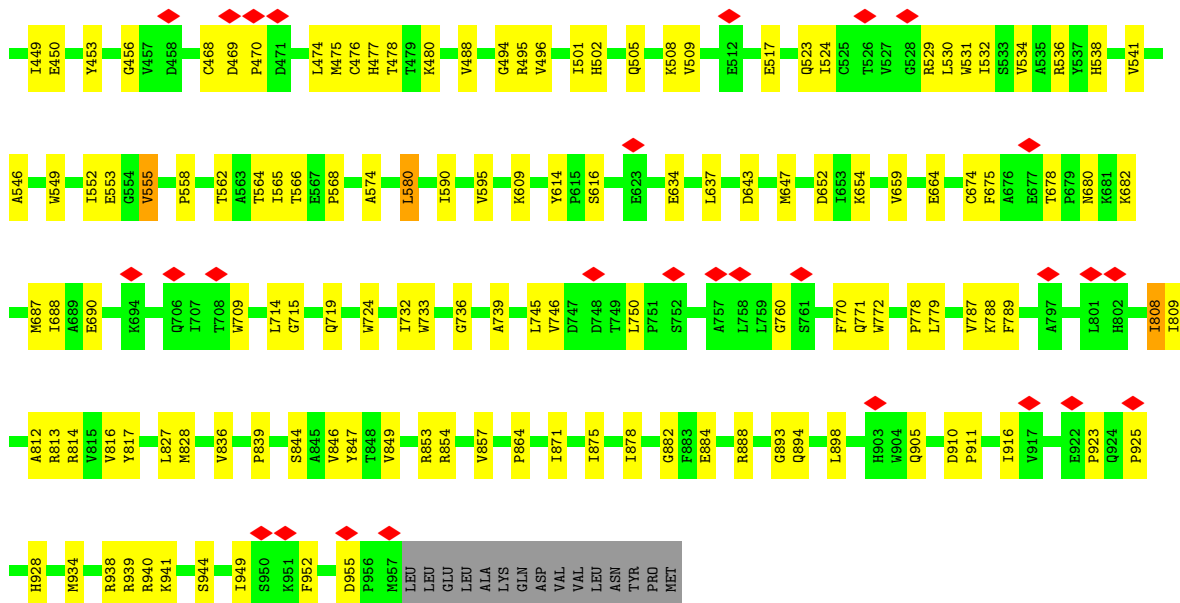
● Molecule 8: Pre-mRNA-processing-splicing factor 8



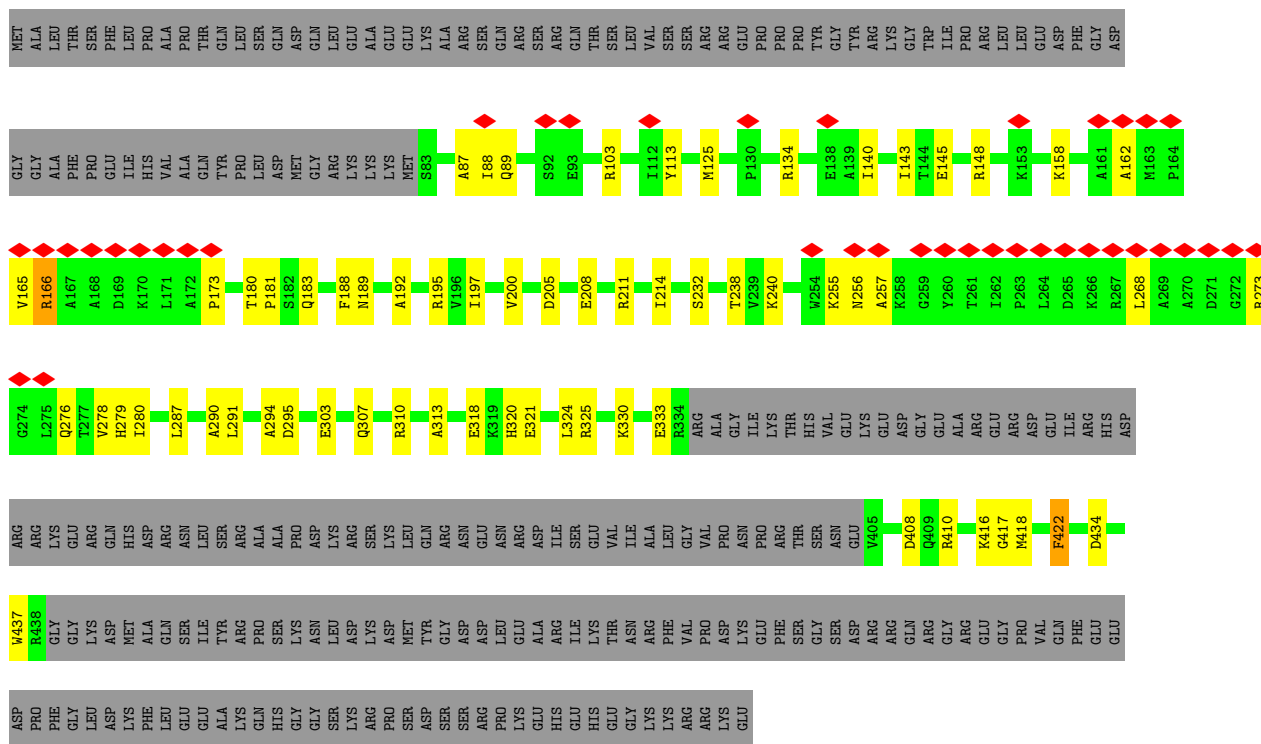
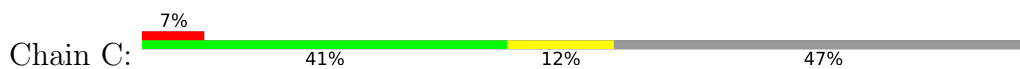


• Molecule 9: 116 kDa U5 small nuclear ribonucleoprotein component

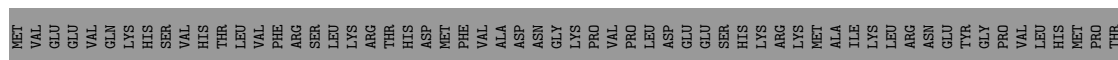




• Molecule 10: SNW domain-containing protein 1

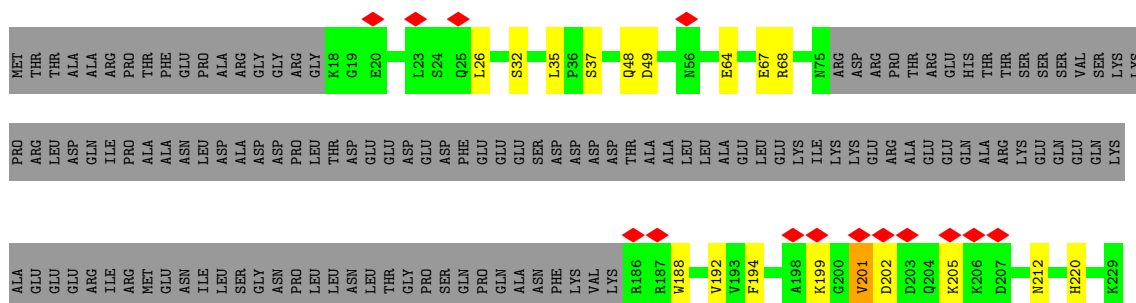
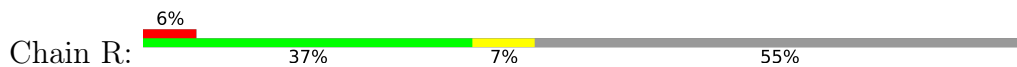


• Molecule 11: Pleiotropic regulator 1





• Molecule 17: Spliceosome-associated protein CWC15 homolog



• Molecule 18: Serine/arginine repetitive matrix protein 2



HIS ARG
ALA ALA
THR THR
GLY GLY
GLU GLY
GLY GLY
ALA ALA
SER ASP
SER ASP
LEU LEU
PRO PRO
GLU GLU
THR THR

● Molecule 24: Splicing factor 3B subunit 1



MET ALA
ALA ALA
LEU LEU
GLU THR
ASP ASP
PRO ASP
THR THR
HIS HIS
ASP ASP
GLU GLU
SER ASP
ASP ASP
LEU LEU
PRO PRO
GLN GLN
ILE ILE
SER SER
PRO PRO
ASP ASP
THR THR

THR GLU
LEU LEU
GLU THR
ASP ASP
PRO ASP
THR THR
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SER SER
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TRP TRP
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GLY THR
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LEU THR
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TRP TRP
ASP ASP
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ALA ALA
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MET MET
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GLY GLY
HIS HIS
ILE ILE
MET MET
THR THR
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ALA ALA
TYR TYR
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GLY GLY
THR THR
PRO PRO
LYS LYS
THR THR
ALA ALA
GLY GLY
PRO PRO
ILE ILE

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L539 L544
H572 I578
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R590 G443
I596 R451
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D458 Q459
P460 N463
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E870 E873
D883 E889
I893 Q901
M910 F914
I1188 M1161
V1169 T1170
P1171 E1174
M1178 Y1214
S1223 P1224

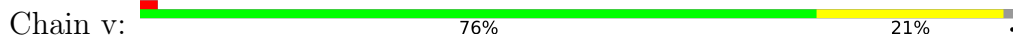
H971 I1000
V1003 I1004
G1005 M1006
P1018 R1027
I1036 R1053
L1065 I1066
K1087 I1073
M1100 R1106
R1109 E1299
L1300 T1112
P1125 L1129
P1130 M1133
R1137 E1140
V1143 I1158
M1161 V1169
T1170 P1171
E1174 M1178
Y1214 S1223
P1224

H1225 V1226
I1227 L1234
R1245 M1246
L1247 Q1248
Y1249 P1257
A1258 V1261
R1280 L1280
I1281 R1286
I1287 Y1288
I1296 R1297
Y1298 R113
E1299 L1300
D1301 Y1302
I1303 L1304

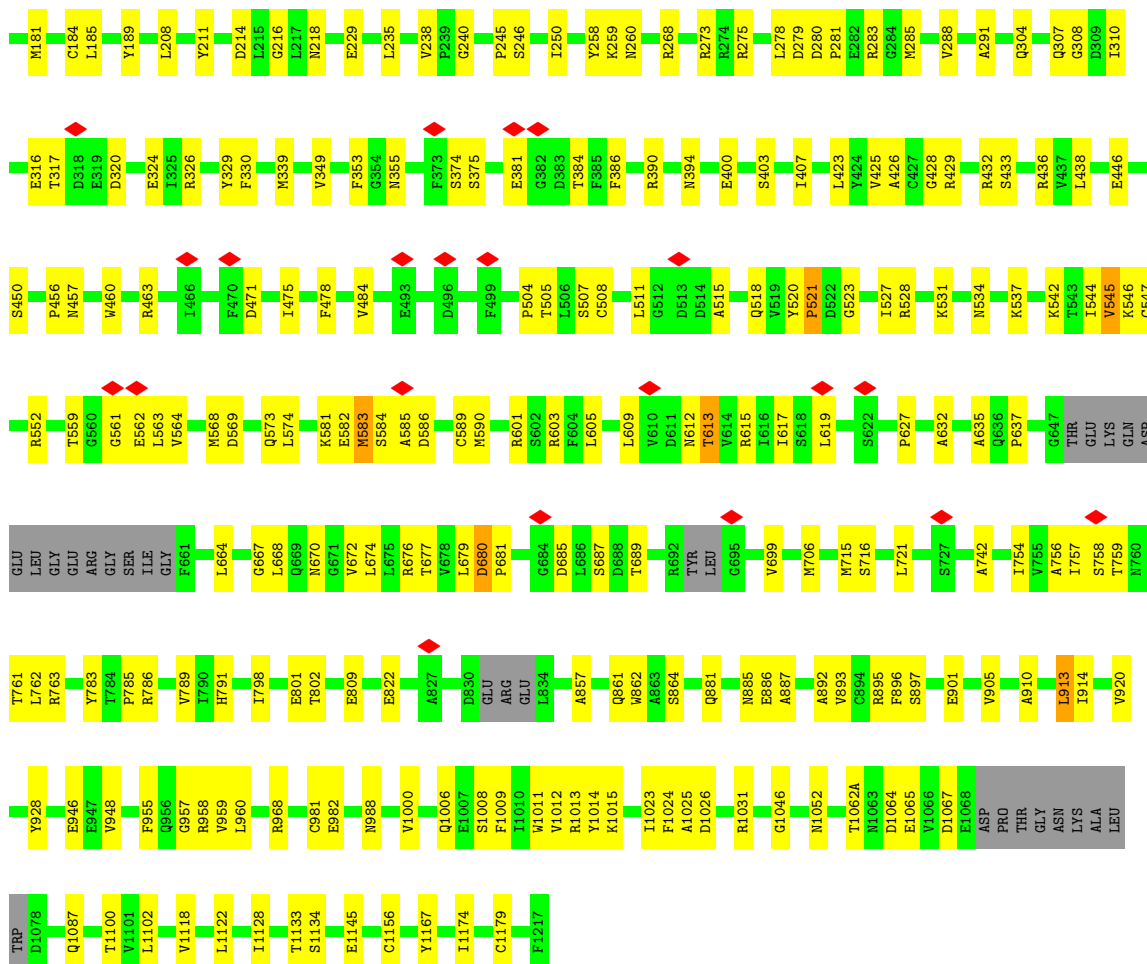
H1225 V1226
I1227 L1234
R1245 M1246
L1247 Q1248
Y1249 P1257
A1258 V1261
R1280 L1280
I1281 R1286
I1287 Y1288
I1296 R1297
Y1298 R113
E1299 L1300
D1301 Y1302
I1303 L1304

H1225 V1226
I1227 L1234
R1245 M1246
L1247 Q1248
Y1249 P1257
A1258 V1261
R1280 L1280
I1281 R1286
I1287 Y1288
I1296 R1297
Y1298 R113
E1299 L1300
D1301 Y1302
I1303 L1304

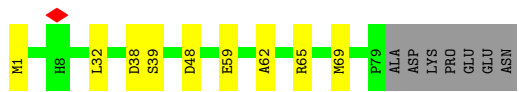
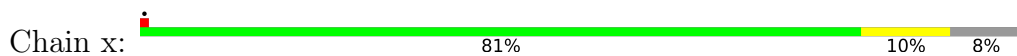
● Molecule 25: Splicing factor 3B subunit 3



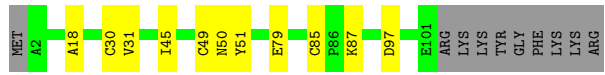
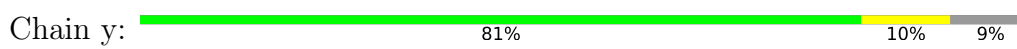
H1 T12
R34 I37
L38 E39
S64 L70
V79 W80
R81 S82
D83 W88
I89 K109
S110 G111
C112 R113
R114 L115
V116 P117
G118 Q119
F120 L121
A122 S133
E136 K137
Q138 K139
L140 V141
R146 R151
L158 H161
V170 V175
E178



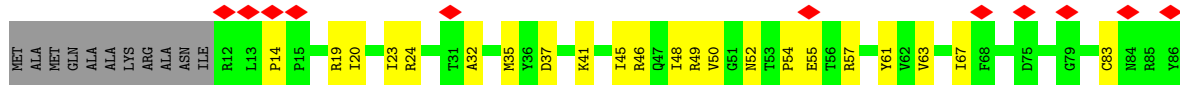
• Molecule 26: Splicing factor 3B subunit 5



• Molecule 27: PHD finger-like domain-containing protein 5A



• Molecule 28: Splicing factor 3B subunit 6



L87	L112
LEU	LYS
LYS	GLU
LYS	LYS
TYR	GLY
ILE	ASN
THR	THR
ASP	ASP
PRO	PRO
PRO	LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.314	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (\AA)	487.19998, 487.19998, 487.19998	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.16, 1.16, 1.16	Depositor

5 Model quality

5.1 Standard geometry

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

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	1	0.38	0/999	0.71	0/1347
2	2	0.39	0/1404	0.49	0/2177
3	3	0.34	0/1002	0.80	1/1341 (0.1%)
4	5	0.49	0/1638	0.57	1/2545 (0.0%)
5	6	0.45	0/2279	0.48	0/3551
6	7	0.44	0/744	0.75	0/993
7	8	0.45	0/1239	0.74	0/1660
8	A	0.54	0/19083	0.82	20/25888 (0.1%)
9	B	0.39	0/7299	0.83	9/9917 (0.1%)
10	C	0.41	0/2328	0.85	2/3128 (0.1%)
11	D	0.59	0/2584	0.89	8/3522 (0.2%)
12	E	0.29	0/1079	0.69	2/1453 (0.1%)
13	L	0.48	0/879	0.82	1/1184 (0.1%)
14	O	0.36	0/2295	0.78	4/3088 (0.1%)
15	P	0.37	0/2354	0.76	0/3176
16	Q	0.45	0/1178	0.79	0/1579
17	R	0.40	0/881	0.88	6/1169 (0.5%)
18	S	0.34	0/265	0.70	0/355
19	V	0.24	0/1268	0.59	0/1714
20	Y	0.33	0/775	0.67	1/1045 (0.1%)
21	Z	0.42	0/1129	0.48	0/1752
22	s	0.45	0/1411	0.72	0/1911
23	t	0.38	0/1447	0.76	0/1945
24	u	0.51	0/7147	0.79	1/9675 (0.0%)
25	v	0.45	0/9504	0.74	2/12894 (0.0%)
26	x	0.53	0/675	0.77	0/912
27	y	0.51	0/779	0.66	0/1047
28	z	0.34	1/857 (0.1%)	0.74	0/1157
All	All	0.47	1/74522 (0.0%)	0.77	58/102125 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	3	0	1
8	A	0	19
9	B	0	8
10	C	0	3
11	D	0	5
13	L	0	1
14	O	0	2
15	P	0	3
22	s	0	1
23	t	0	1
24	u	0	6
25	v	0	5
28	z	0	2
All	All	0	57

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	z	14	PRO	C-N	5.38	1.46	1.33

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	R	201	VAL	CA-C-N	6.92	138.70	126.45
17	R	201	VAL	C-N-CA	6.92	138.70	126.45
8	A	1483	GLY	N-CA-C	-6.86	103.68	115.61
11	D	317	VAL	CA-C-N	6.49	133.93	121.54
11	D	317	VAL	C-N-CA	6.49	133.93	121.54
3	3	587	VAL	N-CA-C	6.44	113.11	106.21
12	E	146	HIS	CA-C-N	6.38	133.72	121.54
12	E	146	HIS	C-N-CA	6.38	133.72	121.54
8	A	705	LYS	CA-C-N	6.28	133.53	121.54
8	A	705	LYS	C-N-CA	6.28	133.53	121.54
9	B	72	VAL	N-CA-C	-6.17	107.23	113.47
20	Y	95	GLY	N-CA-C	-6.16	107.15	114.48
14	O	445	LYS	CA-C-N	6.14	133.28	121.54
14	O	445	LYS	C-N-CA	6.14	133.28	121.54
8	A	253	ASN	N-CA-C	-6.08	106.84	114.56
11	D	381	HIS	CA-C-N	5.94	141.25	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	381	HIS	C-N-CA	5.94	141.25	127.00
8	A	273	ILE	N-CA-C	-5.88	103.56	109.02
11	D	381	HIS	C-N-CD	-5.87	107.68	120.60
8	A	902	TYR	CA-C-N	5.86	132.74	121.54
8	A	902	TYR	C-N-CA	5.86	132.74	121.54
14	O	389	HIS	CA-C-N	5.74	132.51	121.54
14	O	389	HIS	C-N-CA	5.74	132.51	121.54
8	A	166	PHE	N-CA-C	5.64	122.28	109.81
8	A	1497	THR	CA-C-N	5.61	132.25	121.54
8	A	1497	THR	C-N-CA	5.61	132.25	121.54
8	A	1514	LYS	N-CA-C	-5.54	97.97	107.61
8	A	1773	SER	CA-C-N	5.53	132.10	121.54
8	A	1773	SER	C-N-CA	5.53	132.10	121.54
11	D	384	HIS	N-CA-C	5.52	122.55	110.80
8	A	1446	GLN	N-CA-C	-5.51	99.07	110.80
10	C	278	VAL	CA-C-N	5.50	132.04	121.54
10	C	278	VAL	C-N-CA	5.50	132.04	121.54
25	v	137	LYS	CA-C-N	-5.49	112.27	121.94
25	v	137	LYS	C-N-CA	-5.49	112.27	121.94
24	u	695	VAL	N-CA-C	-5.47	107.94	113.20
9	B	138	LEU	N-CA-C	5.47	116.93	110.97
9	B	517	GLU	N-CA-C	-5.45	107.64	114.56
8	A	300	ASN	CA-C-N	5.42	133.80	122.58
8	A	300	ASN	C-N-CA	5.42	133.80	122.58
11	D	400	PHE	N-CA-C	5.41	120.10	112.75
11	D	381	HIS	N-CA-C	5.40	121.73	109.81
17	R	32	SER	CA-C-N	5.36	131.78	121.54
17	R	32	SER	C-N-CA	5.36	131.78	121.54
17	R	49	ASP	CA-C-N	5.36	128.28	120.51
17	R	49	ASP	C-N-CA	5.36	128.28	120.51
9	B	808	ILE	CA-C-N	5.34	125.55	120.43
9	B	808	ILE	C-N-CA	5.34	125.55	120.43
8	A	647	LEU	CA-C-N	-5.17	112.44	122.06
8	A	647	LEU	C-N-CA	-5.17	112.44	122.06
9	B	925	PRO	N-CA-C	-5.16	108.79	114.92
8	A	959	ILE	CA-C-N	-5.12	114.09	122.54
8	A	959	ILE	C-N-CA	-5.12	114.09	122.54
9	B	65	TYR	CA-CB-CG	5.08	123.04	113.90
9	B	816	VAL	CA-C-N	-5.08	111.68	121.58
9	B	816	VAL	C-N-CA	-5.08	111.68	121.58
13	L	62	GLU	CA-CB-CG	5.06	124.23	114.10
4	5	26	A	P-O3'-C3'	5.04	127.76	120.20

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	568	GLY	Peptide
8	A	1075	GLN	Peptide
8	A	1183	PRO	Peptide
8	A	1206	GLU	Peptide
8	A	1213	VAL	Peptide
8	A	1491	LYS	Peptide
8	A	1493	THR	Peptide
8	A	1512	SER	Peptide
8	A	1513	MET	Peptide
8	A	1514	LYS	Peptide
8	A	1547	VAL	Peptide
8	A	1593	LEU	Peptide
8	A	1635	TYR	Peptide
8	A	1636	LYS	Peptide
8	A	165	ARG	Peptide
8	A	1699	THR	Peptide
8	A	1719	PHE	Peptide
8	A	175	PRO	Peptide
8	A	210	HIS	Peptide
8	A	521	ASN	Peptide
9	B	318	PHE	Peptide
9	B	352	LYS	Peptide
9	B	438	ILE	Peptide
9	B	440	SER	Peptide
9	B	469	ASP	Peptide
9	B	65	TYR	Peptide
9	B	750	LEU	Peptide
9	B	941	LYS	Peptide
10	C	103	ARG	Peptide
10	C	166	ARG	Peptide
10	C	422	PHE	Peptide
11	D	187	LYS	Peptide
11	D	380	LEU	Peptide
11	D	383	ARG	Peptide
11	D	393	ASP	Peptide
11	D	455	GLN	Peptide
13	L	91	ARG	Peptide
14	O	391	TYR	Peptide
14	O	405	PHE	Peptide
15	P	112	VAL	Peptide

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Mol	Chain	Res	Type	Group
15	P	113	ASN	Peptide
15	P	276	THR	Peptide
22	s	148	ASP	Peptide
23	t	118	ALA	Peptide
24	u	1125	PRO	Peptide
24	u	460	PRO	Peptide
24	u	463	ASN	Peptide
24	u	464	LEU	Peptide
24	u	483	ASP	Peptide
24	u	494	GLU	Peptide
25	v	259	LYS	Peptide
25	v	544	ILE	Peptide
25	v	582	GLU	Peptide
25	v	584	SER	Peptide
25	v	913	LEU	Peptide
28	z	32	ALA	Peptide
28	z	83	CYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	981	0	976	16	0
2	2	1262	0	640	11	0
3	3	981	0	961	13	0
4	5	1470	0	746	17	0
5	6	2035	0	1028	25	0
6	7	733	0	720	10	0
7	8	1211	0	1248	13	0
8	A	18569	0	18479	309	0
9	B	7137	0	7149	140	0
10	C	2287	0	2314	47	0
11	D	2517	0	2471	46	0
12	E	1054	0	988	10	0
13	L	858	0	868	20	0
14	O	2235	0	2153	30	0
15	P	2305	0	2282	46	0
16	Q	1153	0	1160	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	R	869	0	855	12	0
18	S	261	0	267	1	0
19	V	1236	0	1210	25	0
20	Y	762	0	779	9	0
21	Z	1013	0	515	16	0
22	s	1377	0	1314	15	0
23	t	1415	0	1337	28	0
24	u	7013	0	7199	94	0
25	v	9315	0	9235	156	0
26	x	656	0	622	9	0
27	y	766	0	738	7	0
28	z	839	0	841	15	0
29	6	4	0	0	0	0
30	A	36	0	6	11	0
31	B	32	0	12	1	0
32	P	3	0	0	0	0
32	Q	3	0	0	0	0
32	t	1	0	0	0	0
32	y	3	0	0	0	0
All	All	72392	0	69113	1006	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 7.

All (1006) 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)
8:A:613:TYR:HE2	30:A:3001:IHP:O42	1.25	1.18
8:A:442:LYS:NZ	30:A:3001:IHP:O43	1.76	1.16
8:A:163:ARG:NH2	30:A:3001:IHP:O36	1.84	1.10
8:A:613:TYR:CE2	30:A:3001:IHP:O42	2.16	0.98
2:2:12:G:H1	5:6:86:U:H3	0.91	0.90
8:A:1706:ASP:O	8:A:1710:ASN:HA	1.73	0.89
8:A:613:TYR:CE2	30:A:3001:IHP:H1	2.11	0.85
4:5:24:G:N3	4:5:26:A:N6	2.35	0.75
8:A:1493:THR:HG22	8:A:1744:ARG:HB3	1.69	0.74
15:P:278:GLN:O	15:P:281:GLU:HB3	1.85	0.74
14:O:454:ASN:O	14:O:458:PHE:HB2	1.88	0.73
8:A:1543:ASN:HD21	8:A:1563:HIS:H	1.37	0.71
25:v:304:GLN:HE21	25:v:308:GLY:HA2	1.56	0.70
6:7:6:ARG:NH1	21:Z:243:G:N7	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:468:CYS:HB2	9:B:546:ALA:H	1.58	0.69
24:u:935:THR:O	24:u:939:ARG:HB2	1.93	0.69
8:A:1575:GLN:HB3	23:t:220:LEU:HD11	1.74	0.68
9:B:238:ASN:O	9:B:242:LEU:HB2	1.94	0.68
4:5:27:U:OP1	8:A:635:ARG:NH2	2.27	0.68
8:A:609:LYS:HZ1	30:A:3001:IHP:H4	1.58	0.67
8:A:1160:ARG:HD2	17:R:192:VAL:HG21	1.75	0.67
16:Q:100:LEU:HD11	16:Q:106:ILE:HD11	1.76	0.67
24:u:971:MET:HB3	24:u:1004:ILE:HD11	1.76	0.67
25:v:568:MET:HA	25:v:574:LEU:HA	1.77	0.67
13:L:30:GLN:HE21	13:L:33:ARG:HD2	1.60	0.66
25:v:668:LEU:HD12	25:v:670:ASN:H	1.59	0.66
8:A:946:GLU:HB3	8:A:949:PRO:HD2	1.77	0.66
8:A:1838:LYS:HA	8:A:1868:MET:HE2	1.76	0.66
24:u:806:ILE:HG12	24:u:810:ILE:HD12	1.78	0.66
25:v:664:LEU:HB3	25:v:676:ARG:HB2	1.78	0.66
25:v:615:ARG:HD2	25:v:627:PRO:HB3	1.78	0.66
5:6:64:U:OP2	8:A:663:ARG:NH2	2.28	0.65
9:B:135:CYS:O	9:B:142:LYS:NZ	2.28	0.65
3:3:566:TYR:HB2	3:3:583:ARG:HA	1.78	0.65
23:t:305:GLY:HA2	25:v:632:ALA:HB3	1.78	0.65
4:5:62:G:N2	4:5:63:A:N7	2.45	0.65
15:P:261:ILE:HG22	15:P:272:ILE:HG22	1.79	0.65
8:A:1519:THR:H	8:A:1522:GLN:HE21	1.43	0.65
9:B:509:VAL:HA	9:B:565:ILE:HG22	1.79	0.65
8:A:1553:VAL:HG12	23:t:194:ARG:HB2	1.79	0.65
25:v:783:TYR:HB2	25:v:801:GLU:HB3	1.80	0.64
23:t:296:CYS:SG	23:t:297:TYR:N	2.69	0.64
25:v:981:CYS:SG	25:v:982:GLU:N	2.69	0.64
25:v:456:PRO:HA	25:v:478:PHE:HB3	1.80	0.64
25:v:109:LYS:NZ	27:y:79:GLU:O	2.30	0.64
5:6:19:C:O2'	16:Q:120:ARG:NH1	2.29	0.64
25:v:1052:ASN:HD21	25:v:1167:TYR:HB2	1.63	0.63
7:8:561:MET:HE2	24:u:1053:ARG:HD2	1.81	0.63
8:A:1963:GLU:OE2	8:A:1966:HIS:ND1	2.31	0.63
9:B:476:CYS:HB2	9:B:496:VAL:HA	1.81	0.63
25:v:403:SER:O	25:v:436:ARG:NH1	2.31	0.63
8:A:1491:LYS:HE2	8:A:1710:ASN:HB3	1.81	0.62
25:v:273:ARG:NH1	25:v:285:MET:SD	2.72	0.62
9:B:250:ARG:NH2	9:B:450:GLU:OE1	2.32	0.62
9:B:827:LEU:HD11	9:B:934:MET:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:70:VAL:O	15:P:82:GLN:NE2	2.32	0.62
8:A:951:LEU:HD23	8:A:952:VAL:HG13	1.80	0.62
9:B:134:LEU:HB3	9:B:226:VAL:HG13	1.81	0.62
9:B:222:SER:OG	9:B:223:ASP:N	2.33	0.62
24:u:413:LYS:HG3	28:z:52:ASN:HD21	1.64	0.62
25:v:463:ARG:HG2	25:v:471:ASP:HA	1.82	0.62
12:E:103:GLN:O	12:E:108:ARG:NH2	2.33	0.61
24:u:670:GLN:HA	24:u:673:ILE:HG12	1.82	0.61
8:A:1745:GLU:HB3	8:A:1748:ARG:HH11	1.66	0.61
8:A:1413:ASP:O	8:A:1418:ARG:NH1	2.31	0.61
9:B:502:HIS:HB2	9:B:505:GLN:HE22	1.64	0.61
9:B:674:CYS:SG	9:B:675:PHE:N	2.73	0.61
25:v:893:VAL:HG12	25:v:905:VAL:HG22	1.81	0.61
9:B:157:ILE:HB	9:B:159:LYS:HG3	1.82	0.61
14:O:431:ARG:HH22	14:O:459:GLU:HA	1.64	0.61
5:6:35:A:N7	21:Z:254:G:N1	2.49	0.61
8:A:889:ARG:NH1	8:A:1004:ASN:O	2.33	0.61
9:B:552:ILE:HD13	9:B:555:VAL:H	1.66	0.61
20:Y:94:ASN:ND2	20:Y:97:ASN:OD1	2.34	0.61
9:B:410:LEU:HD23	9:B:414:PRO:HB2	1.82	0.61
8:A:79:ARG:O	8:A:82:ARG:NH1	2.34	0.60
9:B:888:ARG:HG2	9:B:893:GLY:HA2	1.82	0.60
19:V:81:GLN:HG2	19:V:107:THR:HG23	1.84	0.60
24:u:652:CYS:O	24:u:692:HIS:NE2	2.35	0.60
1:1:40:LEU:HD12	1:1:80:CYS:HB3	1.84	0.60
5:6:21:U:H2'	12:E:130:ARG:HE	1.65	0.60
8:A:2127:TYR:HB2	8:A:2146:VAL:HB	1.82	0.60
5:6:93:G:O2'	14:O:347:HIS:NE2	2.30	0.60
8:A:1080:GLU:O	8:A:1086:ARG:NH1	2.34	0.60
19:V:69:GLY:O	19:V:152:ARG:NH1	2.35	0.60
8:A:1000:ILE:HG13	8:A:1001:VAL:HG23	1.84	0.60
8:A:693:ILE:HG21	8:A:709:ILE:HG21	1.83	0.60
1:1:7:VAL:HG22	1:1:108:ARG:HB3	1.82	0.60
8:A:159:ARG:NH2	8:A:160:HIS:O	2.35	0.60
8:A:491:GLU:OE2	8:A:495:GLN:NE2	2.35	0.59
25:v:117:PRO:HD3	25:v:138:GLN:HE21	1.65	0.59
8:A:1611:LYS:HA	8:A:1629:ILE:HG22	1.83	0.59
8:A:1724:PRO:O	8:A:1728:GLN:NE2	2.35	0.59
10:C:318:GLU:O	10:C:321:GLU:HB2	2.02	0.59
13:L:59:LYS:O	13:L:91:ARG:NH2	2.36	0.59
15:P:262:THR:HG22	15:P:271:PHE:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:234:LEU:HD21	15:P:300:VAL:HG13	1.84	0.59
25:v:330:PHE:O	25:v:390:ARG:NH2	2.35	0.59
8:A:162:LYS:O	8:A:573:GLN:NE2	2.36	0.59
9:B:186:VAL:HA	9:B:534:VAL:HA	1.85	0.59
14:O:411:MET:HE3	14:O:441:ASP:HB2	1.84	0.59
25:v:699:VAL:HA	25:v:715:MET:O	2.01	0.59
8:A:1640:SER:OG	8:A:1641:ARG:N	2.35	0.59
25:v:114:ARG:NH1	26:x:38:ASP:OD1	2.36	0.59
9:B:772:TRP:O	9:B:813:ARG:NH2	2.35	0.59
22:s:15:VAL:HG12	22:s:166:VAL:HA	1.83	0.59
8:A:686:ARG:HA	8:A:689:VAL:HG12	1.84	0.59
25:v:12:THR:O	25:v:34:ARG:NH1	2.36	0.59
17:R:199:LYS:HB3	17:R:202:ASP:HA	1.84	0.58
20:Y:55:ARG:NH1	20:Y:58:GLU:OE1	2.36	0.58
1:1:37:TRP:HA	1:1:82:LEU:O	2.03	0.58
8:A:80:LYS:NZ	16:Q:37:HIS:O	2.35	0.58
8:A:300:ASN:O	9:B:939:ARG:NH1	2.36	0.58
30:A:3001:IHP:O44	30:A:3001:IHP:H3	2.02	0.58
24:u:1133:MET:HE1	24:u:1169:VAL:HG12	1.84	0.58
25:v:423:LEU:HB2	25:v:438:LEU:HB2	1.84	0.58
25:v:601:ARG:NH1	25:v:603:ARG:O	2.36	0.58
8:A:940:ILE:HD12	8:A:1090:ARG:HH21	1.67	0.58
8:A:1893:PHE:O	8:A:1896:CYS:HB2	2.03	0.58
15:P:167:PHE:O	15:P:172:GLU:N	2.37	0.58
8:A:2191:GLN:NE2	8:A:2244:LYS:O	2.36	0.58
15:P:227:GLU:HG3	15:P:230:THR:HG22	1.84	0.58
24:u:714:GLU:O	27:y:51:TYR:OH	2.22	0.58
25:v:279:ASP:OD2	25:v:307:GLN:NE2	2.37	0.58
1:1:55:VAL:HG23	3:3:589:ARG:HD3	1.86	0.58
8:A:974:ASN:HB2	8:A:1178:TYR:HB3	1.84	0.58
3:3:574:ASN:HD21	3:3:580:PRO:HG3	1.68	0.58
8:A:689:VAL:HG23	8:A:738:MET:HE2	1.86	0.57
9:B:221:ILE:HG23	9:B:495:ARG:HB2	1.86	0.57
15:P:175:ARG:HE	15:P:179:CYS:HA	1.68	0.57
24:u:398:PRO:HD3	28:z:19:ARG:HH11	1.68	0.57
25:v:609:LEU:HB2	25:v:613:THR:HG23	1.87	0.57
7:8:495:ARG:NH2	25:v:1026:ASP:OD2	2.36	0.57
24:u:901:GLN:O	24:u:939:ARG:NH1	2.37	0.57
25:v:699:VAL:HG12	25:v:716:SER:HB2	1.85	0.57
25:v:79:VAL:HG22	25:v:89:ILE:HG12	1.87	0.57
8:A:512:ASN:ND2	21:Z:254:G:O2'	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:v:664:LEU:HD22	25:v:676:ARG:HD2	1.85	0.57
2:2:12:G:O6	5:6:86:U:O4	2.23	0.57
8:A:762:ARG:HG3	8:A:903:SER:HB3	1.85	0.57
9:B:141:GLY:N	31:B:1500:GTP:O2B	2.38	0.57
19:V:35:THR:HG22	19:V:82:PHE:HE2	1.70	0.57
8:A:362:ARG:HH21	9:B:279:ARG:HD3	1.70	0.57
8:A:470:ARG:HE	10:C:166:ARG:HD3	1.69	0.57
8:A:975:VAL:HG13	8:A:1099:PHE:HD2	1.70	0.57
8:A:1956:PRO:HD2	8:A:1960:THR:HG21	1.86	0.57
9:B:678:THR:HG22	9:B:682:LYS:H	1.69	0.57
8:A:1463:LYS:HE3	10:C:434:ASP:HB3	1.87	0.57
8:A:2002:LEU:HD22	8:A:2006:GLU:HG2	1.85	0.57
9:B:366:GLN:HB3	9:B:370:VAL:HG23	1.87	0.57
25:v:1145:GLU:HG2	25:v:1174:ILE:HG23	1.87	0.57
8:A:787:GLU:OE2	8:A:790:ARG:NH1	2.36	0.56
8:A:2169:LEU:HB2	8:A:2272:MET:HE3	1.86	0.56
25:v:450:SER:HB2	25:v:762:LEU:HB3	1.86	0.56
8:A:909:TYR:HB2	8:A:1033:GLY:HA3	1.87	0.56
8:A:1275:ARG:NH2	8:A:1464:LEU:O	2.38	0.56
9:B:384:VAL:HG23	9:B:392:LEU:HD11	1.86	0.56
8:A:173:GLU:OE2	22:s:90:ARG:NH1	2.38	0.56
17:R:201:VAL:HG21	17:R:205:LYS:HB2	1.86	0.56
25:v:946:GLU:OE2	25:v:968:ARG:NH2	2.37	0.56
9:B:779:LEU:O	9:B:938:ARG:NH1	2.39	0.56
9:B:844:SER:HA	9:B:847:TYR:HD2	1.71	0.56
11:D:381:HIS:ND1	11:D:383:ARG:O	2.38	0.56
15:P:240:GLY:H	15:P:268:GLN:HB3	1.71	0.56
9:B:690:GLU:OE2	9:B:788:LYS:NZ	2.38	0.56
25:v:862:TRP:HB3	25:v:887:ALA:HB2	1.88	0.56
8:A:165:ARG:HG3	23:t:118:ALA:HB3	1.88	0.56
8:A:962:LEU:HB2	8:A:965:VAL:HG22	1.86	0.56
9:B:687:MET:HE1	9:B:789:PHE:HD2	1.70	0.56
15:P:66:LYS:NZ	21:Z:261:A:OP1	2.39	0.56
8:A:857:ASN:OD1	8:A:858:GLN:N	2.38	0.56
8:A:1133:CYS:SG	8:A:1231:ARG:NE	2.79	0.56
8:A:1418:ARG:HE	8:A:1464:LEU:HD23	1.70	0.56
9:B:230:ASP:OD2	9:B:262:ARG:NH1	2.39	0.56
25:v:677:THR:N	25:v:685:ASP:O	2.38	0.56
9:B:100:LYS:NZ	9:B:647:MET:SD	2.76	0.56
15:P:24:CYS:H	15:P:81:CYS:HB2	1.71	0.56
16:Q:139:CYS:SG	16:Q:140:ARG:N	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:v:612:ASN:ND2	25:v:635:ALA:O	2.39	0.56
25:v:680:ASP:OD1	25:v:680:ASP:N	2.35	0.56
5:6:65:G:N7	8:A:663:ARG:NH1	2.51	0.56
8:A:1231:ARG:NH2	8:A:1283:GLU:OE1	2.38	0.56
8:A:1496:PRO:HG2	8:A:1497:THR:HG23	1.88	0.56
9:B:523:GLN:HB3	9:B:558:PRO:HG3	1.87	0.56
15:P:78:LYS:NZ	15:P:203:TYR:OH	2.36	0.56
15:P:163:HIS:HA	15:P:182:ARG:HH21	1.71	0.56
8:A:439:GLN:O	8:A:444:ARG:NH2	2.38	0.55
8:A:1604:LEU:HD23	8:A:1605:GLU:HG3	1.87	0.55
9:B:106:GLU:HG2	9:B:107:GLN:HG2	1.87	0.55
9:B:478:THR:HA	9:B:494:GLY:HA3	1.89	0.55
11:D:220:VAL:HG23	11:D:230:ILE:HG22	1.89	0.55
11:D:370:ASN:HB3	11:D:396:LYS:HE3	1.87	0.55
25:v:245:PRO:HG3	25:v:317:THR:HG21	1.88	0.55
25:v:637:PRO:HA	25:v:668:LEU:HA	1.88	0.55
8:A:1382:SER:HA	8:A:1415:GLY:HA2	1.87	0.55
9:B:94:ILE:HG23	17:R:48:GLN:HG2	1.87	0.55
10:C:238:THR:HG21	10:C:240:LYS:HE3	1.89	0.55
15:P:64:ARG:NH2	21:Z:261:A:OP2	2.39	0.55
25:v:520:TYR:H	25:v:523:GLY:HA2	1.70	0.55
3:3:559:ASN:ND2	3:3:563:ARG:O	2.35	0.55
9:B:916:ILE:HD11	9:B:928:HIS:HB2	1.88	0.55
10:C:134:ARG:NE	11:D:382:PRO:O	2.36	0.55
2:2:13:C:H1'	2:2:14:C:H5	1.72	0.55
5:6:65:G:H21	5:6:69:A:H2	1.53	0.55
8:A:1644:LEU:O	8:A:1723:LYS:NZ	2.40	0.55
15:P:146:MET:HB3	15:P:216:ARG:HH22	1.71	0.55
8:A:1483:GLY:O	8:A:1487:HIS:N	2.31	0.55
8:A:1510:GLU:HG2	8:A:1513:MET:HA	1.88	0.55
19:V:48:TYR:OH	19:V:110:SER:O	2.21	0.55
4:5:36:C:H42	4:5:46:U:H3	1.52	0.55
16:Q:117:CYS:SG	16:Q:118:ILE:N	2.80	0.55
25:v:133:SER:HB2	25:v:139:LYS:HG2	1.87	0.55
25:v:185:LEU:HG	25:v:235:LEU:HD11	1.88	0.55
8:A:305:ARG:HH11	9:B:854:ARG:HH22	1.55	0.55
8:A:945:THR:OG1	8:A:946:GLU:N	2.38	0.55
8:A:2278:SER:OG	8:A:2309:HIS:NE2	2.32	0.55
9:B:733:TRP:HB2	9:B:745:LEU:HD11	1.88	0.55
25:v:1009:PHE:HZ	25:v:1046:GLY:HA3	1.71	0.55
8:A:35:ARG:O	8:A:39:GLN:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:200:ASP:OD1	8:A:240:ARG:NH2	2.39	0.55
25:v:605:LEU:HD22	25:v:619:LEU:HD11	1.88	0.55
8:A:1530:PRO:HA	8:A:1533:ARG:HG2	1.90	0.54
25:v:288:VAL:HG12	26:x:62:ALA:HB3	1.89	0.54
25:v:324:GLU:OE2	25:v:326:ARG:NH1	2.40	0.54
11:D:392:PRO:HG3	11:D:415:ILE:HA	1.90	0.54
1:l:31:GLU:OE2	24:u:821:HIS:N	2.40	0.54
8:A:358:PRO:O	8:A:362:ARG:NH1	2.40	0.54
8:A:1459:ARG:HD2	10:C:417:GLY:HA3	1.90	0.54
9:B:80:ILE:HD11	11:D:200:ILE:HG12	1.89	0.54
15:P:90:TYR:HB3	15:P:92:LEU:HD13	1.89	0.54
19:V:26:GLU:OE1	19:V:131:ARG:NH2	2.40	0.54
23:t:262:CYS:SG	23:t:263:PHE:N	2.80	0.54
25:v:170:VAL:HG23	25:v:184:CYS:HB3	1.89	0.54
8:A:613:TYR:CZ	30:A:3001:IHP:H1	2.42	0.54
8:A:1124:ASN:OD1	8:A:1129:ASN:ND2	2.41	0.54
8:A:1640:SER:HB3	8:A:1718:TRP:H	1.73	0.54
9:B:160:ARG:NH2	9:B:313:GLN:OE1	2.40	0.54
19:V:25:LEU:HG	19:V:132:VAL:HG12	1.90	0.54
19:V:61:MET:HE2	19:V:63:GLN:HB2	1.89	0.54
8:A:386:PRO:HD2	8:A:389:LYS:HZ2	1.72	0.54
12:E:196:TRP:HA	16:Q:139:CYS:HB3	1.90	0.54
19:V:66:ASP:OD2	19:V:71:GLY:N	2.38	0.54
25:v:136:GLU:OE2	25:v:189:TYR:OH	2.23	0.54
8:A:881:ILE:O	8:A:885:LEU:HB2	2.06	0.54
25:v:374:SER:OG	25:v:375:SER:N	2.40	0.54
9:B:508:LYS:HA	9:B:524:ILE:HG22	1.89	0.54
9:B:595:VAL:HG22	9:B:654:LYS:HG3	1.90	0.54
9:B:719:GLN:NE2	9:B:724:TRP:O	2.41	0.54
8:A:1777:ILE:HG13	8:A:1860:GLN:HB3	1.90	0.54
16:Q:31:GLU:OE2	22:s:84:LYS:NZ	2.37	0.54
17:R:64:GLU:HG3	17:R:68:ARG:HE	1.73	0.54
25:v:446:GLU:OE1	25:v:763:ARG:NH1	2.41	0.54
8:A:103:LEU:HB3	8:A:638:LEU:HD11	1.90	0.53
8:A:1543:ASN:HB2	8:A:1569:LEU:HD21	1.90	0.53
9:B:151:GLU:OE1	9:B:159:LYS:NZ	2.40	0.53
22:s:41:ILE:HD13	22:s:169:ASN:HD21	1.73	0.53
25:v:511:LEU:O	25:v:552:ARG:NH2	2.38	0.53
8:A:285:ASP:HB3	8:A:286:ILE:HD12	1.90	0.53
8:A:552:ARG:NH1	8:A:588:LEU:O	2.41	0.53
11:D:422:ASN:OD1	11:D:423:SER:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:u:442:THR:OG1	24:u:443:GLY:N	2.42	0.53
25:v:426:ALA:HB1	25:v:785:PRO:HG2	1.90	0.53
4:5:28:A:H1'	8:A:642:ARG:HD2	1.90	0.53
8:A:1057:ARG:NH1	8:A:1060:GLU:OE1	2.39	0.53
10:C:165:VAL:HG13	10:C:166:ARG:HE	1.71	0.53
17:R:35:LEU:O	17:R:37:SER:N	2.41	0.53
23:t:262:CYS:N	23:t:267:GLN:O	2.42	0.53
7:8:522:PHE:HB3	24:u:1137:ARG:HG2	1.89	0.53
20:Y:49:LYS:NZ	20:Y:68:ILE:O	2.41	0.53
24:u:1174:GLU:HB2	24:u:1214:TYR:HE2	1.74	0.53
9:B:187:THR:H	9:B:534:VAL:HG12	1.74	0.53
25:v:886:GLU:HA	25:v:910:ALA:O	2.08	0.53
8:A:1890:GLN:NE2	8:A:2013:GLY:O	2.41	0.53
23:t:127:GLU:O	23:t:136:ARG:NH2	2.39	0.53
23:t:213:PHE:HB2	23:t:217:CYS:HB3	1.91	0.53
8:A:1206:GLU:O	8:A:1227:GLN:NE2	2.40	0.53
15:P:261:ILE:HA	15:P:271:PHE:O	2.08	0.53
25:v:70:LEU:HD21	25:v:146:ARG:HB2	1.90	0.53
25:v:667:GLY:HA2	25:v:672:VAL:HA	1.90	0.53
9:B:220:ARG:HE	9:B:580:LEU:HB3	1.74	0.53
9:B:678:THR:HG23	9:B:680:ASN:H	1.74	0.53
12:E:181:PHE:HD1	12:E:200:VAL:HG22	1.74	0.53
8:A:1519:THR:OG1	8:A:1520:ASN:N	2.42	0.53
9:B:477:HIS:NE2	9:B:562:THR:OG1	2.42	0.53
25:v:82:SER:OG	25:v:83:ASP:N	2.41	0.53
8:A:28:GLU:OE1	8:A:31:GLN:NE2	2.39	0.53
8:A:379:GLU:HB3	8:A:384:VAL:HG23	1.89	0.53
9:B:133:THR:HG23	9:B:222:SER:HB3	1.90	0.53
11:D:457:GLY:HA3	17:R:212:ASN:H	1.74	0.53
28:z:45:ILE:HD11	28:z:48:ILE:HG23	1.91	0.53
8:A:1124:ASN:O	8:A:1129:ASN:ND2	2.42	0.52
8:A:1491:LYS:HD2	8:A:1744:ARG:HG2	1.90	0.52
8:A:1740:LEU:O	8:A:1744:ARG:NH1	2.42	0.52
10:C:208:GLU:OE1	10:C:211:ARG:NH2	2.42	0.52
25:v:706:MET:HE3	25:v:721:LEU:HD21	1.91	0.52
8:A:1482:GLU:HG3	8:A:1483:GLY:H	1.73	0.52
8:A:2130:GLY:HA3	8:A:2142:ILE:HA	1.91	0.52
12:E:132:PHE:HB2	12:E:138:ALA:HB2	1.91	0.52
15:P:68:THR:HG23	15:P:82:GLN:HG3	1.90	0.52
25:v:240:GLY:HA3	25:v:246:SER:HB2	1.91	0.52
1:1:28:TRP:CD1	24:u:822:ARG:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:509:GLN:O	3:3:513:ASP:HB2	2.10	0.52
5:6:35:A:N6	21:Z:255:C:O2	2.42	0.52
8:A:2200:MET:HG3	8:A:2206:TRP:HB2	1.91	0.52
11:D:481:GLU:HG3	11:D:483:ASP:H	1.74	0.52
25:v:676:ARG:HD3	25:v:685:ASP:HB3	1.91	0.52
8:A:901:LEU:HB2	8:A:904:HIS:HB3	1.92	0.52
9:B:261:ASP:OD1	9:B:261:ASP:N	2.41	0.52
15:P:168:TRP:CD1	15:P:184:GLU:H	2.26	0.52
24:u:497:ILE:HA	24:u:500:LEU:HD12	1.92	0.52
11:D:436:MET:HG3	11:D:450:VAL:HG13	1.92	0.52
25:v:316:GLU:OE1	25:v:326:ARG:NH2	2.42	0.52
25:v:1013:ARG:NH1	25:v:1065:GLU:OE2	2.42	0.52
9:B:911:PRO:HB3	9:B:934:MET:HG2	1.91	0.52
12:E:121:ASN:HB3	12:E:124:MET:HG2	1.91	0.52
8:A:1809:ILE:HB	8:A:1818:PHE:HB2	1.91	0.52
8:A:1876:LEU:HD12	8:A:1879:PHE:HB2	1.91	0.52
15:P:282:VAL:O	15:P:286:LYS:N	2.43	0.52
25:v:757:ILE:HD13	25:v:761:THR:HG23	1.91	0.52
8:A:1271:MET:HE2	8:A:1278:VAL:HG21	1.92	0.52
9:B:474:LEU:HB3	9:B:566:THR:HA	1.91	0.52
15:P:64:ARG:NH1	15:P:161:ARG:O	2.42	0.52
23:t:306:VAL:HG22	25:v:685:ASP:HB2	1.92	0.52
25:v:330:PHE:O	25:v:394:ASN:ND2	2.40	0.52
28:z:37:ASP:O	28:z:41:LYS:HB2	2.10	0.52
6:7:59:CYS:SG	6:7:72:HIS:NE2	2.72	0.52
8:A:1872:LEU:O	8:A:1876:LEU:HB2	2.09	0.52
25:v:1024:PHE:O	25:v:1087:GLN:NE2	2.43	0.52
8:A:104:GLU:HA	8:A:638:LEU:HD21	1.92	0.51
8:A:1664:ILE:HG22	8:A:1703:ILE:HB	1.92	0.51
8:A:2207:ASP:HB3	8:A:2210:LYS:HB2	1.91	0.51
25:v:754:ILE:HG22	25:v:756:ALA:HB2	1.92	0.51
8:A:422:LEU:HD22	8:A:638:LEU:HD23	1.91	0.51
8:A:2178:ILE:HA	8:A:2214:ILE:O	2.10	0.51
25:v:280:ASP:OD1	25:v:283:ARG:N	2.42	0.51
8:A:902:TYR:OH	8:A:1249:MET:SD	2.63	0.51
9:B:181:ILE:HD11	9:B:614:TYR:HE1	1.75	0.51
9:B:508:LYS:HD2	9:B:568:PRO:HA	1.92	0.51
10:C:188:PHE:HB3	15:P:25:GLN:HG2	1.91	0.51
5:6:40:U:H3	21:Z:250:U:H3	1.59	0.51
8:A:1257:THR:O	8:A:1261:ASN:HB2	2.11	0.51
9:B:531:TRP:HE1	9:B:538:HIS:CG	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:158:LYS:O	10:C:162:ALA:N	2.34	0.51
8:A:1776:ILE:HB	8:A:1858:PRO:HA	1.93	0.51
14:O:343:GLU:O	14:O:347:HIS:ND1	2.44	0.51
11:D:475:SER:OG	11:D:476:ARG:NH2	2.44	0.51
15:P:74:CYS:O	15:P:202:TYR:OH	2.28	0.51
8:A:959:ILE:HG22	8:A:1087:LEU:HD11	1.93	0.51
11:D:416:ILE:HA	11:D:431:ALA:HA	1.93	0.51
11:D:476:ARG:NH1	17:R:67:GLU:OE2	2.42	0.51
14:O:433:ARG:O	14:O:438:TYR:N	2.39	0.51
15:P:259:ARG:HG2	15:P:273:GLN:HB2	1.93	0.51
24:u:1258:ALA:HB3	24:u:1261:VAL:HG12	1.93	0.51
8:A:586:GLY:H	8:A:589:THR:HG22	1.76	0.51
8:A:613:TYR:O	8:A:617:ASN:ND2	2.43	0.51
10:C:189:ASN:ND2	15:P:30:GLU:O	2.44	0.51
8:A:339:PHE:N	9:B:266:GLU:OE2	2.44	0.51
8:A:1640:SER:HA	8:A:1652:MET:HA	1.93	0.51
11:D:446:ASN:OD1	11:D:449:ARG:NH2	2.44	0.51
8:A:265:THR:OG1	8:A:328:HIS:O	2.29	0.50
8:A:559:ASP:HA	8:A:562:VAL:HG12	1.92	0.50
8:A:1472:THR:HG22	10:C:437:TRP:HZ3	1.76	0.50
8:A:1682:ALA:HB3	23:t:122:LEU:HD23	1.93	0.50
25:v:527:ILE:HG12	25:v:531:LYS:HA	1.93	0.50
8:A:491:GLU:O	8:A:495:GLN:HB2	2.11	0.50
8:A:1609:VAL:HG12	8:A:1631:LEU:HG	1.93	0.50
8:A:2236:GLU:OE1	8:A:2239:ARG:NE	2.40	0.50
10:C:276:GLN:HB2	10:C:279:HIS:HA	1.93	0.50
24:u:823:MET:HG3	24:u:829:ASN:HB3	1.93	0.50
8:A:231:THR:OG1	9:B:389:ASP:OD2	2.29	0.50
8:A:1136:ARG:NH1	8:A:1345:GLN:OE1	2.43	0.50
9:B:532:ILE:HG23	9:B:541:VAL:HG21	1.93	0.50
25:v:175:VAL:HB	25:v:178:GLU:HB3	1.93	0.50
25:v:229:GLU:OE2	25:v:268:ARG:NH1	2.45	0.50
8:A:291:GLU:O	8:A:295:GLU:HB2	2.11	0.50
8:A:994:ASN:HD22	13:L:79:PRO:HG2	1.76	0.50
11:D:230:ILE:HG13	11:D:239:LYS:HB2	1.93	0.50
14:O:343:GLU:OE1	14:O:378:ASN:ND2	2.44	0.50
14:O:451:LEU:O	14:O:455:TYR:N	2.44	0.50
19:V:14:VAL:HB	19:V:25:LEU:HB2	1.92	0.50
8:A:398:THR:HG22	9:B:386:GLY:HA3	1.92	0.50
8:A:551:LEU:HA	8:A:554:THR:HG22	1.93	0.50
9:B:828:MET:HA	9:B:905:GLN:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:v:353:PHE:O	25:v:432:ARG:NH1	2.40	0.50
8:A:1278:VAL:HG23	8:A:1284:LEU:HD22	1.94	0.50
10:C:145:GLU:OE1	10:C:148:ARG:NH1	2.45	0.50
15:P:165:CYS:HB3	15:P:181:TYR:HB2	1.92	0.50
25:v:329:TYR:HE2	25:v:390:ARG:HG2	1.77	0.50
8:A:1241:HIS:HB2	8:A:1287:LEU:HD21	1.92	0.50
25:v:1118:VAL:HG22	25:v:1128:ILE:HG22	1.94	0.50
10:C:165:VAL:HG22	10:C:166:ARG:HH11	1.76	0.50
24:u:412:TYR:HB3	28:z:49:ARG:HB3	1.93	0.50
25:v:545:VAL:HG22	25:v:546:LYS:HG2	1.93	0.50
25:v:1012:VAL:HG22	25:v:1023:ILE:HG22	1.94	0.50
1:1:121:SER:OG	1:1:122:GLU:OE1	2.29	0.50
8:A:1901:LYS:HD2	8:A:1967:ILE:HG22	1.94	0.50
9:B:305:GLY:HA3	9:B:436:GLN:HG3	1.94	0.50
10:C:87:ALA:O	10:C:89:GLN:NE2	2.43	0.50
15:P:213:LEU:HA	15:P:216:ARG:HG2	1.93	0.50
22:s:106:SER:OG	22:s:107:HIS:N	2.45	0.50
9:B:384:VAL:HG21	9:B:419:VAL:HG11	1.94	0.49
25:v:561:GLY:HA3	25:v:583:MET:HB3	1.93	0.49
6:7:49:ASN:ND2	6:7:53:SER:OG	2.40	0.49
13:L:48:ALA:O	13:L:52:GLU:HB2	2.12	0.49
15:P:159:ARG:NE	21:Z:262:G:OP2	2.38	0.49
24:u:1234:LEU:HD22	24:u:1246:MET:HE1	1.94	0.49
25:v:80:VAL:HB	25:v:88:VAL:HG13	1.94	0.49
25:v:913:LEU:HG	25:v:920:VAL:HG12	1.94	0.49
8:A:995:ARG:NH2	10:C:295:ASP:OD2	2.45	0.49
8:A:1335:ILE:HD12	8:A:1354:ARG:HH21	1.76	0.49
20:Y:67:VAL:HA	20:Y:70:PHE:HB2	1.94	0.49
25:v:534:ASN:HB2	25:v:574:LEU:HD21	1.94	0.49
8:A:35:ARG:NH2	12:E:170:THR:OG1	2.46	0.49
8:A:775:ASN:O	8:A:775:ASN:ND2	2.43	0.49
13:L:30:GLN:HE21	13:L:33:ARG:HH11	1.61	0.49
14:O:428:GLU:HG3	14:O:431:ARG:HD3	1.94	0.49
24:u:1245:ARG:NH2	24:u:1248:GLN:OE1	2.43	0.49
25:v:857:ALA:O	25:v:861:GLN:NE2	2.33	0.49
7:8:571:LEU:HD22	24:u:1130:PRO:HG2	1.94	0.49
9:B:174:GLU:HB3	9:B:181:ILE:HG22	1.95	0.49
9:B:219:LEU:HG	9:B:251:LEU:HD22	1.94	0.49
9:B:739:ALA:H	9:B:771:GLN:HE22	1.60	0.49
12:E:101:THR:HG23	12:E:104:MET:H	1.76	0.49
1:1:38:ILE:HD11	1:1:82:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:303:ILE:HD13	9:B:659:VAL:HG21	1.94	0.49
9:B:134:LEU:HD13	9:B:142:LYS:HB2	1.94	0.49
15:P:294:ASN:ND2	19:V:120:GLN:OE1	2.46	0.49
10:C:183:GLN:NE2	12:E:112:SER:OG	2.46	0.49
24:u:621:ASP:HB3	24:u:624:VAL:HG22	1.95	0.49
7:8:587:HIS:HD2	24:u:1249:TYR:HE1	1.61	0.49
8:A:1128:TYR:HB3	8:A:1139:ARG:HD2	1.94	0.49
8:A:1549:VAL:HG11	23:t:186:PRO:HD2	1.95	0.49
10:C:310:ARG:O	10:C:313:ALA:HB3	2.13	0.49
15:P:67:LYS:HG3	15:P:68:THR:H	1.78	0.49
23:t:279:HIS:ND1	23:t:296:CYS:SG	2.71	0.49
8:A:378:PHE:H	9:B:354:ARG:HH22	1.60	0.49
2:2:43:U:H1'	21:Z:384:G:H22	1.78	0.48
8:A:1745:GLU:HA	8:A:1748:ARG:HE	1.76	0.48
8:A:1757:GLU:HB2	24:u:938:TRP:HH2	1.77	0.48
24:u:1247:LEU:HD22	24:u:1280:LEU:HD22	1.95	0.48
25:v:113:ARG:HB2	25:v:116:VAL:HG22	1.93	0.48
25:v:1000:VAL:HB	25:v:1012:VAL:HB	1.93	0.48
4:5:51:A:O2'	4:5:52:U:O5'	2.31	0.48
8:A:377:GLU:H	9:B:354:ARG:HH12	1.61	0.48
8:A:886:LEU:O	8:A:889:ARG:NH2	2.37	0.48
10:C:321:GLU:O	10:C:325:ARG:N	2.46	0.48
11:D:343:PRO:HG3	11:D:356:LEU:HD23	1.95	0.48
15:P:256:GLY:HA3	15:P:274:PHE:HE1	1.77	0.48
19:V:14:VAL:O	19:V:24:VAL:HA	2.14	0.48
25:v:605:LEU:HB3	25:v:617:ILE:O	2.13	0.48
25:v:955:PHE:HB3	25:v:960:LEU:HD13	1.95	0.48
8:A:1472:THR:O	8:A:1476:GLN:NE2	2.46	0.48
25:v:542:LYS:HG2	25:v:559:THR:HB	1.95	0.48
8:A:1634:SER:OG	8:A:1635:TYR:N	2.47	0.48
10:C:330:LYS:HG3	10:C:333:GLU:HB3	1.95	0.48
24:u:494:GLU:HG2	24:u:530:PRO:HG2	1.96	0.48
25:v:601:ARG:CZ	25:v:619:LEU:H	2.26	0.48
25:v:1011:TRP:HB2	25:v:1025:ALA:HB3	1.94	0.48
27:y:30:CYS:SG	27:y:31:VAL:N	2.86	0.48
8:A:55:ASP:O	16:Q:109:ARG:NH1	2.46	0.48
8:A:2108:LYS:HA	8:A:2111:LEU:HB3	1.95	0.48
9:B:772:TRP:CD1	9:B:813:ARG:HH21	2.32	0.48
24:u:492:GLN:O	24:u:496:LYS:N	2.47	0.48
24:u:586:ASP:OD1	24:u:586:ASP:N	2.42	0.48
25:v:801:GLU:O	25:v:864:SER:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1726:ILE:HA	8:A:1729:ALA:HB3	1.94	0.48
16:Q:102:CYS:SG	16:Q:103:LEU:N	2.87	0.48
25:v:339:MET:HG2	25:v:349:VAL:HG12	1.95	0.48
25:v:407:ILE:HG23	25:v:425:VAL:HG13	1.95	0.48
27:y:18:ALA:HB1	27:y:50:ASN:HD22	1.78	0.48
1:1:39:PHE:HD1	1:1:81:PHE:HE1	1.60	0.48
8:A:516:LEU:HD13	8:A:524:LEU:HD21	1.95	0.48
9:B:652:ASP:N	9:B:652:ASP:OD1	2.46	0.48
11:D:350:HIS:HA	11:D:374:SER:HB2	1.94	0.48
23:t:274:VAL:N	23:t:308:ASN:O	2.45	0.48
24:u:781:ASP:OD1	24:u:781:ASP:N	2.47	0.48
8:A:355:LEU:HA	9:B:864:PRO:HB3	1.96	0.48
9:B:114:TYR:OH	9:B:189:VAL:N	2.38	0.48
9:B:132:VAL:HG12	9:B:224:GLY:HA3	1.95	0.48
25:v:64:SER:OG	25:v:119:GLN:O	2.23	0.48
5:6:14:C:H2'	5:6:15:A:H8	1.78	0.48
5:6:28:A:N6	21:Z:258:A:O2'	2.36	0.48
8:A:1014:ASN:HA	8:A:1026:ASN:HB3	1.95	0.48
8:A:1537:TRP:HD1	8:A:1751:LEU:HD11	1.78	0.48
8:A:1742:VAL:O	8:A:1746:ARG:HB2	2.14	0.48
13:L:19:LEU:HD23	13:L:54:LEU:HD22	1.96	0.48
14:O:454:ASN:O	14:O:458:PHE:CB	2.61	0.48
20:Y:110:LEU:HA	20:Y:113:GLN:HG2	1.95	0.48
23:t:217:CYS:SG	23:t:221:HIS:NE2	2.87	0.48
24:u:539:LEU:HA	24:u:544:LEU:HD11	1.95	0.48
25:v:88:VAL:HG11	25:v:1156:CYS:HA	1.96	0.48
2:2:28:C:H2'	8:A:857:ASN:HD22	1.79	0.48
8:A:1848:LEU:HD13	8:A:1914:MET:HE2	1.96	0.47
13:L:55:ASP:HB3	13:L:58:ILE:HG13	1.96	0.47
25:v:508:CYS:HB2	25:v:518:GLN:HG2	1.96	0.47
8:A:608:LEU:O	8:A:611:LEU:HB2	2.14	0.47
8:A:1061:MET:HE1	8:A:1088:PHE:HB3	1.96	0.47
8:A:1701:VAL:HA	8:A:1716:GLY:HA3	1.95	0.47
20:Y:51:TRP:HZ3	20:Y:105:LEU:HD23	1.80	0.47
8:A:2248:PRO:HG2	8:A:2251:TYR:HB2	1.96	0.47
25:v:246:SER:O	25:v:260:ASN:ND2	2.48	0.47
1:1:85:GLU:O	3:3:500:GLY:N	2.48	0.47
2:2:41:U:OP1	6:7:72:HIS:ND1	2.48	0.47
4:5:51:A:O2'	4:5:52:U:O4'	2.33	0.47
8:A:850:TYR:OH	8:A:863:GLU:OE1	2.31	0.47
8:A:952:VAL:O	8:A:956:CYS:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2072:GLU:HG3	8:A:2076:ARG:HH21	1.79	0.47
9:B:213:ASP:OD2	9:B:616:SER:N	2.43	0.47
9:B:475:MET:HE2	9:B:574:ALA:HB2	1.95	0.47
25:v:786:ARG:HE	25:v:802:THR:HB	1.79	0.47
8:A:442:LYS:NZ	30:A:3001:IHP:O44	2.43	0.47
8:A:951:LEU:HD12	8:A:1190:CYS:HB3	1.96	0.47
8:A:2105:ILE:HB	8:A:2141:GLU:HG2	1.96	0.47
11:D:297:HIS:HD1	11:D:299:THR:H	1.63	0.47
25:v:291:ALA:HB2	25:v:339:MET:HB2	1.96	0.47
1:1:101:LYS:HB3	1:1:106:THR:HG22	1.97	0.47
8:A:952:VAL:HG11	8:A:1214:TRP:HE1	1.80	0.47
8:A:1536:LEU:HB2	8:A:1572:SER:HB2	1.96	0.47
24:u:910:MET:HE3	24:u:910:MET:HB2	1.84	0.47
1:1:57:SER:OG	3:3:583:ARG:O	2.32	0.47
4:5:26:A:H4'	8:A:425:PRO:HG3	1.97	0.47
8:A:908:VAL:HG21	8:A:1448:LEU:HG	1.95	0.47
8:A:1897:LEU:HD22	8:A:1906:ILE:HG21	1.96	0.47
9:B:634:GLU:OE2	9:B:882:GLY:N	2.43	0.47
9:B:732:ILE:HG22	9:B:746:VAL:HG22	1.97	0.47
13:L:48:ALA:O	13:L:52:GLU:CB	2.63	0.47
25:v:561:GLY:H	25:v:563:LEU:HD13	1.80	0.47
25:v:563:LEU:HB3	25:v:564:VAL:H	1.58	0.47
28:z:54:PRO:HA	28:z:57:ARG:HB3	1.95	0.47
8:A:1211:ASP:N	8:A:1211:ASP:OD1	2.45	0.47
8:A:1221:THR:HG23	8:A:1223:GLU:HG2	1.97	0.47
8:A:1648:SER:OG	8:A:1880:PRO:O	2.29	0.47
8:A:1791:HIS:NE2	8:A:1799:THR:O	2.48	0.47
13:L:71:LEU:HA	13:L:74:LEU:HB3	1.97	0.47
14:O:369:PHE:HE2	14:O:378:ASN:HB3	1.80	0.47
24:u:451:ARG:HG3	24:u:453:MET:H	1.78	0.47
25:v:138:GLN:HB2	25:v:161:HIS:ND1	2.30	0.47
8:A:291:GLU:O	8:A:295:GLU:CB	2.63	0.47
8:A:1519:THR:HG23	8:A:1522:GLN:HE21	1.80	0.47
24:u:572:HIS:NE2	24:u:616:ASP:OD2	2.48	0.47
24:u:664:GLY:HA2	24:u:667:ILE:HD12	1.97	0.47
24:u:826:ASP:O	24:u:830:TYR:N	2.47	0.47
25:v:1008:SER:OG	25:v:1009:PHE:N	2.41	0.47
4:5:9:G:N2	4:5:10:U:O4	2.38	0.47
8:A:782:LEU:HD23	17:R:220:HIS:HE1	1.80	0.47
10:C:303:GLU:O	10:C:307:GLN:NE2	2.48	0.47
14:O:253:GLU:HG3	14:O:285:MET:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:v:504:PRO:HG2	25:v:521:PRO:HD2	1.97	0.47
15:P:101:LEU:HD21	15:P:143:THR:HG22	1.95	0.46
24:u:413:LYS:N	28:z:50:VAL:O	2.42	0.46
5:6:48:A:N7	10:C:256:ASN:ND2	2.62	0.46
8:A:166:PHE:HZ	8:A:577:GLY:HA2	1.80	0.46
8:A:605:CYS:SG	8:A:637:TRP:NE1	2.87	0.46
25:v:181:MET:HA	25:v:211:TYR:O	2.15	0.46
28:z:35:MET:HE1	28:z:50:VAL:HG22	1.96	0.46
10:C:125:MET:O	11:D:442:ARG:NH1	2.47	0.46
22:s:84:LYS:HA	22:s:107:HIS:HB3	1.96	0.46
2:2:42:G:N2	21:Z:385:U:O2	2.39	0.46
4:5:55:C:O2	8:A:642:ARG:NH1	2.49	0.46
8:A:1084:PRO:HD2	17:R:188:TRP:CD1	2.51	0.46
8:A:1456:THR:HG23	10:C:422:PHE:HE2	1.80	0.46
9:B:119:LEU:HA	9:B:122:LEU:HB2	1.97	0.46
9:B:736:GLY:HA2	9:B:770:PHE:HE2	1.81	0.46
9:B:938:ARG:NH2	9:B:944:SER:O	2.34	0.46
8:A:375:ASP:O	9:B:354:ARG:NH1	2.49	0.46
8:A:1275:ARG:HB2	8:A:1375:TRP:CD1	2.50	0.46
8:A:1807:ILE:HB	8:A:1820:LYS:HB3	1.96	0.46
10:C:214:ILE:HG21	17:R:26:LEU:HB3	1.98	0.46
10:C:287:LEU:O	10:C:290:ALA:HB3	2.15	0.46
24:u:480:VAL:HG11	28:z:55:GLU:HB2	1.97	0.46
24:u:578:ILE:HG13	24:u:596:ILE:HD11	1.97	0.46
25:v:569:ASP:N	25:v:573:GLN:O	2.49	0.46
28:z:19:ARG:NH2	28:z:67:ILE:HG13	2.31	0.46
3:3:580:PRO:HG2	3:3:582:TYR:HD1	1.80	0.46
8:A:2131:VAL:HG13	8:A:2172:MET:HG2	1.98	0.46
9:B:115:GLU:HG2	9:B:117:ASP:H	1.81	0.46
9:B:531:TRP:HA	9:B:541:VAL:HB	1.97	0.46
19:V:25:LEU:HD23	19:V:98:LEU:HD22	1.97	0.46
22:s:9:PRO:O	22:s:29:TRP:NE1	2.42	0.46
24:u:870:GLU:HA	24:u:873:GLU:HG2	1.97	0.46
25:v:122:ALA:HB2	25:v:170:VAL:HG13	1.98	0.46
7:8:503:HIS:CD2	7:8:510:TYR:HB2	2.51	0.46
8:A:1522:GLN:HB3	23:t:214:GLY:HA3	1.97	0.46
9:B:357:THR:OG1	9:B:359:LYS:O	2.27	0.46
10:C:173:PRO:HB2	10:C:200:VAL:HA	1.98	0.46
11:D:349:SER:OG	11:D:350:HIS:N	2.49	0.46
14:O:385:PHE:O	14:O:390:ALA:N	2.48	0.46
19:V:13:ASN:O	19:V:165:SER:OG	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:s:56:ARG:HG3	22:s:153:GLU:HB2	1.98	0.46
23:t:263:PHE:HA	23:t:266:ARG:HD3	1.97	0.46
8:A:941:LYS:HB3	8:A:950:LEU:HD11	1.96	0.46
10:C:181:PRO:HB2	15:P:25:GLN:HE22	1.81	0.46
24:u:476:ASP:OD1	28:z:24:ARG:NH2	2.49	0.46
25:v:120:PHE:HB3	25:v:170:VAL:HG12	1.97	0.46
25:v:457:ASN:O	25:v:758:SER:OG	2.30	0.46
8:A:593:ARG:NE	21:Z:239:C:OP1	2.41	0.46
8:A:269:LEU:HB3	8:A:271:MET:HE3	1.97	0.46
8:A:843:LEU:HD22	8:A:867:ILE:HG23	1.97	0.46
8:A:972:GLU:OE1	8:A:1100:ARG:NH2	2.40	0.46
8:A:1072:LEU:HD22	8:A:1087:LEU:HB2	1.97	0.46
8:A:1459:ARG:HD2	10:C:418:MET:H	1.80	0.46
15:P:48:CYS:SG	15:P:119:GLN:NE2	2.88	0.46
24:u:807:LYS:HA	24:u:811:LEU:HG	1.98	0.46
25:v:896:PHE:HE1	25:v:959:VAL:HG13	1.81	0.46
6:7:55:GLU:HG2	6:7:62:LEU:HD23	1.98	0.45
8:A:1878:ASP:OD1	8:A:1878:ASP:N	2.49	0.45
9:B:130:ARG:HH12	9:B:435:VAL:HG12	1.80	0.45
15:P:231:ILE:O	15:P:277:ARG:NE	2.36	0.45
19:V:41:GLU:OE2	19:V:44:ARG:NH2	2.35	0.45
25:v:34:ARG:HB2	25:v:37:ILE:HB	1.98	0.45
25:v:114:ARG:NE	25:v:136:GLU:OE1	2.34	0.45
25:v:905:VAL:HB	25:v:928:TYR:HB2	1.98	0.45
7:8:498:VAL:HG22	24:u:1249:TYR:HA	1.97	0.45
8:A:513:LEU:HD23	8:A:516:LEU:HD12	1.98	0.45
8:A:692:ASP:HB3	8:A:738:MET:HE1	1.99	0.45
9:B:162:ASP:OD1	9:B:162:ASP:N	2.48	0.45
9:B:337:GLN:HA	9:B:340:ALA:HB3	1.98	0.45
9:B:480:LYS:HE2	9:B:480:LYS:HB2	1.83	0.45
11:D:467:ALA:HB3	11:D:480:ALA:HB3	1.99	0.45
14:O:284:GLU:O	14:O:288:LYS:HB2	2.17	0.45
25:v:116:VAL:HA	25:v:138:GLN:HE21	1.81	0.45
25:v:988:ASN:HD22	25:v:1006:GLN:HB3	1.80	0.45
8:A:271:MET:SD	8:A:310:THR:OG1	2.74	0.45
8:A:1244:VAL:HA	8:A:1247:ILE:HG12	1.98	0.45
9:B:488:VAL:HA	9:B:609:LYS:HZ1	1.81	0.45
24:u:649:LYS:HZ3	24:u:653:LYS:HD2	1.81	0.45
24:u:785:LYS:HD3	24:u:823:MET:HE1	1.99	0.45
1:1:53:ILE:O	1:1:57:SER:HB2	2.17	0.45
8:A:1804:ASN:N	8:A:1804:ASN:OD1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2207:ASP:O	8:A:2211:THR:N	2.49	0.45
14:O:391:TYR:HB3	14:O:395:ALA:HB2	1.97	0.45
23:t:107:LYS:HD3	23:t:108:PRO:HD2	1.98	0.45
25:v:450:SER:O	25:v:762:LEU:N	2.49	0.45
7:8:462:VAL:O	7:8:466:LYS:HB2	2.17	0.45
8:A:735:ILE:HA	8:A:738:MET:HG2	1.98	0.45
8:A:947:PRO:HG2	8:A:1455:TRP:HB2	1.99	0.45
10:C:434:ASP:OD1	10:C:434:ASP:N	2.47	0.45
10:C:195:ARG:HG3	15:P:32:PRO:HA	1.98	0.45
13:L:61:THR:O	13:L:91:ARG:NH2	2.49	0.45
24:u:1140:GLU:HB2	24:u:1143:VAL:HG22	1.99	0.45
25:v:208:LEU:HD22	25:v:250:ILE:HD11	1.98	0.45
8:A:1514:LYS:HB3	24:u:1027:ARG:HB2	1.98	0.45
8:A:1676:ILE:HG21	8:A:1706:ASP:HB2	1.98	0.45
8:A:2148:VAL:HG23	8:A:2150:GLN:HB3	1.99	0.45
9:B:324:ALA:HA	9:B:327:TYR:HB2	1.98	0.45
11:D:394:ASN:ND2	11:D:409:LEU:O	2.50	0.45
24:u:601:ALA:HA	24:u:609:MET:HE3	1.99	0.45
24:u:862:GLU:OE1	24:u:865:ARG:NH2	2.50	0.45
8:A:530:LEU:HB3	8:A:534:GLU:HG3	1.98	0.45
8:A:609:LYS:NZ	30:A:3001:IHP:H4	2.31	0.45
8:A:929:GLU:OE2	8:A:933:ARG:NH1	2.50	0.45
10:C:205:ASP:OD1	10:C:205:ASP:N	2.49	0.45
11:D:410:SER:OG	11:D:411:GLY:N	2.45	0.45
20:Y:99:ARG:NE	26:x:1:MET:SD	2.80	0.45
24:u:804:ASN:HA	24:u:807:LYS:HG2	1.97	0.45
5:6:94:C:H5'	14:O:347:HIS:CD2	2.51	0.45
9:B:164:ASP:N	9:B:164:ASP:OD1	2.47	0.45
11:D:207:VAL:HG22	11:D:480:ALA:HB1	1.99	0.45
3:3:559:ASN:HD21	3:3:583:ARG:HH11	1.65	0.45
8:A:246:LEU:HG	8:A:408:PRO:HG2	1.98	0.45
8:A:982:GLU:OE1	8:A:1172:ASN:ND2	2.48	0.45
8:A:1162:PRO:HG2	8:A:1165:VAL:HG22	1.99	0.45
9:B:137:HIS:HB3	9:B:140:HIS:CD2	2.51	0.45
9:B:836:VAL:HB	9:B:871:ILE:HB	1.98	0.45
9:B:846:VAL:HA	9:B:849:VAL:HG22	1.98	0.45
11:D:210:ILE:HD13	11:D:221:THR:HB	1.98	0.45
24:u:1223:SER:HB3	24:u:1226:VAL:HG12	1.98	0.45
25:v:679:LEU:HD23	25:v:681:PRO:HD2	1.99	0.45
9:B:715:GLY:O	9:B:719:GLN:HB2	2.18	0.44
10:C:88:ILE:O	19:V:141:ARG:NH2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:89:ILE:HG22	13:L:91:ARG:H	1.81	0.44
15:P:95:GLN:HE22	15:P:206:ASN:HB2	1.83	0.44
19:V:48:TYR:OH	19:V:110:SER:OG	2.28	0.44
19:V:56:ILE:HD12	19:V:153:PRO:HG3	1.98	0.44
25:v:1100:THR:N	26:x:48:ASP:OD2	2.39	0.44
27:y:45:ILE:HA	27:y:85:CYS:HB2	1.99	0.44
3:3:604:LYS:HD3	3:3:605:LYS:HD2	1.99	0.44
9:B:590:ILE:HG12	9:B:637:LEU:HD21	1.99	0.44
16:Q:52:ILE:HA	16:Q:55:GLN:HG2	1.98	0.44
25:v:757:ILE:HG23	25:v:759:THR:H	1.82	0.44
1:1:62:ILE:HG21	1:1:82:LEU:HD22	1.98	0.44
6:7:16:VAL:HG12	8:A:1519:THR:HG22	1.98	0.44
8:A:1871:PRO:O	8:A:1875:HIS:ND1	2.37	0.44
8:A:2310:ARG:HB3	8:A:2313:HIS:HD1	1.83	0.44
9:B:309:PHE:HB2	9:B:318:PHE:CG	2.51	0.44
11:D:352:THR:HA	11:D:374:SER:HA	1.99	0.44
13:L:65:ARG:HH12	13:L:69:GLU:HB3	1.82	0.44
14:O:391:TYR:O	14:O:395:ALA:N	2.44	0.44
24:u:585:GLU:O	24:u:590:ARG:NH2	2.51	0.44
11:D:385:TYR:HB3	11:D:386:THR:H	1.65	0.44
24:u:1036:ILE:HD11	24:u:1073:ILE:HA	2.00	0.44
8:A:107:PRO:HG3	8:A:114:ARG:HB3	1.99	0.44
8:A:388:LEU:HD22	9:B:379:LYS:HB3	1.99	0.44
8:A:1667:ARG:NH1	8:A:1706:ASP:OD1	2.51	0.44
8:A:2129:TYR:HB2	8:A:2144:CYS:HB3	2.00	0.44
9:B:93:ILE:HG12	11:D:278:ASN:HD21	1.83	0.44
24:u:1297:ARG:NH1	26:x:39:SER:OG	2.40	0.44
25:v:355:ASN:ND2	25:v:400:GLU:OE2	2.51	0.44
25:v:507:SER:OG	25:v:547:CYS:SG	2.56	0.44
25:v:674:LEU:HD22	25:v:689:THR:HG22	2.00	0.44
25:v:742:ALA:HA	25:v:756:ALA:HA	1.98	0.44
8:A:1198:PRO:HA	8:A:1226:ALA:HA	2.00	0.44
8:A:1666:LEU:HD22	8:A:1707:LEU:HD11	1.99	0.44
14:O:262:ARG:NH2	14:O:291:GLN:HG3	2.33	0.44
23:t:304:ASN:O	25:v:687:SER:OG	2.30	0.44
6:7:56:CYS:O	6:7:60:LEU:N	2.51	0.44
8:A:555:LYS:NZ	8:A:559:ASP:OD2	2.36	0.44
8:A:1365:ILE:HG23	8:A:1474:MET:HE1	1.99	0.44
8:A:1789:THR:HG22	8:A:1801:LYS:HB2	1.98	0.44
13:L:28:LYS:O	13:L:31:TRP:NE1	2.50	0.44
24:u:686:LEU:HD12	24:u:689:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:u:1174:GLU:O	24:u:1178:MET:HB2	2.16	0.44
25:v:83:ASP:O	25:v:111:GLY:N	2.51	0.44
8:A:856:LEU:HD23	8:A:857:ASN:H	1.83	0.44
8:A:1418:ARG:HG3	8:A:1462:GLY:HA3	2.00	0.44
8:A:2109:ASN:OD1	8:A:2110:VAL:N	2.46	0.44
9:B:222:SER:HB2	9:B:549:TRP:HZ3	1.83	0.44
19:V:35:THR:HG21	19:V:127:THR:HG21	1.99	0.44
8:A:1678:ARG:NH2	23:t:121:GLU:HB2	2.33	0.44
11:D:260:TYR:HB3	11:D:274:ASP:HA	1.98	0.44
24:u:405:ASP:HA	28:z:49:ARG:HH22	1.83	0.44
24:u:1158:ILE:HB	24:u:1161:MET:HE3	2.00	0.44
25:v:381:GLU:O	25:v:384:THR:OG1	2.36	0.44
1:1:92:LEU:HD11	3:3:576:PHE:HB2	1.99	0.43
2:2:16:U:N3	5:6:82:A:OP1	2.32	0.43
9:B:244:LYS:HD3	9:B:244:LYS:HA	1.77	0.43
10:C:189:ASN:HB3	10:C:192:ALA:HB2	1.99	0.43
25:v:897:SER:HB2	25:v:957:GLY:HA3	2.00	0.43
7:8:488:LEU:HD11	24:u:1257:PRO:HD3	2.01	0.43
9:B:474:LEU:HD11	9:B:501:ILE:HG13	2.00	0.43
9:B:709:TRP:HB2	9:B:714:LEU:HD23	1.99	0.43
11:D:386:THR:HG22	11:D:441:TRP:HZ2	1.82	0.43
20:Y:40:MET:HB2	20:Y:78:LYS:HA	2.00	0.43
22:s:30:SER:HB2	22:s:171:PHE:HE1	1.82	0.43
5:6:91:A:H2'	5:6:92:A:C8	2.54	0.43
8:A:952:VAL:HG21	8:A:1214:TRP:CZ2	2.53	0.43
8:A:1260:VAL:HG13	8:A:1327:MET:HB3	2.00	0.43
24:u:826:ASP:HB3	24:u:829:ASN:HB2	2.00	0.43
25:v:1013:ARG:HD2	25:v:1064:ASP:HB3	2.01	0.43
4:5:17:U:H2'	4:5:18:C:H6	1.82	0.43
5:6:16:G:OP1	8:A:35:ARG:NH2	2.52	0.43
8:A:1513:MET:HG2	8:A:1514:LYS:H	1.82	0.43
10:C:291:LEU:O	10:C:294:ALA:HB3	2.18	0.43
14:O:423:GLU:HG3	14:O:431:ARG:HB3	2.00	0.43
15:P:167:PHE:O	15:P:173:CYS:N	2.52	0.43
15:P:237:GLY:HA2	15:P:269:CYS:HA	2.00	0.43
6:7:37:THR:HG21	13:L:21:ALA:HB1	2.00	0.43
9:B:320:LEU:H	9:B:320:LEU:HG	1.44	0.43
14:O:341:PRO:HD2	14:O:346:TRP:NE1	2.33	0.43
7:8:557:VAL:HB	23:t:208:THR:HG23	2.00	0.43
11:D:471:ASP:OD1	11:D:472:GLN:N	2.51	0.43
28:z:46:ARG:HB3	28:z:63:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:147:MET:HE2	8:A:147:MET:HB3	1.55	0.43
8:A:312:TYR:OH	9:B:853:ARG:NH2	2.46	0.43
8:A:856:LEU:H	8:A:860:GLN:HE21	1.66	0.43
9:B:69:ALA:HA	9:B:72:VAL:HG12	2.01	0.43
9:B:808:ILE:O	9:B:812:ALA:N	2.51	0.43
11:D:182:ALA:HB3	11:D:185:MET:HB2	2.01	0.43
24:u:490:GLU:O	24:u:493:LYS:HB3	2.19	0.43
25:v:475:ILE:HD11	25:v:505:THR:HG21	1.99	0.43
5:6:73:A:OP1	5:6:75:G:O2'	2.36	0.43
8:A:1144:LYS:HA	8:A:1147:VAL:HG12	2.00	0.43
8:A:1554:GLN:HA	8:A:1561:PHE:HA	2.01	0.43
8:A:2124:ILE:HD12	8:A:2147:MET:HE1	2.00	0.43
8:A:2281:TYR:HD2	8:A:2288:HIS:HD2	1.66	0.43
14:O:384:ARG:HA	14:O:387:GLU:HG2	1.99	0.43
15:P:239:LEU:HG	15:P:243:ILE:HB	2.00	0.43
24:u:1287:ILE:HG21	26:x:32:LEU:HD11	1.99	0.43
25:v:34:ARG:HE	25:v:39:GLU:CD	2.26	0.43
5:6:29:A:H62	21:Z:258:A:H8	1.66	0.43
8:A:109:PRO:HG3	8:A:630:TRP:HE1	1.83	0.43
8:A:339:PHE:HZ	8:A:403:ALA:HA	1.82	0.43
8:A:820:ARG:HA	8:A:820:ARG:HD3	1.72	0.43
8:A:1160:ARG:HA	17:R:194:PHE:HB2	1.99	0.43
8:A:1267:LEU:HD22	8:A:1368:LEU:HD23	2.01	0.43
8:A:1678:ARG:HG3	23:t:124:THR:HA	2.01	0.43
9:B:530:LEU:HD22	9:B:552:ILE:HG22	2.01	0.43
9:B:664:GLU:HG2	9:B:827:LEU:HD23	2.00	0.43
9:B:814:ARG:NE	9:B:952:PHE:O	2.52	0.43
10:C:408:ASP:OD2	10:C:410:ARG:NH1	2.52	0.43
11:D:205:GLY:H	11:D:484:LYS:HD2	1.84	0.43
14:O:283:ALA:HA	14:O:298:ILE:HD11	2.01	0.43
19:V:9:TRP:HZ2	19:V:164:PRO:HB2	1.84	0.43
25:v:208:LEU:HA	25:v:208:LEU:HD12	1.83	0.43
9:B:529:ARG:HD3	9:B:553:GLU:HG3	2.00	0.43
10:C:113:TYR:OH	11:D:402:ASP:O	2.37	0.43
13:L:53:TRP:HD1	13:L:54:LEU:HD12	1.84	0.43
25:v:958:ARG:NH2	25:v:1014:TYR:OH	2.52	0.43
2:2:49:U:H3	2:2:63:G:H1	1.67	0.42
8:A:150:MET:HB2	8:A:193:LEU:HB2	2.00	0.42
8:A:784:LEU:HD21	8:A:896:ILE:HG21	2.00	0.42
8:A:1489:LEU:C	8:A:1492:GLY:H	2.27	0.42
9:B:122:LEU:HA	9:B:125:ASN:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:614:TYR:OH	9:B:643:ASP:OD2	2.28	0.42
9:B:745:LEU:HB3	9:B:789:PHE:CZ	2.54	0.42
12:E:178:ARG:HG2	12:E:199:TYR:CZ	2.54	0.42
21:Z:253:A:O2'	21:Z:254:G:O4'	2.37	0.42
25:v:320:ASP:N	25:v:320:ASP:OD1	2.51	0.42
25:v:562:GLU:HB3	25:v:581:LYS:HB3	2.01	0.42
2:2:26:A:OP1	8:A:1020:LYS:NZ	2.47	0.42
8:A:1676:ILE:HD13	8:A:1706:ASP:HB2	2.01	0.42
8:A:1824:THR:O	8:A:1827:TRP:HB2	2.20	0.42
9:B:227:LEU:HB3	9:B:255:VAL:HG23	2.01	0.42
15:P:66:LYS:HE3	15:P:66:LYS:HB3	1.87	0.42
24:u:519:ILE:HD11	24:u:531:LEU:HD11	2.01	0.42
25:v:586:ASP:HB3	25:v:609:LEU:HB3	2.01	0.42
25:v:895:ARG:NH1	25:v:901:GLU:OE2	2.52	0.42
27:y:49:CYS:HB3	27:y:87:LYS:HG2	1.99	0.42
8:A:856:LEU:N	8:A:860:GLN:HE21	2.17	0.42
8:A:1264:ASN:O	8:A:1268:ILE:HD12	2.19	0.42
8:A:2128:LEU:HB3	8:A:2142:ILE:HD13	2.02	0.42
26:x:32:LEU:HD23	26:x:32:LEU:HA	1.88	0.42
8:A:2078:ILE:H	8:A:2078:ILE:HG13	1.67	0.42
9:B:477:HIS:HA	9:B:564:THR:HG22	2.01	0.42
9:B:955:ASP:OD1	9:B:955:ASP:N	2.52	0.42
10:C:140:ILE:HA	10:C:143:ILE:HG22	2.00	0.42
13:L:9:GLY:H	13:L:40:ARG:HH12	1.67	0.42
24:u:846:ALA:HB3	24:u:883:ASP:HB3	2.01	0.42
24:u:893:ILE:HD13	24:u:893:ILE:HA	1.89	0.42
24:u:1133:MET:HB2	24:u:1133:MET:HE2	1.81	0.42
25:v:1015:LYS:NZ	25:v:1067:ASP:OD1	2.35	0.42
8:A:1699:THR:OG1	8:A:1700:GLY:N	2.53	0.42
9:B:129:ILE:HG22	9:B:199:LEU:HD13	2.02	0.42
9:B:204:ASP:N	9:B:204:ASP:OD1	2.49	0.42
9:B:884:GLU:O	9:B:888:ARG:HB2	2.20	0.42
13:L:16:ASP:OD1	13:L:49:ARG:NE	2.53	0.42
24:u:1224:PRO:HA	24:u:1227:ILE:HG22	2.01	0.42
25:v:475:ILE:HA	25:v:484:VAL:HA	2.01	0.42
25:v:861:GLN:HA	25:v:885:ASN:HD22	1.84	0.42
25:v:1008:SER:OG	25:v:1031:ARG:NH1	2.52	0.42
8:A:167:PRO:HG2	23:t:190:ARG:HG3	2.00	0.42
8:A:1557:LEU:HD13	8:A:1580:HIS:CD2	2.55	0.42
24:u:1027:ARG:HH12	24:u:1067:LYS:NZ	2.18	0.42
4:5:9:G:N2	4:5:67:A:H61	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:414:ARG:NH1	9:B:410:LEU:O	2.52	0.42
8:A:1425:LYS:HB3	10:C:416:LYS:HA	2.02	0.42
8:A:1649:LYS:HE2	8:A:1880:PRO:HB3	2.02	0.42
14:O:264:ILE:O	14:O:268:ALA:HB2	2.20	0.42
15:P:78:LYS:HA	15:P:78:LYS:HD3	1.77	0.42
19:V:87:HIS:CE1	19:V:89:ASP:HB2	2.55	0.42
20:Y:52:ILE:HG21	20:Y:71:ILE:HG12	2.02	0.42
24:u:798:THR:OG1	24:u:799:ASP:N	2.47	0.42
25:v:310:ILE:HG12	25:v:339:MET:HE1	2.02	0.42
10:C:232:SER:HB2	11:D:372:LYS:NZ	2.34	0.42
14:O:293:ASN:O	14:O:297:ASN:HB2	2.20	0.42
14:O:303:ILE:HD12	14:O:313:TRP:CZ3	2.55	0.42
23:t:232:ILE:O	23:t:236:LEU:HB2	2.20	0.42
24:u:477:LYS:O	24:u:495:ARG:NH1	2.53	0.42
24:u:1129:LEU:O	24:u:1133:MET:HB2	2.19	0.42
4:5:19:A:O2'	4:5:21:A:N1	2.51	0.42
4:5:29:A:H2'	4:5:30:A:H8	1.84	0.42
8:A:251:ASP:N	8:A:251:ASP:OD1	2.53	0.42
8:A:304:ILE:HG23	9:B:923:PRO:HG3	2.02	0.42
8:A:989:ASP:OD1	8:A:989:ASP:N	2.51	0.42
9:B:160:ARG:HB3	9:B:164:ASP:HA	2.02	0.42
19:V:66:ASP:OD2	19:V:70:THR:N	2.52	0.42
24:u:491:GLU:O	24:u:495:ARG:N	2.53	0.42
25:v:79:VAL:HG12	25:v:121:LEU:HD21	2.01	0.42
25:v:275:ARG:HH11	25:v:386:PHE:HB2	1.84	0.42
25:v:460:TRP:HE3	25:v:475:ILE:HG23	1.84	0.42
26:x:65:ARG:O	26:x:69:MET:HB2	2.19	0.42
8:A:463:PRO:HA	8:A:464:PRO:HD3	1.83	0.42
8:A:1126:VAL:HG23	8:A:1151:ARG:HH11	1.84	0.42
11:D:425:GLY:O	11:D:441:TRP:N	2.46	0.42
13:L:49:ARG:HG2	13:L:54:LEU:HD13	2.01	0.42
24:u:943:LYS:HB3	24:u:945:ALA:HB2	2.02	0.42
25:v:1133:THR:OG1	25:v:1134:SER:N	2.53	0.42
2:2:17:U:H3	10:C:256:ASN:HA	1.84	0.41
4:5:9:G:O6	4:5:69:A:O2'	2.27	0.41
4:5:26:A:H1'	4:5:27:U:H5'	2.01	0.41
5:6:49:G:O2'	6:7:29:ARG:NH2	2.53	0.41
5:6:91:A:H2'	5:6:92:A:H8	1.85	0.41
8:A:1653:ASP:OD1	8:A:1653:ASP:N	2.52	0.41
9:B:778:PRO:HB3	9:B:817:TYR:CG	2.55	0.41
10:C:255:LYS:HG2	10:C:257:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:320:HIS:O	10:C:324:LEU:N	2.53	0.41
8:A:115:ASP:OD1	8:A:115:ASP:N	2.53	0.41
8:A:664:HIS:NE2	10:C:214:ILE:O	2.52	0.41
8:A:731:LEU:HD11	8:A:735:ILE:HD11	2.02	0.41
8:A:1832:ARG:HB2	8:A:1835:GLN:HB2	2.02	0.41
9:B:130:ARG:NH2	9:B:431:VAL:O	2.52	0.41
24:u:1174:GLU:HB2	24:u:1214:TYR:CE2	2.54	0.41
25:v:589:CYS:SG	25:v:590:MET:N	2.93	0.41
7:8:566:ILE:HG23	7:8:567:ASP:H	1.86	0.41
8:A:377:GLU:H	9:B:354:ARG:NH1	2.17	0.41
11:D:399:LYS:HD2	11:D:406:ILE:HD11	2.03	0.41
21:Z:393:G:OP2	24:u:1106:ARG:NE	2.53	0.41
25:v:238:VAL:HG21	25:v:258:TYR:HE1	1.84	0.41
25:v:1145:GLU:HB3	25:v:1179:CYS:SG	2.60	0.41
7:8:478:HIS:O	7:8:481:THR:OG1	2.32	0.41
8:A:371:LEU:HG	8:A:373:ASP:HB2	2.02	0.41
8:A:1755:SER:O	24:u:943:LYS:N	2.53	0.41
9:B:453:TYR:HE2	9:B:456:GLY:HA3	1.85	0.41
15:P:264:VAL:HG13	15:P:269:CYS:HB2	2.02	0.41
24:u:954:LEU:HA	24:u:954:LEU:HD12	1.87	0.41
25:v:428:GLY:HA3	25:v:433:SER:HA	2.02	0.41
25:v:429:ARG:NH2	26:x:59:GLU:O	2.52	0.41
8:A:583:ALA:HB1	8:A:609:LYS:HD3	2.02	0.41
8:A:790:ARG:NH2	8:A:986:GLU:HB3	2.36	0.41
8:A:1340:LEU:HB2	18:S:5:ILE:HG22	2.02	0.41
8:A:1555:LEU:HD23	8:A:1574:ILE:HD13	2.02	0.41
8:A:1649:LYS:HB2	8:A:1880:PRO:HB3	2.01	0.41
9:B:167:TYR:HB2	9:B:536:ARG:HH11	1.84	0.41
10:C:268:LEU:O	10:C:273:ARG:NH2	2.53	0.41
22:s:85:ASP:OD1	22:s:109:ASN:ND2	2.39	0.41
22:s:134:THR:O	22:s:137:THR:OG1	2.39	0.41
25:v:791:HIS:HB2	25:v:798:ILE:HD11	2.03	0.41
3:3:579:TRP:HA	3:3:580:PRO:HD3	1.99	0.41
5:6:14:C:H2'	5:6:15:A:C8	2.55	0.41
6:7:7:PRO:HG3	8:A:1524:SER:HB2	2.01	0.41
8:A:397:ASN:OD1	8:A:397:ASN:N	2.52	0.41
8:A:591:MET:HG2	8:A:598:LEU:HD21	2.02	0.41
8:A:863:GLU:HG3	8:A:913:PRO:HB3	2.03	0.41
8:A:1605:GLU:OE2	8:A:1634:SER:N	2.39	0.41
8:A:2278:SER:OG	8:A:2279:TRP:N	2.53	0.41
9:B:129:ILE:HD12	9:B:131:ASN:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:839:PRO:HG2	9:B:894:GLN:HB3	2.03	0.41
11:D:223:SER:HB3	11:D:225:ASP:H	1.85	0.41
11:D:371:HIS:ND1	11:D:391:SER:OG	2.52	0.41
24:u:720:GLY:N	25:v:216:GLY:O	2.47	0.41
11:D:289:SER:OG	11:D:290:ALA:N	2.54	0.41
15:P:280:ALA:O	15:P:283:ALA:HB3	2.20	0.41
22:s:103:ASN:OD1	22:s:104:ALA:N	2.54	0.41
28:z:23:ILE:HG23	28:z:87:LEU:HD12	2.02	0.41
8:A:640:PHE:CE1	8:A:644:ILE:HG13	2.55	0.41
8:A:2160:PRO:HB3	8:A:2290:PRO:HA	2.02	0.41
14:O:317:THR:O	14:O:321:GLU:HG2	2.21	0.41
22:s:2:SER:HB2	23:t:118:ALA:HB1	2.03	0.41
24:u:732:TRP:CD1	24:u:736:ARG:HE	2.38	0.41
24:u:1000:ILE:HA	24:u:1003:VAL:HG12	2.03	0.41
25:v:523:GLY:HA3	25:v:537:LYS:HD3	2.03	0.41
1:1:97:PHE:HD1	1:1:100:ILE:HD13	1.85	0.41
5:6:45:A:H2'	7:8:554:ARG:HH22	1.85	0.41
8:A:82:ARG:NH2	21:Z:258:A:N1	2.50	0.41
8:A:118:VAL:HA	8:A:129:VAL:HA	2.02	0.41
8:A:1947:ASN:O	8:A:1951:LYS:HB2	2.21	0.41
8:A:2069:SER:HA	8:A:2072:GLU:HG2	2.01	0.41
30:A:3001:IHP:O42	30:A:3001:IHP:P1	2.78	0.41
9:B:898:LEU:HD23	9:B:898:LEU:HA	1.93	0.41
9:B:910:ASP:OD1	9:B:910:ASP:N	2.53	0.41
14:O:276:ILE:H	14:O:276:ILE:HG13	1.69	0.41
14:O:313:TRP:CE3	14:O:336:TRP:HB2	2.56	0.41
15:P:204:GLY:HA2	15:P:205:ILE:HA	1.78	0.41
19:V:58:LYS:HE2	19:V:144:MET:HG2	2.02	0.41
19:V:133:CYS:SG	19:V:134:GLN:N	2.94	0.41
24:u:1281:ILE:HD13	24:u:1281:ILE:HA	1.92	0.41
24:u:1299:GLU:HA	24:u:1302:TYR:CE1	2.56	0.41
8:A:154:GLU:HG2	8:A:572:PHE:CG	2.56	0.41
8:A:1988:LEU:HD21	8:A:2007:ILE:HG23	2.03	0.41
9:B:238:ASN:O	9:B:242:LEU:CB	2.65	0.41
24:u:465:PRO:HD2	24:u:502:LEU:HG	2.03	0.41
24:u:1288:TYR:HA	24:u:1296:ILE:HD11	2.02	0.41
25:v:789:VAL:HG11	25:v:892:ALA:HA	2.03	0.41
28:z:49:ARG:HB2	28:z:61:TYR:HB2	2.02	0.41
8:A:891:PHE:O	13:L:83:ARG:NE	2.54	0.40
8:A:1475:ILE:O	8:A:1479:GLY:N	2.51	0.40
8:A:1553:VAL:HG11	23:t:194:ARG:HH11	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:375:GLU:HG3	9:B:376:PRO:HD3	2.02	0.40
11:D:422:ASN:HB3	11:D:426:VAL:HG12	2.02	0.40
14:O:333:PHE:O	14:O:337:MET:HG2	2.21	0.40
15:P:240:GLY:HA3	15:P:296:ARG:HH12	1.85	0.40
19:V:141:ARG:HE	19:V:144:MET:HE3	1.86	0.40
24:u:1171:PRO:HA	24:u:1174:GLU:HG2	2.03	0.40
3:3:563:ARG:HA	3:3:564:PRO:HD3	1.93	0.40
4:5:26:A:OP1	8:A:419:ARG:NH1	2.43	0.40
8:A:1705:ILE:HD13	8:A:1705:ILE:HG21	1.88	0.40
8:A:2072:GLU:HA	8:A:2075:VAL:HG22	2.02	0.40
9:B:201:ASN:N	9:B:201:ASN:OD1	2.54	0.40
23:t:271:ASN:ND2	23:t:283:GLU:OE1	2.54	0.40
24:u:509:PRO:HA	24:u:512:ARG:HB2	2.02	0.40
25:v:141:VAL:HB	25:v:158:LEU:HB2	2.04	0.40
25:v:515:ALA:HA	25:v:528:ARG:HB3	2.02	0.40
25:v:809:GLU:OE2	25:v:881:GLN:NE2	2.55	0.40
5:6:55:C:OP2	5:6:74:U:O2'	2.31	0.40
8:A:1090:ARG:NH1	8:A:1092:ILE:O	2.54	0.40
8:A:1095:ILE:HD12	8:A:1097:ILE:HD11	2.03	0.40
8:A:1529:ILE:HA	8:A:1532:ARG:HG2	2.02	0.40
8:A:1766:GLN:HG3	8:A:1768:TYR:H	1.85	0.40
8:A:2103:THR:HG23	8:A:2139:VAL:HG23	2.02	0.40
9:B:63:LYS:O	9:B:65:TYR:N	2.51	0.40
11:D:194:TRP:HA	11:D:490:ARG:O	2.21	0.40
11:D:297:HIS:HA	11:D:298:PRO:HD3	1.94	0.40
11:D:301:ASP:OD1	11:D:301:ASP:N	2.48	0.40
14:O:300:ASP:OD1	14:O:300:ASP:N	2.53	0.40
23:t:223:ARG:HE	24:u:1018:PRO:HB2	1.86	0.40
24:u:1006:MET:HE3	24:u:1006:MET:HB2	2.00	0.40
24:u:1109:ARG:HA	24:u:1112:THR:HG22	2.03	0.40
24:u:1286:ARG:NH2	24:u:1301:ASP:OD1	2.43	0.40
25:v:214:ASP:O	25:v:218:ASN:N	2.47	0.40
25:v:1062(A):THR:HG22	25:v:1087:GLN:HB3	2.04	0.40
8:A:959:ILE:HD11	8:A:1196:ILE:HD13	2.02	0.40
10:C:279:HIS:HB3	13:L:88:ILE:HG12	2.02	0.40
11:D:213:GLU:OE2	11:D:218:TRP:NE1	2.55	0.40
22:s:25:ASP:OD1	22:s:25:ASP:N	2.53	0.40
22:s:25:ASP:OD1	22:s:137:THR:OG1	2.32	0.40
24:u:914:PHE:CD2	24:u:954:LEU:HD11	2.56	0.40
8:A:362:ARG:HE	9:B:279:ARG:HE	1.68	0.40
9:B:129:ILE:H	9:B:129:ILE:HG13	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:327:TYR:OH	9:B:372:PHE:O	2.32	0.40
9:B:910:ASP:HA	9:B:911:PRO:HD3	1.94	0.40
11:D:356:LEU:HD13	11:D:368:LEU:HD13	2.03	0.40
19:V:82:PHE:HZ	19:V:100:MET:HE3	1.85	0.40
24:u:617:ILE:HD13	24:u:651:VAL:HG21	2.03	0.40
24:u:889:GLU:OE1	24:u:924:ARG:NE	2.55	0.40
25:v:1102:LEU:HD11	25:v:1122:LEU:HD13	2.03	0.40
27:y:97:ASP:OD1	27:y:97:ASP:N	2.52	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 PDB entries followed by that with respect to all EM entries.

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	1	120/322 (37%)	105 (88%)	15 (12%)	0	100	100
3	3	116/619 (19%)	93 (80%)	23 (20%)	0	100	100
6	7	91/464 (20%)	85 (93%)	6 (7%)	0	100	100
7	8	142/895 (16%)	122 (86%)	18 (13%)	2 (1%)	9	31
8	A	2232/2335 (96%)	1953 (88%)	274 (12%)	5 (0%)	43	71
9	B	900/972 (93%)	747 (83%)	149 (17%)	4 (0%)	30	59
10	C	282/536 (53%)	221 (78%)	61 (22%)	0	100	100
11	D	318/514 (62%)	269 (85%)	47 (15%)	2 (1%)	21	50
12	E	126/579 (22%)	112 (89%)	14 (11%)	0	100	100
13	L	101/802 (13%)	87 (86%)	13 (13%)	1 (1%)	12	40
14	O	251/848 (30%)	219 (87%)	31 (12%)	1 (0%)	30	59
15	P	282/420 (67%)	236 (84%)	45 (16%)	1 (0%)	30	59
16	Q	136/144 (94%)	115 (85%)	21 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	R	98/229 (43%)	79 (81%)	19 (19%)	0	100	100
18	S	32/2752 (1%)	24 (75%)	8 (25%)	0	100	100
19	V	157/166 (95%)	148 (94%)	9 (6%)	0	100	100
20	Y	93/904 (10%)	90 (97%)	3 (3%)	0	100	100
22	s	173/472 (37%)	152 (88%)	21 (12%)	0	100	100
23	t	166/343 (48%)	145 (87%)	20 (12%)	1 (1%)	21	50
24	u	877/1304 (67%)	803 (92%)	70 (8%)	4 (0%)	24	54
25	v	1179/1217 (97%)	1022 (87%)	153 (13%)	4 (0%)	36	65
26	x	77/86 (90%)	66 (86%)	11 (14%)	0	100	100
27	y	98/110 (89%)	90 (92%)	8 (8%)	0	100	100
28	z	99/125 (79%)	85 (86%)	14 (14%)	0	100	100
All	All	8146/17158 (48%)	7068 (87%)	1053 (13%)	25 (0%)	37	65

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	D	384	HIS
24	u	464	LEU
8	A	1519	THR
11	D	385	TYR
15	P	67	LYS
23	t	154	ARG
7	8	595	LYS
9	B	66	TYR
24	u	465	PRO
24	u	946	LYS
25	v	583	MET
25	v	585	ALA
13	L	80	THR
8	A	1084	PRO
8	A	1419	ILE
9	B	940	ARG
14	O	444	SER
7	8	521	PRO
8	A	1077	ILE
8	A	1118	PRO
9	B	470	PRO
9	B	760	GLY

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Mol	Chain	Res	Type
25	v	281	PRO
25	v	914	ILE
24	u	489	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1	109/291 (38%)	108 (99%)	1 (1%)	70	76
3	3	102/545 (19%)	101 (99%)	1 (1%)	68	75
6	7	77/382 (20%)	77 (100%)	0	100	100
7	8	132/776 (17%)	132 (100%)	0	100	100
8	A	2026/2108 (96%)	1991 (98%)	35 (2%)	53	67
9	B	802/866 (93%)	785 (98%)	17 (2%)	47	64
10	C	242/459 (53%)	239 (99%)	3 (1%)	63	72
11	D	275/441 (62%)	266 (97%)	9 (3%)	33	57
12	E	111/502 (22%)	111 (100%)	0	100	100
13	L	88/709 (12%)	88 (100%)	0	100	100
14	O	229/751 (30%)	225 (98%)	4 (2%)	53	67
15	P	254/361 (70%)	251 (99%)	3 (1%)	63	72
16	Q	126/130 (97%)	124 (98%)	2 (2%)	55	68
17	R	94/203 (46%)	94 (100%)	0	100	100
18	S	27/2432 (1%)	27 (100%)	0	100	100
19	V	129/134 (96%)	129 (100%)	0	100	100
20	Y	86/831 (10%)	84 (98%)	2 (2%)	44	63
22	s	149/416 (36%)	147 (99%)	2 (1%)	61	71
23	t	153/294 (52%)	153 (100%)	0	100	100
24	u	763/1104 (69%)	759 (100%)	4 (0%)	81	81
25	v	1028/1051 (98%)	1021 (99%)	7 (1%)	76	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	x	71/77 (92%)	71 (100%)	0	100	100
27	y	86/95 (90%)	86 (100%)	0	100	100
28	z	90/109 (83%)	89 (99%)	1 (1%)	65	74
All	All	7249/15067 (48%)	7158 (99%)	91 (1%)	59	71

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	38	ILE
3	3	501	LEU
8	A	70	ILE
8	A	129	VAL
8	A	258	PHE
8	A	338	VAL
8	A	422	LEU
8	A	450	LEU
8	A	574	LEU
8	A	578	LEU
8	A	585	VAL
8	A	647	LEU
8	A	648	LEU
8	A	709	ILE
8	A	735	ILE
8	A	767	VAL
8	A	856	LEU
8	A	871	TYR
8	A	917	ILE
8	A	946	GLU
8	A	975	VAL
8	A	1047	VAL
8	A	1087	LEU
8	A	1099	PHE
8	A	1246	GLN
8	A	1260	VAL
8	A	1434	LYS
8	A	1467	LEU
8	A	1487	HIS
8	A	1531	ASN
8	A	1547	VAL
8	A	1629	ILE
8	A	1711	LEU

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Mol	Chain	Res	Type
8	A	1743	LEU
8	A	1777	ILE
8	A	1967	ILE
8	A	2010	ILE
9	B	97	VAL
9	B	111	VAL
9	B	134	LEU
9	B	226	VAL
9	B	264	ILE
9	B	320	LEU
9	B	380	ILE
9	B	449	ILE
9	B	555	VAL
9	B	580	LEU
9	B	688	ILE
9	B	787	VAL
9	B	809	ILE
9	B	857	VAL
9	B	875	ILE
9	B	878	ILE
9	B	949	ILE
10	C	180	THR
10	C	197	ILE
10	C	280	ILE
11	D	187	LYS
11	D	242	LEU
11	D	380	LEU
11	D	385	TYR
11	D	394	ASN
11	D	427	LEU
11	D	428	VAL
11	D	459	LEU
11	D	478	LEU
14	O	258	ILE
14	O	350	ILE
14	O	404	GLU
14	O	443	ILE
15	P	150	LEU
15	P	263	VAL
15	P	264	VAL
16	Q	60	ILE
16	Q	132	ILE

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Mol	Chain	Res	Type
20	Y	70	PHE
20	Y	71	ILE
22	s	63	VAL
22	s	174	ILE
24	u	596	ILE
24	u	1065	LEU
24	u	1100	ASN
24	u	1303	ILE
25	v	278	LEU
25	v	521	PRO
25	v	545	VAL
25	v	613	THR
25	v	680	ASP
25	v	822	GLU
25	v	948	VAL
28	z	20	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
6	7	74	GLN
7	8	496	ASN
7	8	569	GLN
7	8	587	HIS
8	A	39	GLN
8	A	210	HIS
8	A	243	ASN
8	A	270	ASN
8	A	289	GLN
8	A	325	HIS
8	A	328	HIS
8	A	368	GLN
8	A	483	GLN
8	A	505	ASN
8	A	512	ASN
8	A	561	HIS
8	A	563	GLN
8	A	860	GLN
8	A	873	ASN
8	A	974	ASN
8	A	994	ASN
8	A	1096	HIS

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Mol	Chain	Res	Type
8	A	1169	GLN
8	A	1293	ASN
8	A	1332	HIS
8	A	1399	GLN
8	A	1476	GLN
8	A	1522	GLN
8	A	1531	ASN
8	A	1543	ASN
8	A	1599	GLN
8	A	1712	HIS
8	A	1728	GLN
8	A	1752	GLN
8	A	1918	ASN
8	A	1998	ASN
8	A	2123	GLN
8	A	2138	GLN
9	B	502	HIS
9	B	557	GLN
9	B	583	ASN
9	B	706	GLN
9	B	771	GLN
10	C	157	GLN
10	C	183	GLN
10	C	279	HIS
10	C	307	GLN
11	D	245	HIS
11	D	278	ASN
11	D	283	HIS
11	D	344	GLN
11	D	350	HIS
11	D	413	ASN
11	D	451	HIS
13	L	29	ASN
13	L	30	GLN
14	O	294	HIS
14	O	389	HIS
14	O	425	ASN
15	P	268	GLN
15	P	273	GLN
16	Q	95	GLN
16	Q	136	HIS
17	R	196	ASN

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Mol	Chain	Res	Type
19	V	134	GLN
20	Y	44	ASN
20	Y	74	GLN
22	s	42	GLN
22	s	88	HIS
22	s	127	HIS
22	s	169	ASN
23	t	158	ASN
23	t	289	HIS
24	u	445	HIS
24	u	832	GLN
24	u	903	GLN
24	u	919	ASN
24	u	942	ASN
24	u	1091	HIS
24	u	1100	ASN
24	u	1209	ASN
25	v	9	GLN
25	v	138	GLN
25	v	169	HIS
25	v	219	HIS
25	v	254	ASN
25	v	304	GLN
25	v	526	HIS
25	v	553	GLN
25	v	795	ASN
25	v	796	ASN
25	v	814	GLN
25	v	817	GLN
25	v	885	ASN
25	v	988	ASN
25	v	1147	HIS
25	v	1188	ASN
26	x	8	HIS
26	x	46	HIS
27	y	50	ASN
28	z	52	ASN
28	z	76	HIS
28	z	99	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	57/188 (30%)	16 (28%)	1 (1%)
21	Z	46/478 (9%)	19 (41%)	1 (2%)
4	5	69/116 (59%)	31 (44%)	1 (1%)
5	6	94/107 (87%)	30 (31%)	1 (1%)
All	All	266/889 (29%)	96 (36%)	4 (1%)

All (96) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	13	C
2	2	14	C
2	2	16	U
2	2	18	U
2	2	19	G
2	2	23	A
2	2	24	A
2	2	25	G
2	2	27	U
2	2	30	A
2	2	31	G
2	2	36	G
2	2	37	U
2	2	45	C
2	2	49	U
2	2	50	C
4	5	8	G
4	5	9	G
4	5	10	U
4	5	14	U
4	5	16	U
4	5	17	U
4	5	19	A
4	5	20	G
4	5	21	A
4	5	22	U
4	5	24	G
4	5	26	A
4	5	27	U
4	5	34	U
4	5	35	U
4	5	37	G
4	5	39	C
4	5	40	U

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Mol	Chain	Res	Type
4	5	41	U
4	5	43	U
4	5	44	A
4	5	45	C
4	5	47	A
4	5	52	U
4	5	53	U
4	5	61	A
4	5	62	G
4	5	68	C
4	5	69	A
4	5	72	U
4	5	73	C
5	6	6	C
5	6	7	G
5	6	9	U
5	6	13	G
5	6	21	U
5	6	22	A
5	6	24	A
5	6	25	C
5	6	26	U
5	6	28	A
5	6	29	A
5	6	30	A
5	6	31	U
5	6	34	G
5	6	35	A
5	6	36	A
5	6	44	G
5	6	45	A
5	6	49	G
5	6	54	G
5	6	56	A
5	6	59	G
5	6	69	A
5	6	70	A
5	6	74	U
5	6	78	A
5	6	81	C
5	6	82	A
5	6	83	A

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Mol	Chain	Res	Type
5	6	84	A
21	Z	234	G
21	Z	235	C
21	Z	236	C
21	Z	239	C
21	Z	243	G
21	Z	244	U
21	Z	247	G
21	Z	251	C
21	Z	253	A
21	Z	254	G
21	Z	258	A
21	Z	259	C
21	Z	260	A
21	Z	261	A
21	Z	262	G
21	Z	385	U
21	Z	388	U
21	Z	394	A
21	Z	397	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	23	A
4	5	26	A
5	6	58	G
21	Z	261	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 for Mogul analysis.

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
30	IHP	A	3001	-	36,36,36	0.74	0	60,60,60	1.34	4 (6%)
31	GTP	B	1500	-	33,34,34	0.94	1 (3%)	50,54,54	1.67	10 (20%)

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
30	IHP	A	3001	-	-	2/30/54/54	0/1/1/1
31	GTP	B	1500	-	-	5/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	1500	GTP	C5-N7	-2.13	1.34	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	1500	GTP	C5-C4-N3	-4.75	120.83	128.39
31	B	1500	GTP	C2-N3-C4	4.66	120.33	112.30
30	A	3001	IHP	O12-C2-C1	3.24	115.66	108.76
31	B	1500	GTP	C2-N1-C6	-3.12	119.45	125.11
31	B	1500	GTP	N9-C4-N3	3.11	132.18	125.95
31	B	1500	GTP	N9-C8-N7	-3.00	107.83	113.40
31	B	1500	GTP	C5-C6-N1	2.81	120.39	113.25
30	A	3001	IHP	P4-O14-C4	-2.75	116.09	123.43
30	A	3001	IHP	C5-C6-C1	2.54	116.00	110.43
31	B	1500	GTP	O3B-PB-O1B	-2.51	103.14	110.70
31	B	1500	GTP	O6-C6-C5	-2.47	120.00	126.53
30	A	3001	IHP	C4-C3-C2	-2.41	105.14	110.43
31	B	1500	GTP	C8-N7-C5	2.40	108.54	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	1500	GTP	O2G-PG-O3B	2.08	111.62	104.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

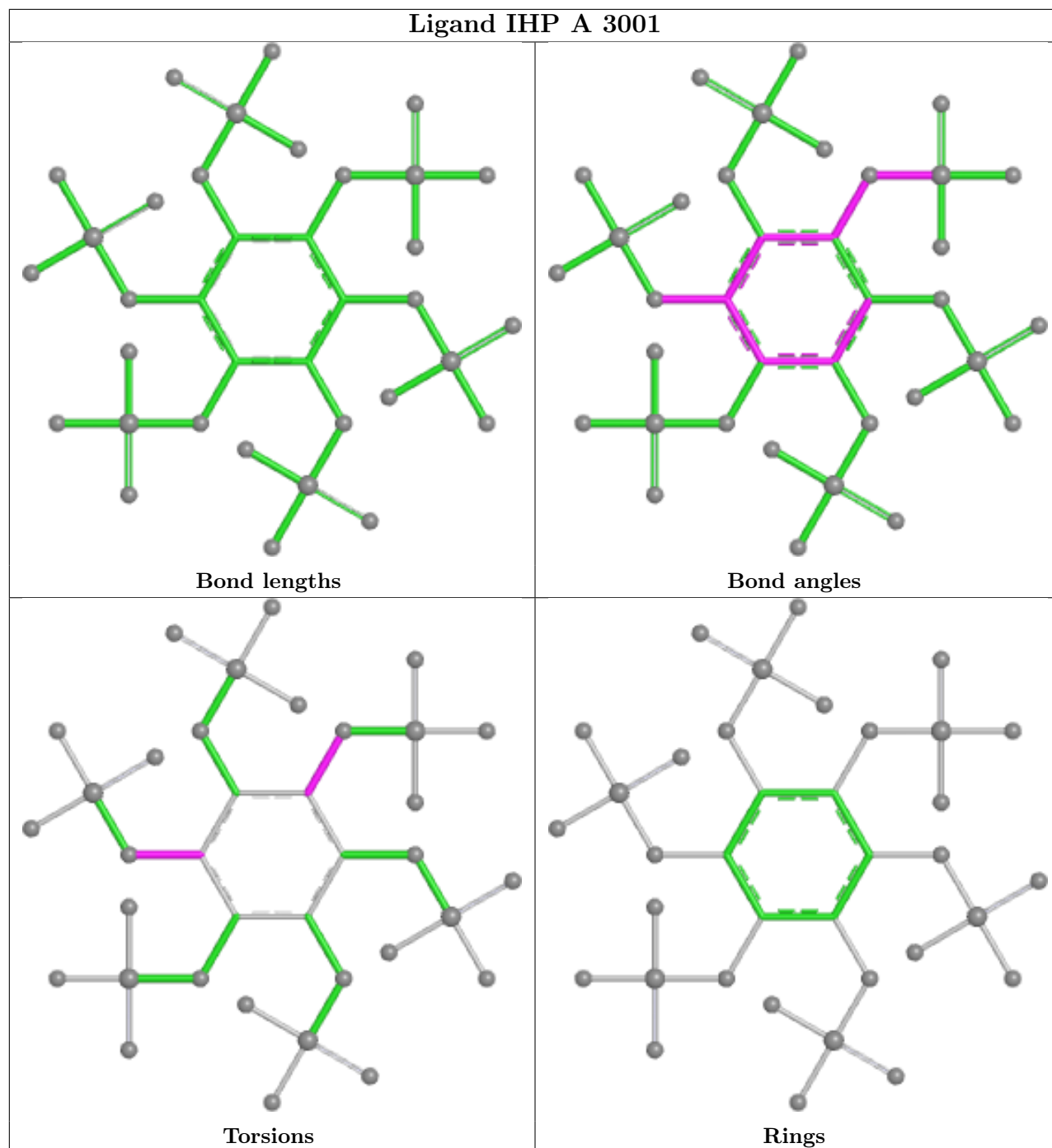
Mol	Chain	Res	Type	Atoms
30	A	3001	IHP	C1-C2-O12-P2
31	B	1500	GTP	C5'-O5'-PA-O3A
31	B	1500	GTP	C5'-O5'-PA-O1A
31	B	1500	GTP	PA-O3A-PB-O1B
31	B	1500	GTP	C4'-C5'-O5'-PA
31	B	1500	GTP	O4'-C4'-C5'-O5'
30	A	3001	IHP	C3-C4-O14-P4

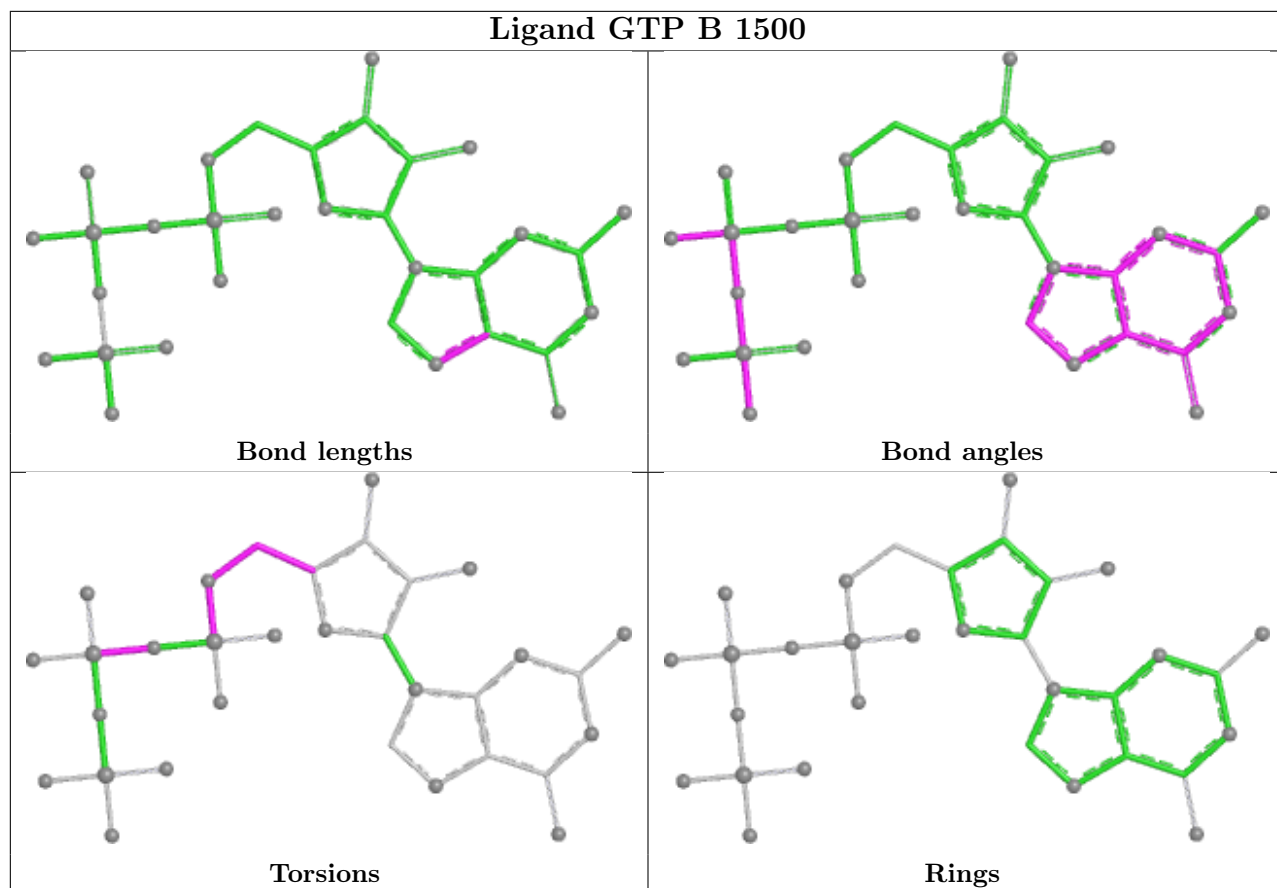
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	A	3001	IHP	11	0
31	B	1500	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	59:A	O3'	60:U	P	4.39

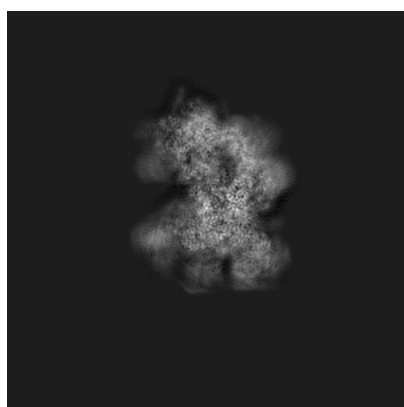
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4255. These allow visual inspection of the internal detail of the map and identification of artifacts.

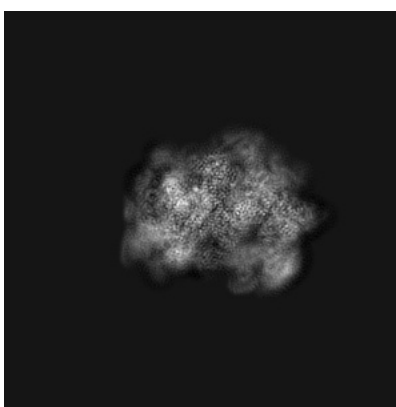
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

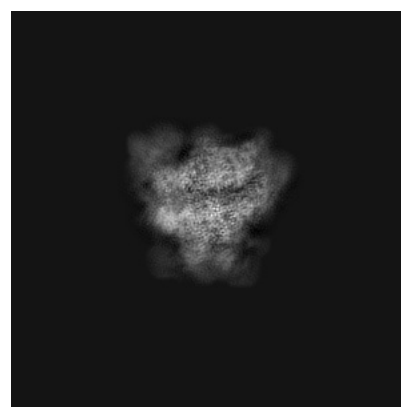
6.1.1 Primary map



X



Y

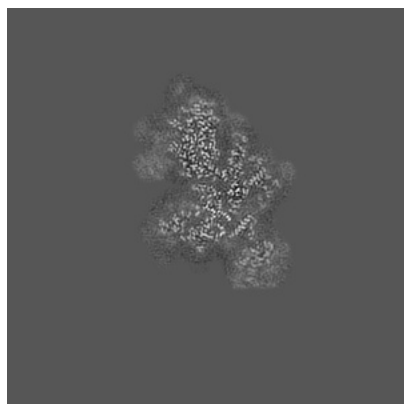


Z

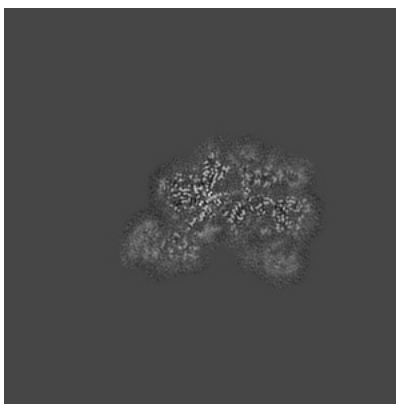
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

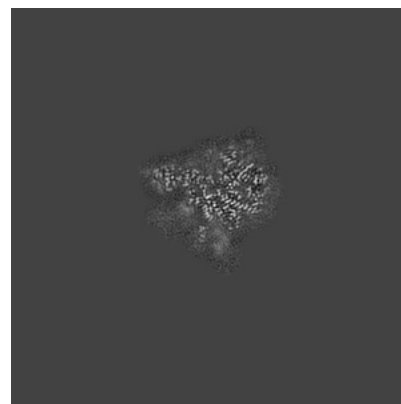
6.2.1 Primary map



X Index: 210



Y Index: 210

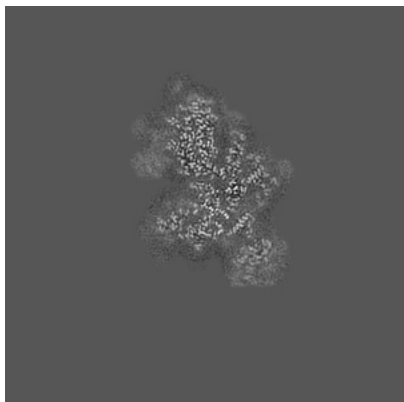


Z Index: 210

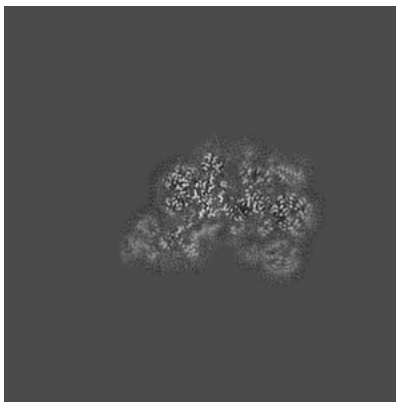
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

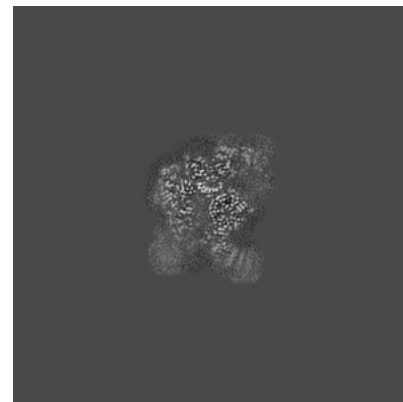
6.3.1 Primary map



X Index: 210



Y Index: 207

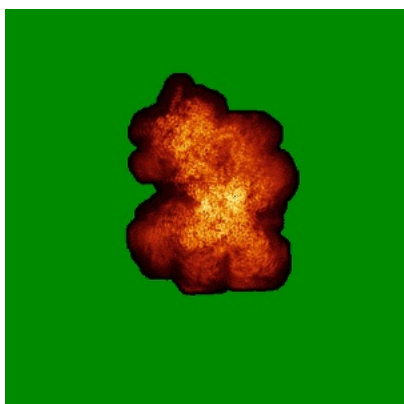


Z Index: 184

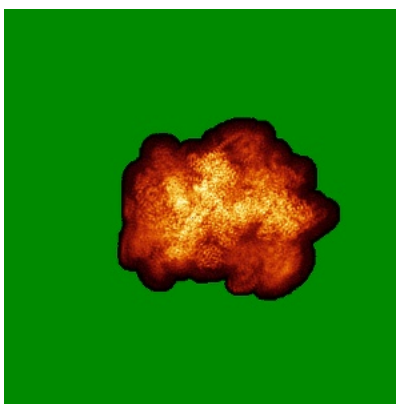
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

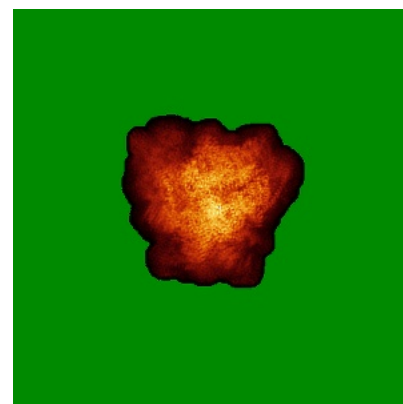
6.4.1 Primary map



X



Y

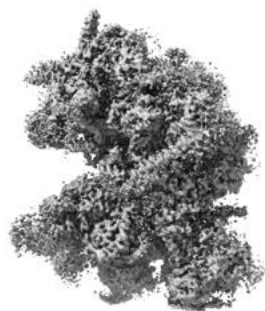


Z

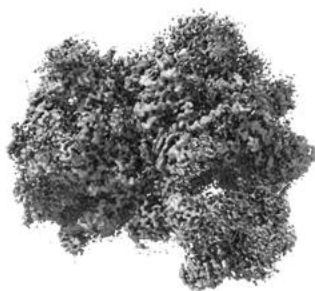
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

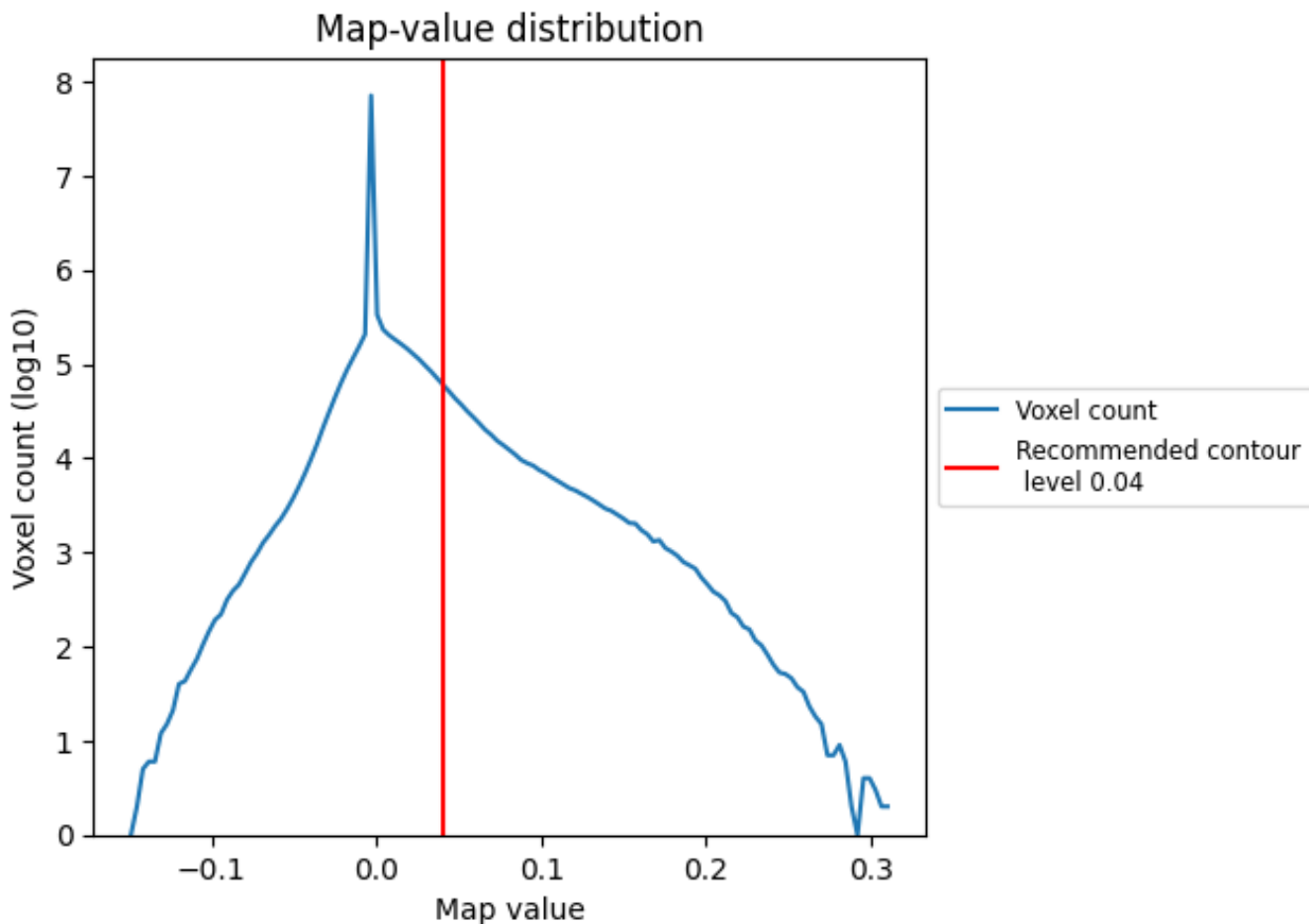
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

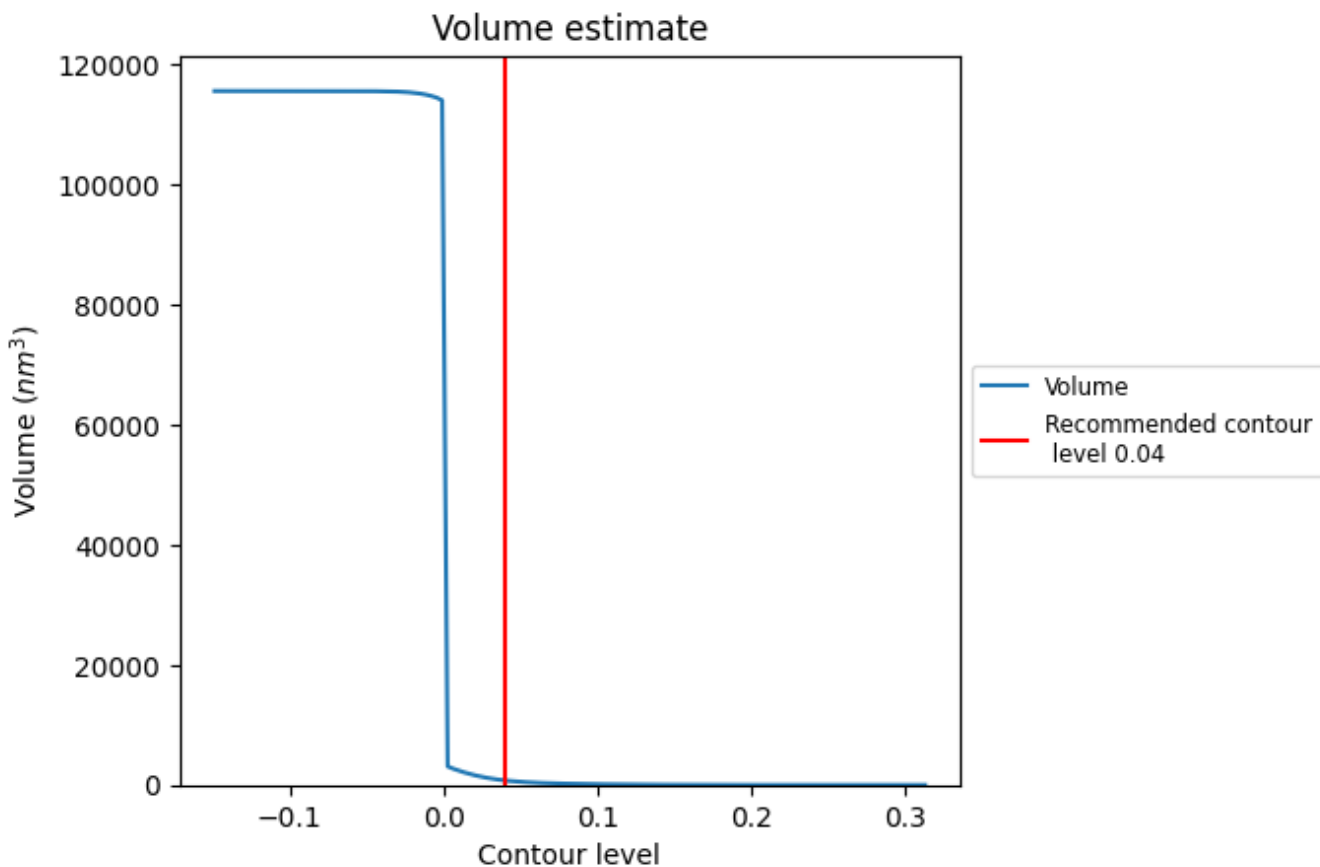
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

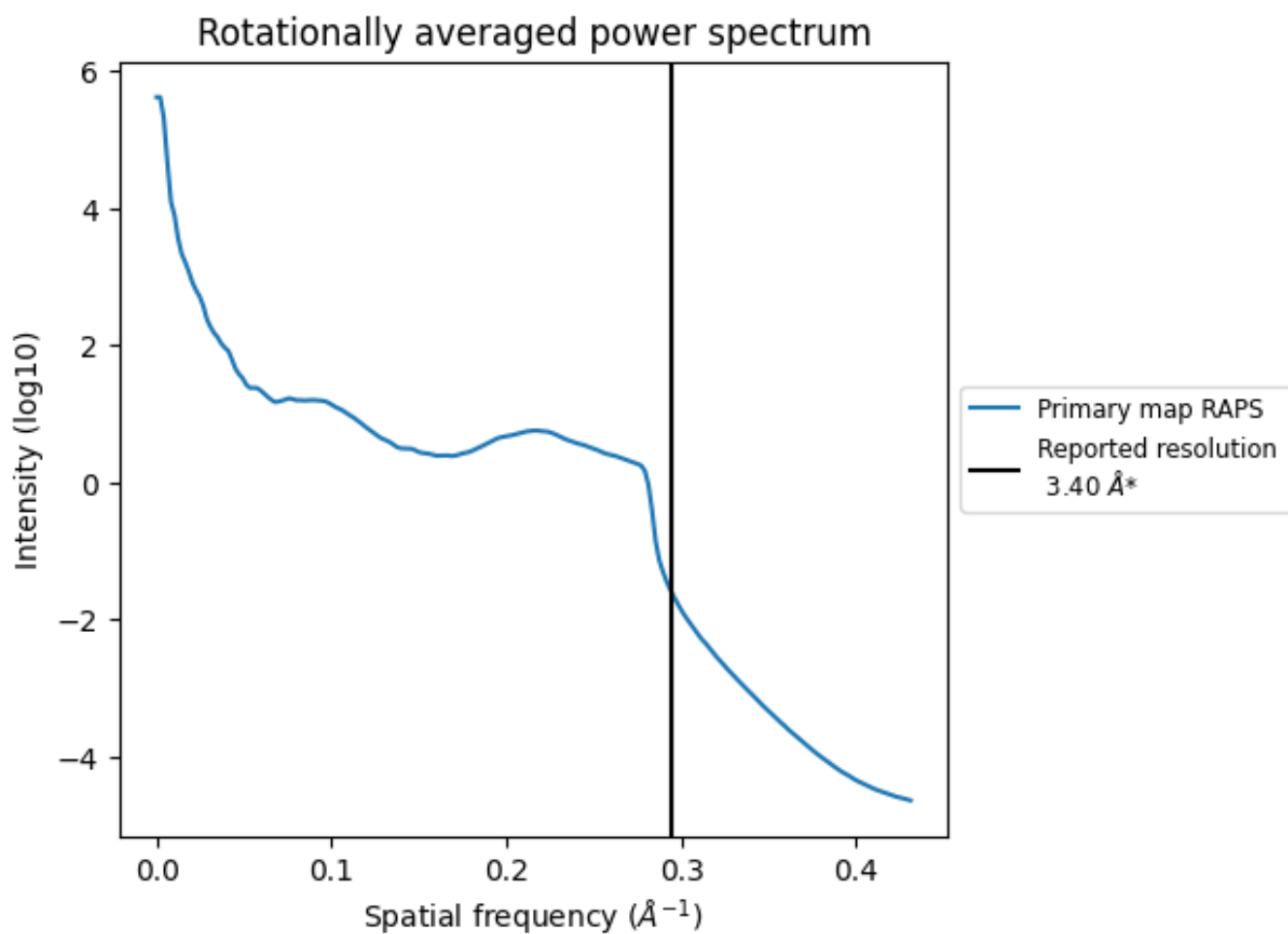
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 759 nm³; this corresponds to an approximate mass of 686 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

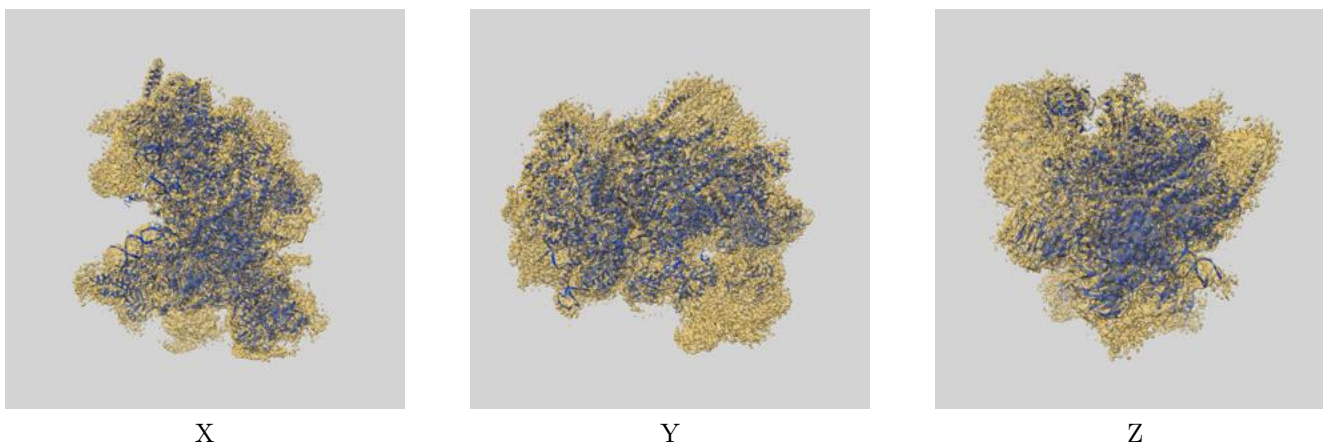
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

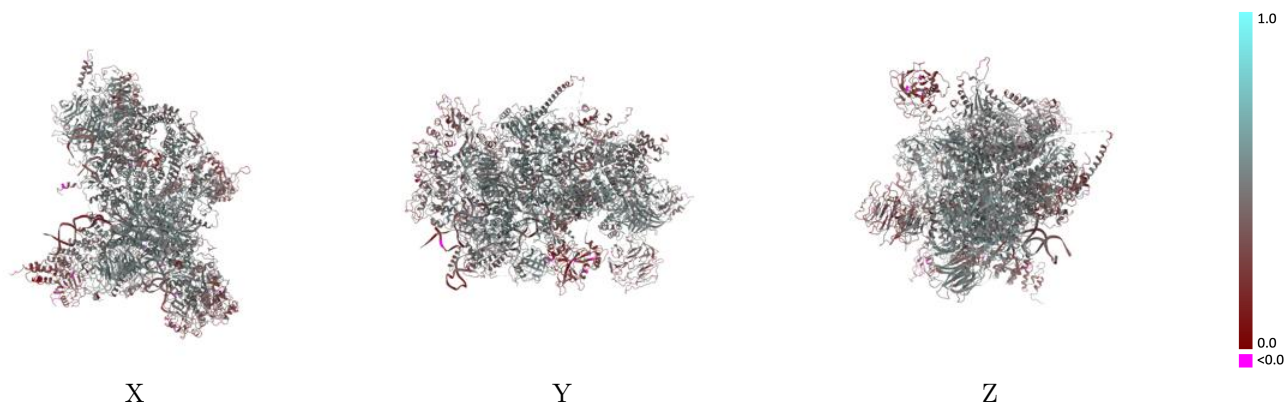
This section contains information regarding the fit between EMDB map EMD-4255 and PDB model 6FF4. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



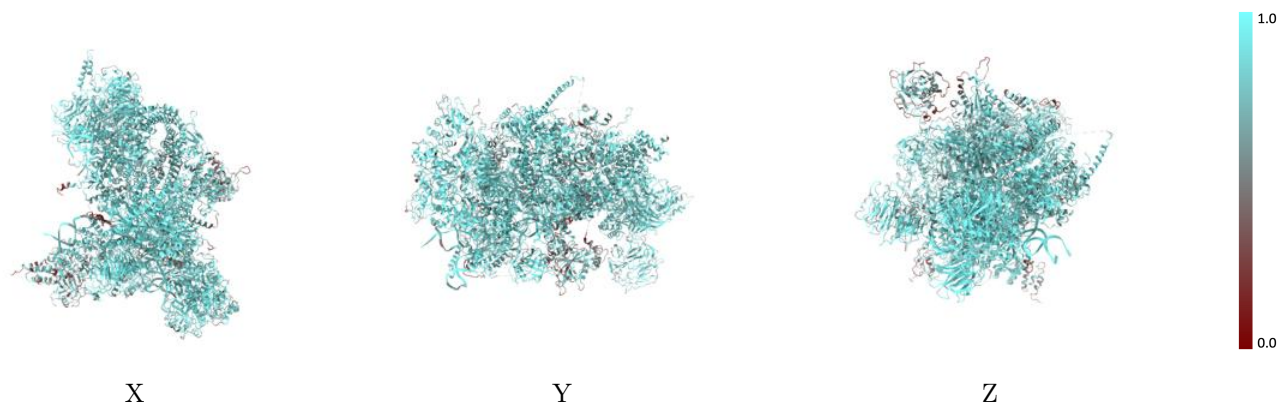
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



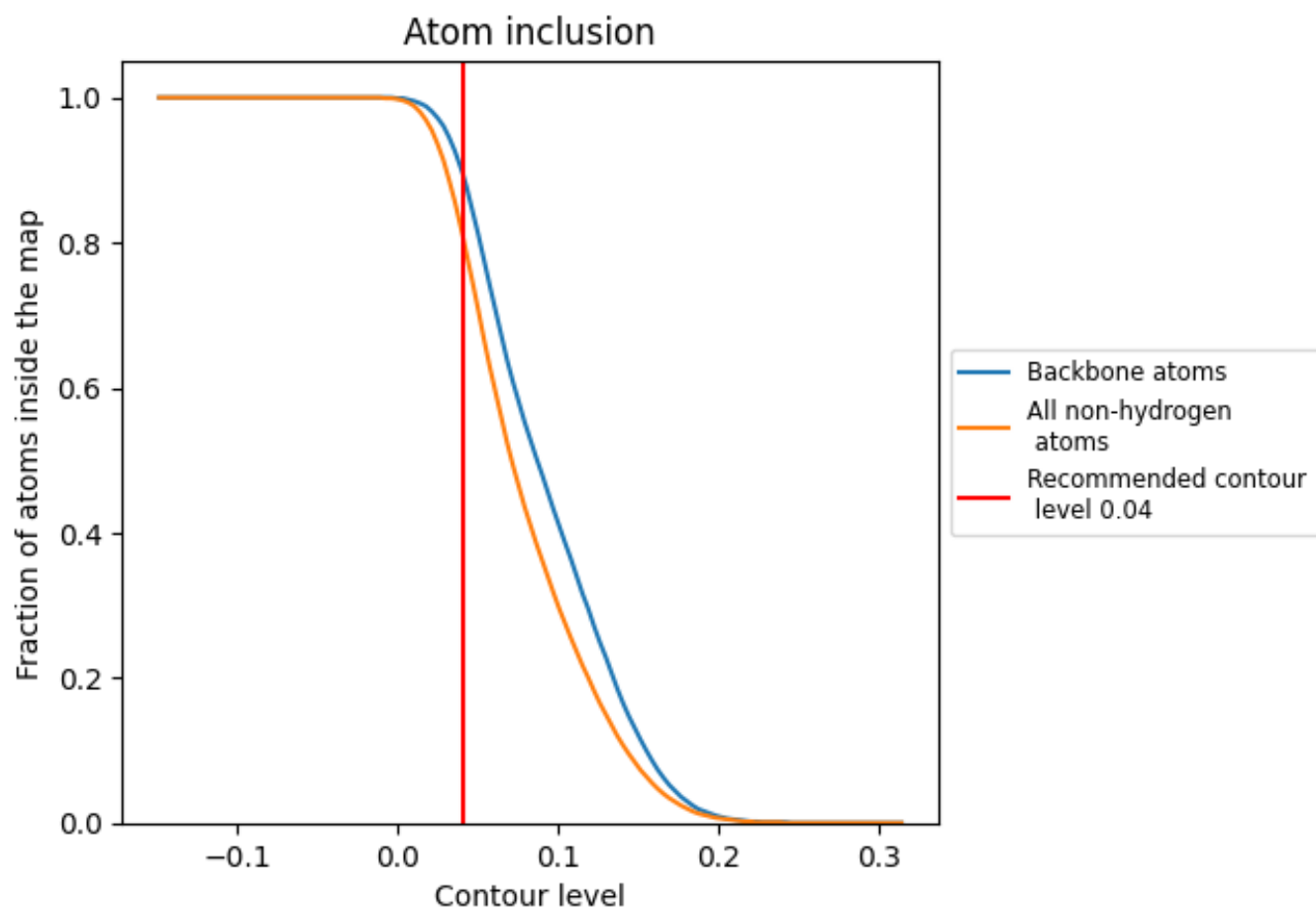
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8120	 0.4430
1	 0.7840	 0.4600
2	 0.8790	 0.3980
3	 0.6360	 0.3860
5	 0.9210	 0.4110
6	 0.8970	 0.3970
7	 0.7870	 0.4660
8	 0.8410	 0.4890
A	 0.8170	 0.4700
B	 0.7990	 0.4050
C	 0.7260	 0.4190
D	 0.9220	 0.5210
E	 0.6100	 0.3610
L	 0.8220	 0.4690
O	 0.7280	 0.3770
P	 0.6410	 0.3540
Q	 0.8840	 0.4650
R	 0.6960	 0.4550
S	 0.6760	 0.4570
V	 0.6450	 0.2470
Y	 0.7920	 0.3720
Z	 0.9230	 0.4510
s	 0.8790	 0.4940
t	 0.6740	 0.4330
u	 0.8420	 0.4910
v	 0.8660	 0.4530
x	 0.8810	 0.4890
y	 0.8740	 0.5160
z	 0.7090	 0.3410

