



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 11:56 pm GMT

PDB ID : 6FSZ
EMDB ID : EMD-4301
Title : Structure of the nuclear RNA exosome
Authors : Schuller, J.M.; Falk, S.; Conti, E.
Deposited on : 2018-02-20
Resolution : 4.60 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:

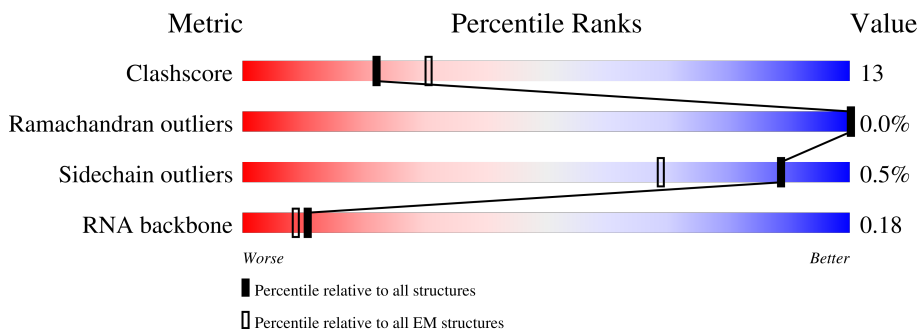
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.60 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.



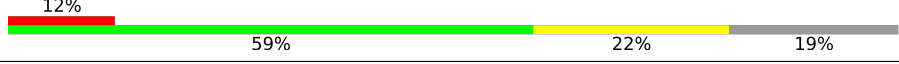
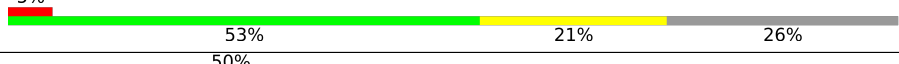
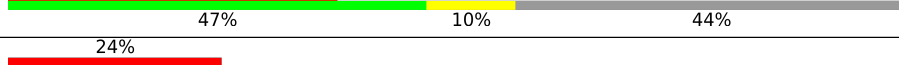
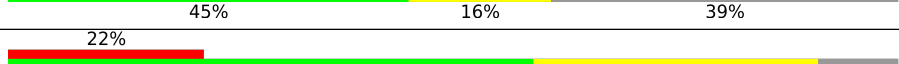
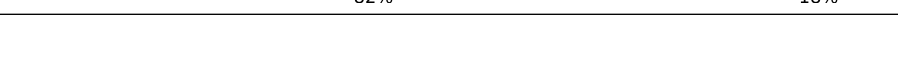
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	2	23	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">17%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 17%, orange 35%, yellow 43%, green 60%, grey 68%);"></div> <div style="text-align: left;">35% 43% 22%</div> </div>
2	AA	303	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">6%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 6%, orange 6%, yellow 68%, green 98%, grey 100%);"></div> <div style="text-align: left;">68% 30%</div> </div>
3	BB	248	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">6%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 6%, orange 6%, yellow 68%, green 98%, grey 100%);"></div> <div style="text-align: left;">68% 30%</div> </div>
4	CC	393	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">9%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 9%, orange 9%, yellow 60%, green 85%, grey 94%);"></div> <div style="text-align: left;">60% 25% 14%</div> </div>
5	DD	245	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">60%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, green 60%, yellow 91%, grey 99%);"></div> <div style="text-align: left;">31% 9%</div> </div>
6	EE	267	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">5%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 5%, orange 5%, yellow 69%, green 99%);"></div> <div style="text-align: left;">69% 31%</div> </div>
7	FF	250	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">6%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 6%, orange 6%, yellow 62%, green 85%, grey 99%);"></div> <div style="text-align: left;">62% 23% 14%</div> </div>

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Mol	Chain	Length	Quality of chain
8	GG	242	
9	HH	361	
10	II	301	
11	JJ	1003	
12	KK	733	
13	LL	184	
14	MM	1073	
15	NN	40	

2 Entry composition i

There are 15 unique types of molecules in this entry. The entry contains 36972 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 RNA chain called RNA (5'-R(P*AP*AP*AP*AP*UP*UP*UP*AP*AP*AP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	23	378	166	43	146	23	0	0

- Molecule 2 is a protein called Exosome complex component RRP45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AA	299	2304	1444	393	451	16	0	0

- Molecule 3 is a protein called Exosome complex component SKI6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	BB	244	1886	1177	335	366	8	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	-1	GLY	-	expression tag	UNP P46948
BB	0	HIS	-	expression tag	UNP P46948

- Molecule 4 is a protein called Exosome complex component RRP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	CC	339	2589	1640	441	497	11	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	102	SER	ALA	conflict	UNP P25359
CC	363	MET	VAL	conflict	UNP P25359

- Molecule 5 is a protein called Exosome complex component RRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	DD	223	1701	1072	285	334	10	1	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DD	-21	GLY	-	expression tag	UNP P53256
DD	-20	HIS	-	expression tag	UNP P53256
DD	-19	GLY	-	expression tag	UNP P53256
DD	-18	ASN	-	expression tag	UNP P53256
DD	-17	ASN	-	expression tag	UNP P53256
DD	-16	LYS	-	expression tag	UNP P53256
DD	-15	GLU	-	expression tag	UNP P53256
DD	-14	PRO	-	expression tag	UNP P53256
DD	-13	ASN	-	expression tag	UNP P53256
DD	-12	THR	-	expression tag	UNP P53256
DD	-11	LYS	-	expression tag	UNP P53256
DD	-10	ASN	-	expression tag	UNP P53256
DD	-9	ARG	-	expression tag	UNP P53256
DD	-8	LEU	-	expression tag	UNP P53256
DD	-7	ASP	-	expression tag	UNP P53256
DD	-6	SER	-	expression tag	UNP P53256
DD	-5	ALA	-	expression tag	UNP P53256
DD	-4	GLU	-	expression tag	UNP P53256
DD	-3	LYS	-	expression tag	UNP P53256
DD	-2	LYS	-	expression tag	UNP P53256
DD	-1	LYS	-	expression tag	UNP P53256
DD	0	LYS	-	expression tag	UNP P53256

- Molecule 6 is a protein called Exosome complex component RRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	EE	267	2050	1308	338	399	5	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EE	-1	GLY	-	expression tag	UNP Q12277
EE	0	HIS	-	expression tag	UNP Q12277
EE	138	ILE	VAL	conflict	UNP Q12277

- Molecule 7 is a protein called Exosome complex component MTR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	FF	215	1638	1023	273	332	10	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FF	75	SER	THR	conflict	UNP P48240
FF	161	THR	MET	conflict	UNP P48240

- Molecule 8 is a protein called Exosome complex component RRP40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	GG	237	1792	1143	295	344	10	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
GG	-1	GLY	-	expression tag	UNP Q08285
GG	0	HIS	-	expression tag	UNP Q08285

- Molecule 9 is a protein called Exosome complex component RRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	HH	293	2236	1393	403	428	12	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
HH	-1	ARG	-	expression tag	UNP P38792
HH	0	SER	-	expression tag	UNP P38792

- Molecule 10 is a protein called Exosome complex component CSL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	II	222	1653	1034	287	325	7	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
II	-8	MET	-	initiating methionine	UNP P53859
II	-7	LYS	-	expression tag	UNP P53859
II	-6	HIS	-	expression tag	UNP P53859
II	-5	HIS	-	expression tag	UNP P53859
II	-4	HIS	-	expression tag	UNP P53859
II	-3	HIS	-	expression tag	UNP P53859
II	-2	HIS	-	expression tag	UNP P53859
II	-1	HIS	-	expression tag	UNP P53859
II	0	PRO	-	expression tag	UNP P53859

- Molecule 11 is a protein called Exosome complex exonuclease DIS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	JJ	948	7430	4693	1310	1392	35	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
JJ	-1	GLY	-	expression tag	UNP Q08162
JJ	0	ALA	-	expression tag	UNP Q08162
JJ	171	ASN	ASP	conflict	UNP Q08162
JJ	551	ASN	ASP	conflict	UNP Q08162

- Molecule 12 is a protein called Exosome complex exonuclease RRP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	KK	414	2517	1544	469	498	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
KK	296	ASN	ASP	engineered mutation	UNP Q12149

- Molecule 13 is a protein called Exosome complex protein LRP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	LL	113	894	565	151	174	4	0	0

- Molecule 14 is a protein called ATP-dependent RNA helicase DOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	MM	978	7627	4871	1294	1419	43	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
MM	80	MET	VAL	conflict	UNP P47047

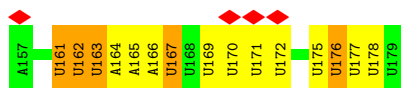
- Molecule 15 is a protein called M-phase phosphoprotein 6 homolog,M-phase phosphoprotein 6 homolog,Nuclear exosome-associated RNA binding protein,M-phase phosphoprotein 6 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	NN	40	277	172	51	54	0	0

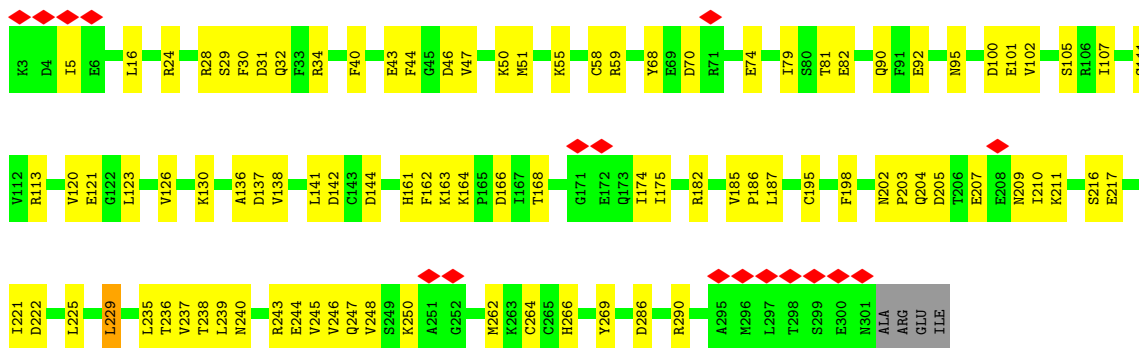
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

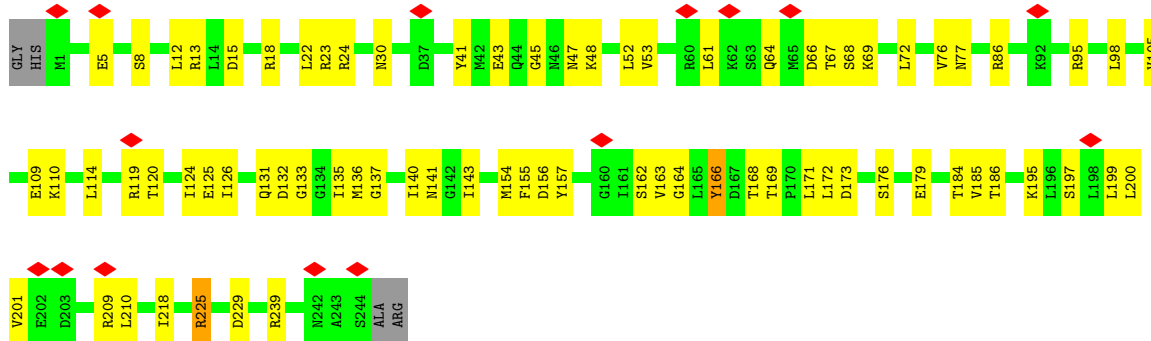
- Molecule 1: RNA (5'-R(P*AP*AP*AP*AP*UP*UP*UP*AP*AP*AP*UP*UP*UP*UP*UP*U P*UP*UP*UP*UP*UP*UP*U)-3')



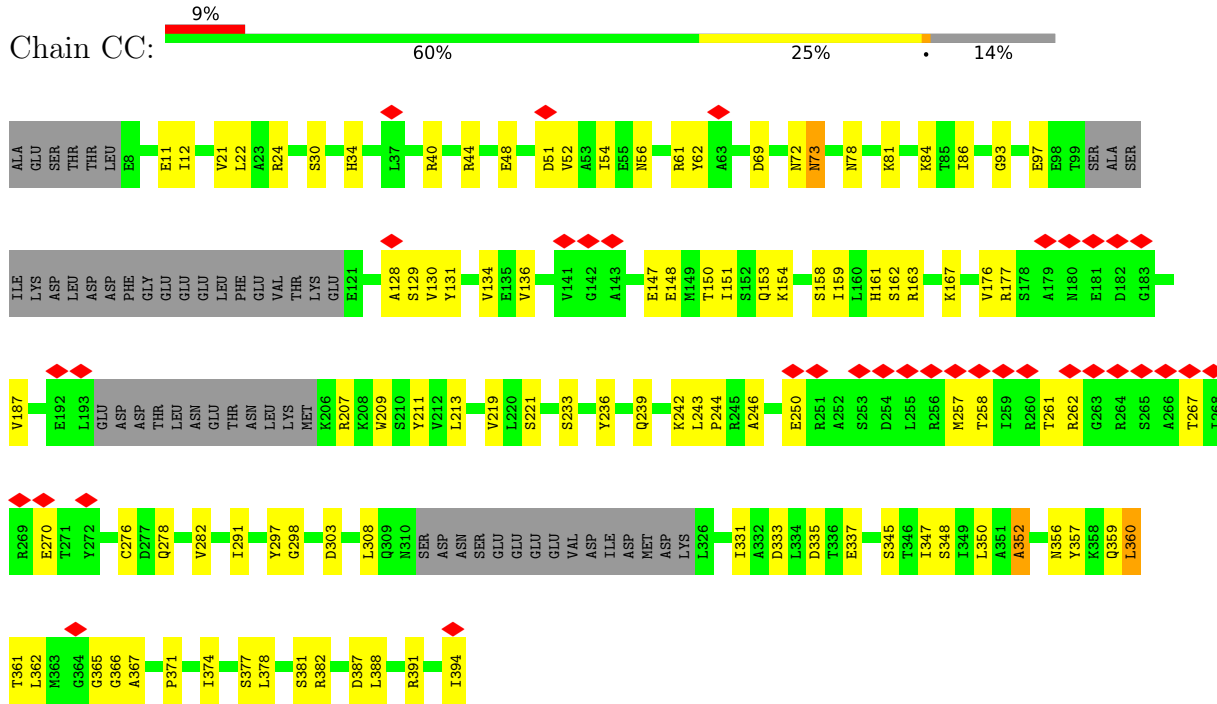
- Molecule 2: Exosome complex component RRP45



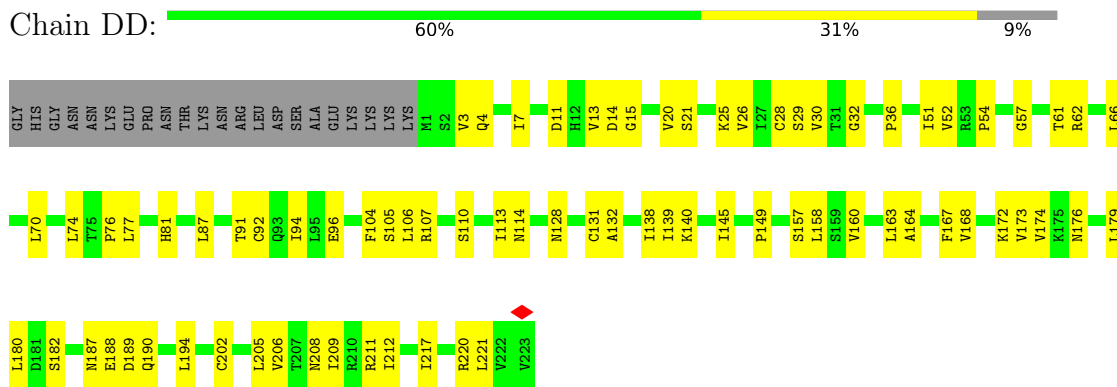
- Molecule 3: Exosome complex component SKI6



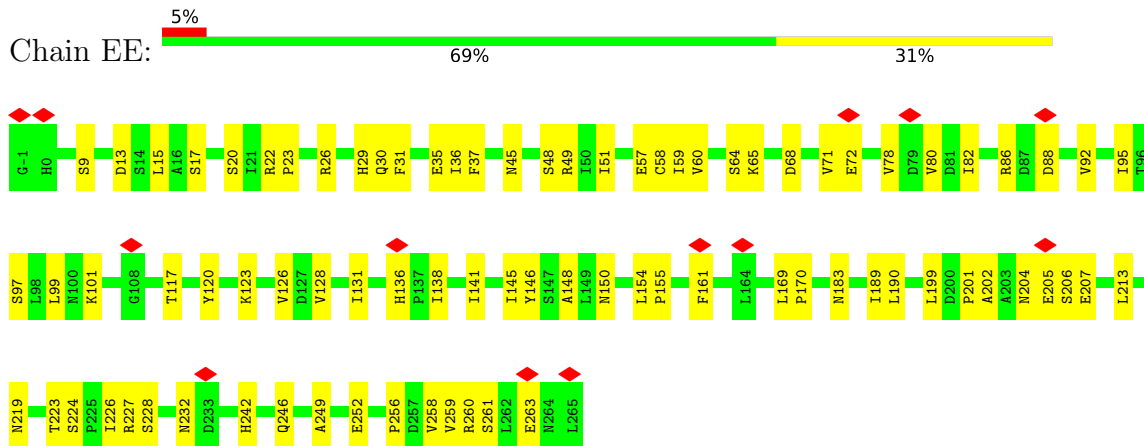
• Molecule 4: Exosome complex component RRP43



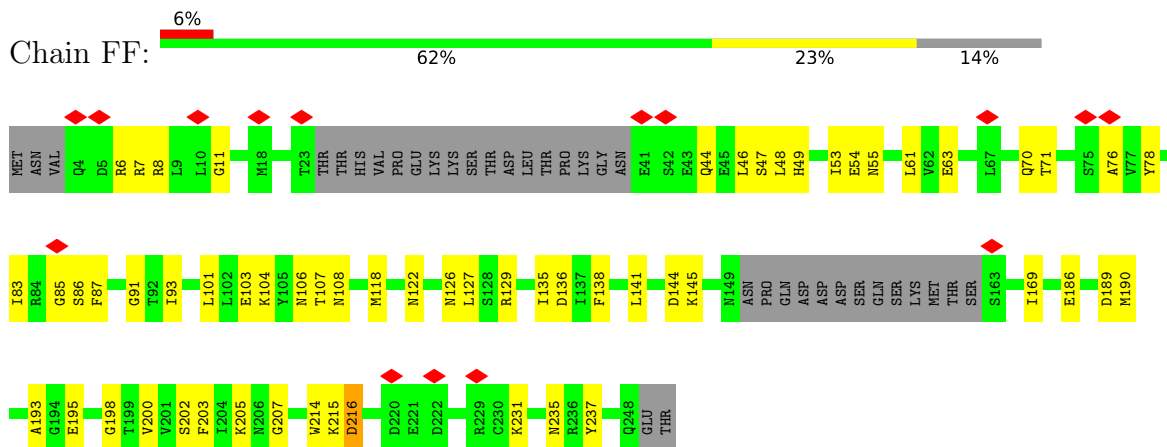
• Molecule 5: Exosome complex component RRP46



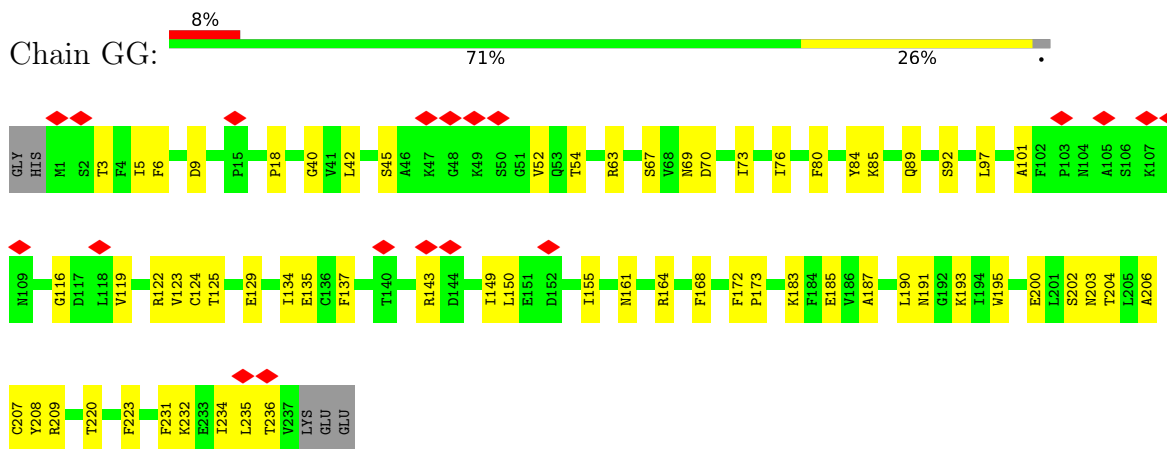
• Molecule 6: Exosome complex component RRP42



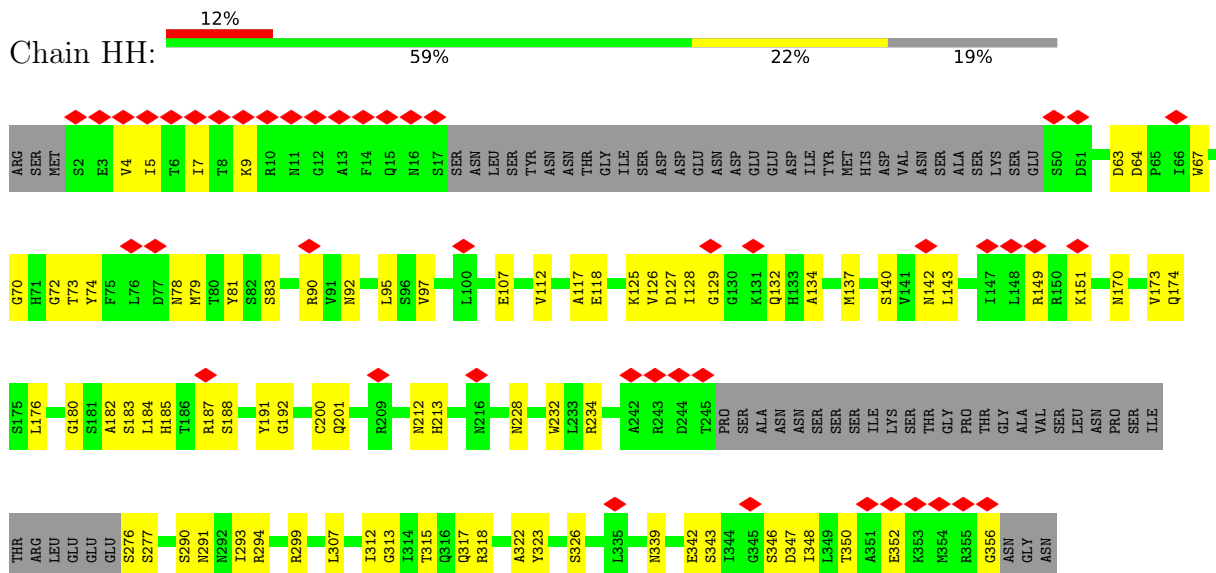
- Molecule 7: Exosome complex component MTR3



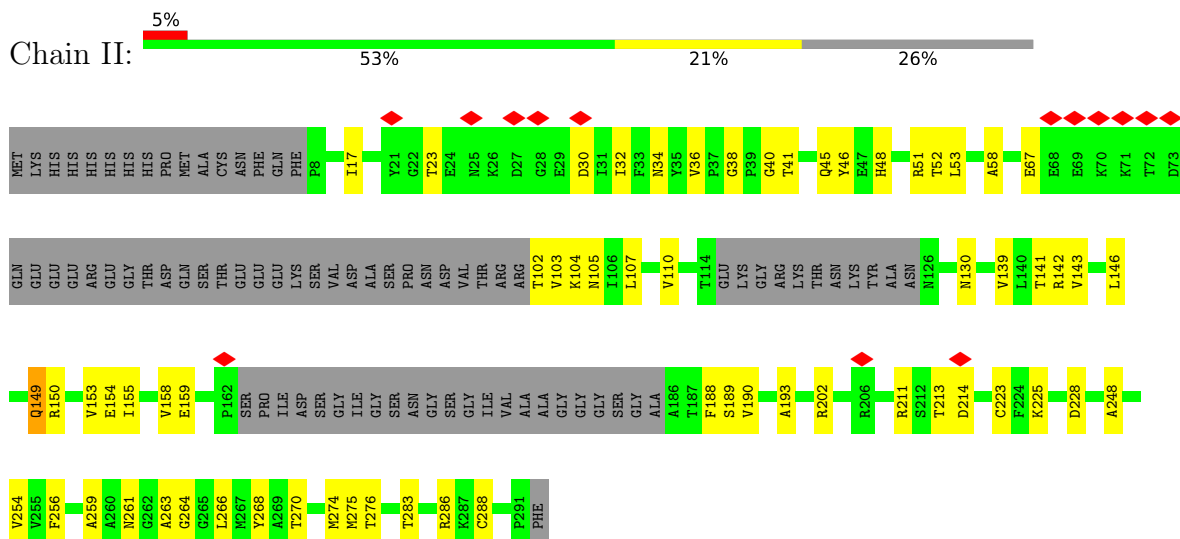
- Molecule 8: Exosome complex component RRP40



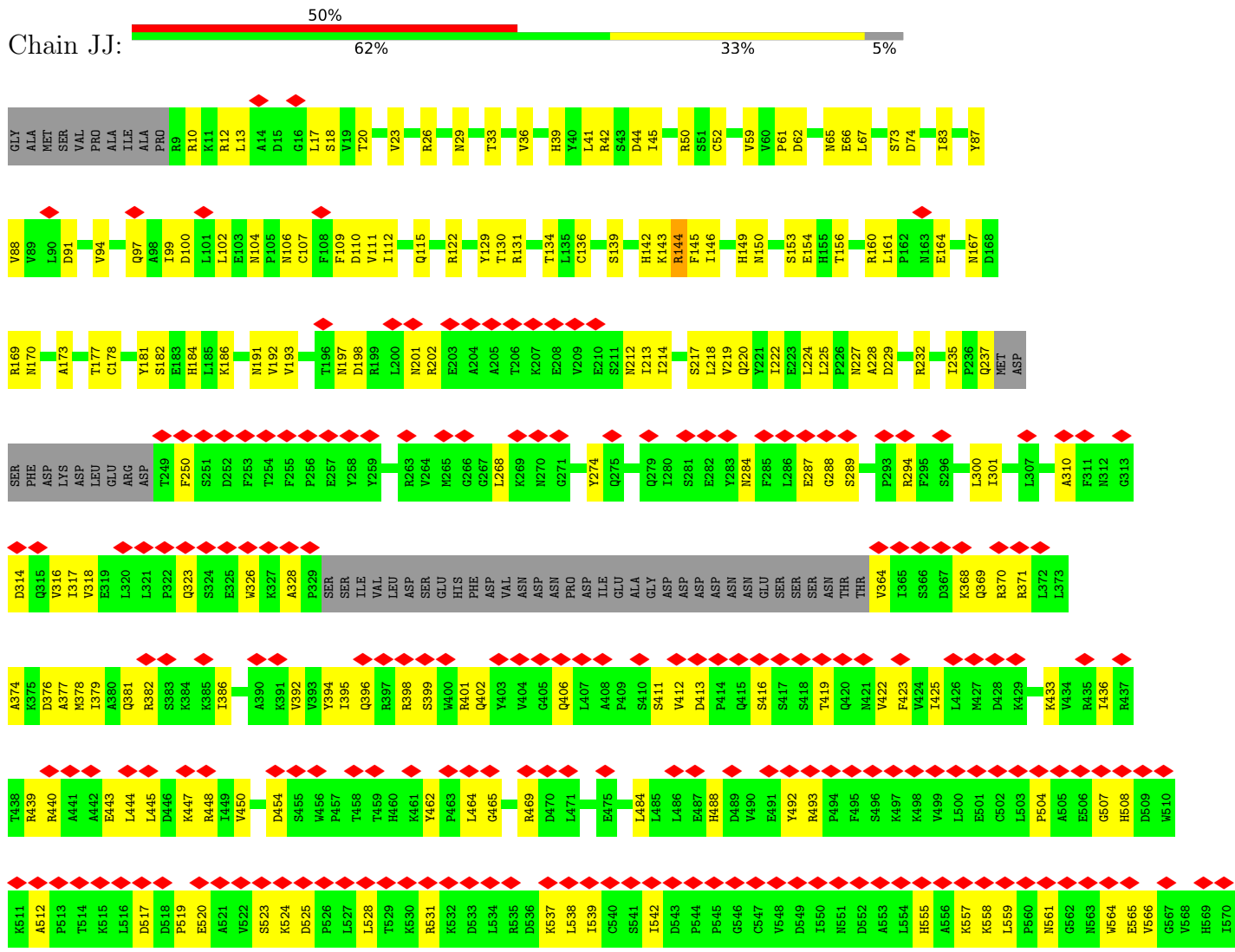
- Molecule 9: Exosome complex component RRP4

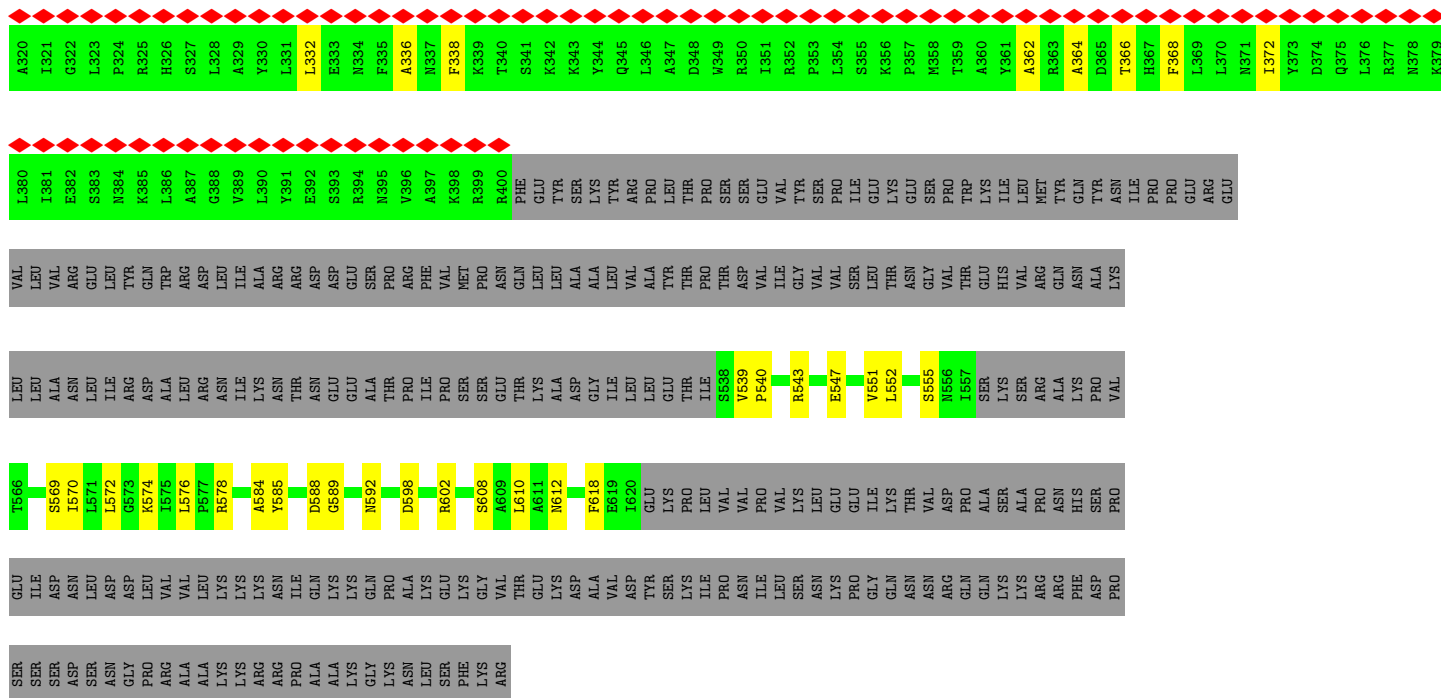


- Molecule 10: Exosome complex component CSL4

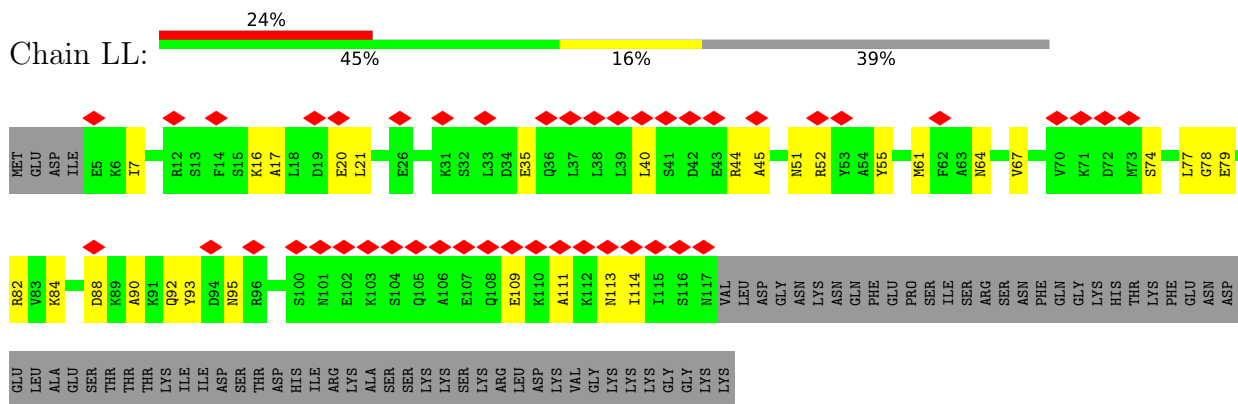


• Molecule 11: Exosome complex exonuclease DIS3

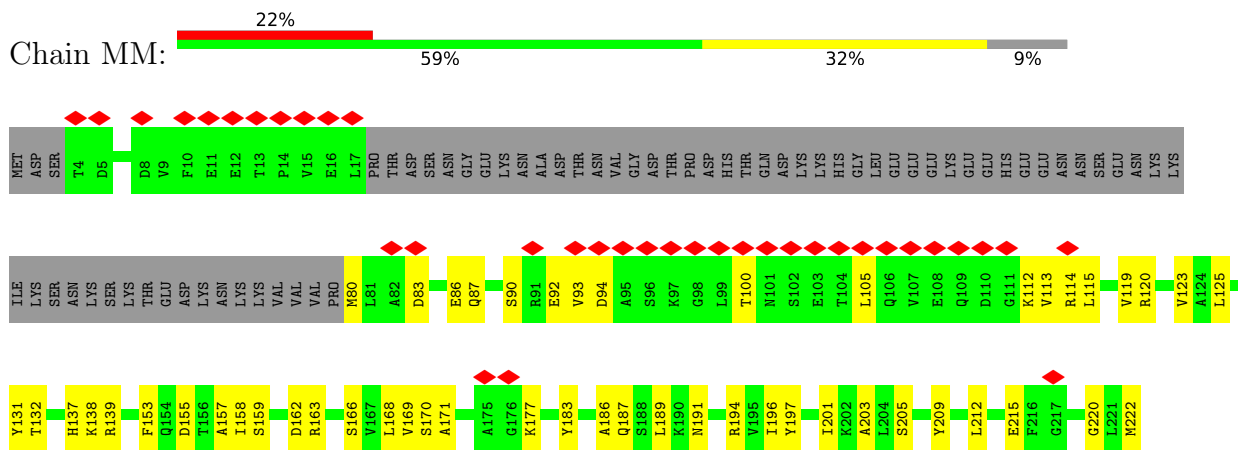




• Molecule 13: Exosome complex protein LRP1



• Molecule 14: ATP-dependent RNA helicase DOB1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22439	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.117	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	594.0, 594.0, 594.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	2	0.76	0/418	1.51	6/645 (0.9%)
2	AA	0.57	0/2340	0.64	1/3161 (0.0%)
3	BB	0.53	0/1910	0.68	0/2579
4	CC	0.50	0/2629	0.69	2/3569 (0.1%)
5	DD	0.54	0/1722	0.70	0/2339
6	EE	0.51	0/2093	0.69	0/2849
7	FF	0.53	0/1660	0.65	0/2241
8	GG	0.55	0/1828	0.68	0/2486
9	HH	0.52	0/2269	0.66	0/3066
10	II	0.48	0/1676	0.66	0/2277
11	JJ	0.42	0/7575	0.60	1/10290 (0.0%)
12	KK	0.35	0/2540	0.51	0/3497
13	LL	0.39	0/903	0.58	0/1210
14	MM	0.49	0/7773	0.66	3/10521 (0.0%)
15	NN	0.44	0/225	0.68	0/301
All	All	0.49	0/37561	0.66	13/51031 (0.0%)

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	BB	0	1
4	CC	0	3
5	DD	0	1
6	EE	0	1
7	FF	0	2
9	HH	0	1
10	II	0	1
11	JJ	0	1
14	MM	0	3
All	All	0	14

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	167	U	N1-C2-O2	13.94	132.56	122.80
1	2	167	U	N3-C2-O2	-11.19	114.36	122.20
1	2	167	U	C2-N1-C1'	11.17	131.10	117.70
1	2	167	U	C6-N1-C1'	-8.17	109.77	121.20
14	MM	940	LEU	CA-CB-CG	-6.03	101.43	115.30
1	2	167	U	C5-C6-N1	5.59	125.50	122.70
4	CC	360	LEU	CB-CG-CD2	-5.47	101.70	111.00
1	2	161	U	C5-C6-N1	5.39	125.39	122.70
2	AA	229	LEU	CA-CB-CG	-5.22	103.30	115.30
14	MM	919	LEU	CB-CG-CD2	-5.10	102.34	111.00
11	JJ	786	LEU	CA-CB-CG	5.08	126.98	115.30
14	MM	440	LEU	CA-CB-CG	5.07	126.95	115.30
4	CC	303	ASP	CB-CG-OD1	5.03	122.82	118.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	BB	166	TYR	Peptide
4	CC	335	ASP	Peptide
4	CC	352	ALA	Peptide
4	CC	54	ILE	Peptide
5	DD	188	GLU	Peptide
6	EE	136	HIS	Peptide
7	FF	141	LEU	Peptide
7	FF	216	ASP	Peptide
9	HH	92	ASN	Peptide
10	II	149	GLN	Peptide
11	JJ	504	PRO	Peptide
14	MM	541	SER	Peptide
14	MM	573	LYS	Peptide
14	MM	874	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	378	0	190	3	0
2	AA	2304	0	2265	65	0
3	BB	1886	0	1904	55	0
4	CC	2589	0	2607	73	0
5	DD	1701	0	1755	49	0
6	EE	2050	0	2063	57	0
7	FF	1638	0	1590	39	0
8	GG	1792	0	1747	42	0
9	HH	2236	0	2215	54	0
10	II	1653	0	1616	41	0
11	JJ	7430	0	7350	215	0
12	KK	2517	0	1819	57	0
13	LL	894	0	917	22	0
14	MM	7627	0	7521	227	0
15	NN	277	0	238	6	0
All	All	36972	0	35797	932	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 13.

All (932) 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)
5:DD:25:LYS:H	5:DD:96:GLU:HB3	1.50	0.76
9:HH:356:GLY:HA2	13:LL:35:GLU:HB2	1.70	0.73
5:DD:138:ILE:HG12	5:DD:145:ILE:HG12	1.68	0.73
11:JJ:732:LEU:HD23	11:JJ:735:ASN:HD22	1.53	0.73
14:MM:939:LEU:HD11	14:MM:966:MET:HG2	1.70	0.73
3:BB:30:ASN:HD22	3:BB:239:ARG:HH12	1.38	0.72
12:KK:241:HIS:HA	12:KK:252:CYS:H	1.55	0.70
12:KK:239:LEU:HA	12:KK:254:MET:HA	1.74	0.70
14:MM:611:GLN:HE22	14:MM:876:VAL:HG22	1.57	0.69
10:II:34:ASN:HB3	10:II:105:ASN:HA	1.74	0.69
3:BB:52:LEU:HB2	3:BB:125:GLU:HB2	1.75	0.67
8:GG:69:ASN:HA	8:GG:122:ARG:HH11	1.58	0.66
14:MM:1025:ILE:HA	14:MM:1028:PHE:HB2	1.76	0.66
11:JJ:83:ILE:O	11:JJ:191:ASN:ND2	2.27	0.66
11:JJ:868:SER:HB3	11:JJ:871:HIS:HD2	1.61	0.66
11:JJ:857:GLN:HE21	11:JJ:871:HIS:HB3	1.60	0.66
6:EE:227:ARG:NH2	7:FF:215:LYS:O	2.30	0.65
14:MM:628:LEU:HB3	14:MM:863:MET:HG2	1.77	0.65
8:GG:3:THR:OG1	8:GG:42:LEU:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:MM:475:HIS:HE1	14:MM:504:THR:HB	1.60	0.64
14:MM:260:ILE:HA	14:MM:290:VAL:HB	1.80	0.64
6:EE:35:GLU:HB2	6:EE:51:ILE:HB	1.77	0.64
4:CC:297:TYR:HB2	4:CC:347:ILE:HB	1.78	0.64
10:II:143:VAL:HA	10:II:153:VAL:HG12	1.80	0.64
14:MM:480:LEU:H	14:MM:483:LEU:HD12	1.62	0.64
3:BB:69:LYS:HB2	3:BB:114:LEU:HB3	1.80	0.64
11:JJ:142:HIS:O	11:JJ:144:ARG:NH2	2.31	0.64
11:JJ:450:VAL:HB	11:JJ:469:ARG:H	1.62	0.64
14:MM:401:ILE:HG23	14:MM:406:TYR:HB2	1.79	0.63
9:HH:143:LEU:HB3	9:HH:149:ARG:HD3	1.80	0.63
6:EE:15:LEU:HD11	6:EE:23:PRO:HD3	1.80	0.63
12:KK:16:VAL:HG21	13:LL:21:LEU:HB2	1.81	0.63
2:AA:237:VAL:HG23	2:AA:248:VAL:HG22	1.80	0.62
11:JJ:104:ASN:ND2	11:JJ:107:CYS:SG	2.72	0.62
14:MM:448:ILE:HG22	14:MM:456:ARG:HG2	1.81	0.62
11:JJ:274:TYR:HE1	11:JJ:294:ARG:HD2	1.63	0.62
14:MM:1042:ALA:HB2	14:MM:1050:LEU:HD23	1.81	0.62
4:CC:56:ASN:HD22	4:CC:394:ILE:HG13	1.63	0.62
6:EE:31:PHE:HB2	9:HH:5:ILE:HB	1.80	0.62
1:2:162:U:H5'	14:MM:224:GLY:HA3	1.81	0.62
4:CC:163:ARG:NH1	5:DD:158:LEU:O	2.33	0.62
14:MM:436:GLU:O	14:MM:440:LEU:N	2.32	0.62
14:MM:139:ARG:NH1	14:MM:159:SER:OG	2.32	0.62
4:CC:177:ARG:HA	4:CC:187:VAL:HA	1.82	0.61
14:MM:614:ASN:ND2	14:MM:873:SER:O	2.33	0.61
4:CC:176:VAL:HB	4:CC:250:GLU:HA	1.82	0.61
11:JJ:112:ILE:HG12	11:JJ:146:ILE:HD11	1.83	0.61
4:CC:352:ALA:HB3	4:CC:356:ASN:HB2	1.81	0.61
7:FF:78:TYR:HB2	7:FF:136:ASP:HB2	1.83	0.61
10:II:154:GLU:HA	10:II:202:ARG:HA	1.82	0.61
10:II:276:THR:HA	10:II:283:THR:HA	1.83	0.61
2:AA:262:MET:O	2:AA:266:HIS:ND1	2.33	0.61
11:JJ:663:ASP:OD1	11:JJ:675:ARG:NH1	2.33	0.61
2:AA:28:ARG:NH2	2:AA:32:GLN:O	2.34	0.61
2:AA:34:ARG:NH1	2:AA:51:MET:O	2.33	0.61
8:GG:155:ILE:HD11	8:GG:193:LYS:HB3	1.83	0.61
10:II:270:THR:H	10:II:275:MET:HA	1.64	0.61
11:JJ:182:SER:O	11:JJ:186:LYS:N	2.34	0.61
8:GG:124:CYS:SG	8:GG:125:THR:N	2.74	0.61
4:CC:61:ARG:NH1	4:CC:69:ASP:O	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AA:209:ASN:O	3:BB:195:LYS:NZ	2.32	0.60
2:AA:250:LYS:HB3	3:BB:199:LEU:HB3	1.83	0.60
5:DD:131:CYS:SG	5:DD:132:ALA:N	2.74	0.60
9:HH:299:ARG:NH1	9:HH:326:SER:OG	2.35	0.60
11:JJ:198:ASP:HB3	11:JJ:201:ASN:HB2	1.83	0.60
11:JJ:857:GLN:NE2	11:JJ:871:HIS:O	2.35	0.60
9:HH:200:CYS:SG	9:HH:201:GLN:N	2.75	0.60
4:CC:207:ARG:NH1	4:CC:270:GLU:O	2.35	0.60
14:MM:288:ARG:NH1	14:MM:312:GLN:OE1	2.34	0.60
4:CC:84:LYS:HD2	7:FF:54:GLU:HG3	1.84	0.60
11:JJ:368:LYS:HA	11:JJ:371:ARG:HH21	1.67	0.60
4:CC:78:ASN:ND2	4:CC:233:SER:O	2.32	0.60
12:KK:574:LYS:O	12:KK:578:ARG:NH2	2.35	0.60
2:AA:24:ARG:O	8:GG:209:ARG:NH2	2.34	0.59
2:AA:92:GLU:HB2	2:AA:95:ASN:HB2	1.84	0.59
3:BB:53:VAL:HG22	3:BB:124:ILE:HG12	1.84	0.59
8:GG:185:GLU:HG2	15:NN:114:THR:HG22	1.83	0.59
9:HH:187:ARG:NH1	14:MM:250:SER:O	2.35	0.59
4:CC:246:ALA:HA	4:CC:276:CYS:HA	1.84	0.59
6:EE:95:ILE:HG23	6:EE:138:ILE:HD13	1.85	0.59
7:FF:200:VAL:HB	7:FF:214:TRP:HB3	1.85	0.59
11:JJ:713:ASN:HA	11:JJ:906:VAL:HA	1.85	0.59
14:MM:132:THR:O	14:MM:163:ARG:NH1	2.35	0.59
6:EE:260:ARG:HA	6:EE:263:GLU:HB3	1.84	0.59
4:CC:61:ARG:NH2	4:CC:72:ASN:O	2.36	0.59
4:CC:128:ALA:HB2	4:CC:167:LYS:HE3	1.83	0.59
11:JJ:100:ASP:OD1	11:JJ:131:ARG:NH2	2.34	0.59
2:AA:239:LEU:HG	2:AA:245:VAL:HA	1.84	0.58
11:JJ:858:LEU:HD12	11:JJ:861:ALA:HB3	1.85	0.58
13:LL:90:ALA:HA	13:LL:93:TYR:HB3	1.84	0.58
9:HH:313:GLY:O	9:HH:318:ARG:NH1	2.35	0.58
14:MM:197:TYR:HB3	14:MM:236:VAL:HG22	1.84	0.58
6:EE:80:VAL:HA	6:EE:128:VAL:HB	1.84	0.58
9:HH:63:ASP:HB2	9:HH:78:ASN:HB3	1.85	0.58
12:KK:543:ARG:O	12:KK:547:GLU:N	2.36	0.58
14:MM:92:GLU:HB3	14:MM:112:LYS:HB3	1.84	0.58
14:MM:139:ARG:NH1	14:MM:155:ASP:O	2.28	0.58
2:AA:210:ILE:HG22	2:AA:211:LYS:HG2	1.86	0.58
7:FF:44:GLN:OE1	7:FF:237:TYR:OH	2.22	0.58
14:MM:794:LEU:O	14:MM:798:ASN:N	2.35	0.58
11:JJ:52:CYS:HG	11:JJ:184:HIS:HE2	1.40	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:MM:251:GLU:OE1	14:MM:254:ARG:NE	2.36	0.58
14:MM:647:HIS:O	14:MM:651:GLN:N	2.31	0.58
3:BB:120:THR:HG23	9:HH:132:GLN:HE21	1.67	0.58
14:MM:80:MET:HB2	14:MM:125:LEU:HB2	1.86	0.58
14:MM:742:LEU:HD12	14:MM:746:ILE:HG21	1.85	0.58
9:HH:151:LYS:HE3	14:MM:194:ARG:HD2	1.85	0.58
11:JJ:83:ILE:HD11	11:JJ:224:LEU:HD13	1.86	0.58
11:JJ:617:PRO:HA	11:JJ:648:SER:HB3	1.86	0.58
14:MM:225:ASP:HB3	14:MM:226:ILE:HD12	1.85	0.58
7:FF:7:ARG:HG3	7:FF:8:ARG:HG3	1.84	0.58
14:MM:1009:THR:HG22	14:MM:1011:THR:H	1.69	0.57
4:CC:371:PRO:HA	4:CC:374:ILE:HD12	1.87	0.57
5:DD:52:VAL:HG22	5:DD:92:CYS:HB2	1.86	0.57
11:JJ:692:GLY:HA2	11:JJ:784:LYS:HB2	1.86	0.57
10:II:158:VAL:O	10:II:189:SER:N	2.37	0.57
11:JJ:316:VAL:HG12	11:JJ:395:ILE:HG23	1.87	0.57
11:JJ:566:VAL:HB	11:JJ:628:TRP:HB2	1.86	0.57
11:JJ:985:SER:HA	11:JJ:997:GLU:H	1.69	0.57
14:MM:492:GLN:NE2	14:MM:510:ASN:O	2.37	0.57
3:BB:13:ARG:HD3	3:BB:171:LEU:HD22	1.86	0.57
3:BB:95:ARG:HA	3:BB:98:LEU:HD12	1.86	0.57
6:EE:226:ILE:HD12	7:FF:215:LYS:HD3	1.85	0.57
14:MM:926:GLY:O	14:MM:929:ASN:ND2	2.37	0.57
14:MM:970:ALA:HA	14:MM:973:ILE:HD12	1.85	0.57
2:AA:202:ASN:ND2	2:AA:205:ASP:O	2.35	0.57
7:FF:103:GLU:HG3	7:FF:144:ASP:HB3	1.85	0.57
11:JJ:444:LEU:HA	11:JJ:447:LYS:HD2	1.85	0.57
14:MM:441:THR:OG1	14:MM:469:ARG:NH1	2.37	0.57
14:MM:747:ARG:NH1	14:MM:750:GLU:OE1	2.37	0.57
9:HH:315:THR:HG22	9:HH:317:GLN:H	1.68	0.57
11:JJ:900:GLU:O	11:JJ:904:GLY:N	2.35	0.57
11:JJ:881:CYS:O	11:JJ:885:ASN:ND2	2.38	0.57
14:MM:265:HIS:ND1	14:MM:293:SER:OG	2.35	0.57
4:CC:24:ARG:NH2	10:II:193:ALA:O	2.38	0.57
8:GG:122:ARG:NH1	8:GG:123:VAL:O	2.38	0.57
11:JJ:537:LYS:O	11:JJ:649:ARG:NH2	2.38	0.57
11:JJ:867:LEU:O	11:JJ:872:ARG:NH2	2.38	0.57
5:DD:62:ARG:NH2	5:DD:104:PHE:O	2.36	0.57
9:HH:318:ARG:O	9:HH:322:ALA:N	2.38	0.57
4:CC:11:GLU:HA	12:KK:618:PHE:HA	1.87	0.56
5:DD:107:ARG:NH2	5:DD:149:PRO:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:EE:259:VAL:O	6:EE:263:GLU:N	2.32	0.56
12:KK:86:ASP:O	12:KK:90:GLU:N	2.35	0.56
6:EE:227:ARG:NH1	7:FF:216:ASP:OD1	2.39	0.56
2:AA:235:LEU:HD13	2:AA:250:LYS:HB2	1.88	0.56
4:CC:81:LYS:NZ	12:KK:576:LEU:O	2.37	0.56
7:FF:76:ALA:HB3	7:FF:138:PHE:HB2	1.88	0.56
9:HH:142:ASN:ND2	9:HH:188:SER:O	2.37	0.56
11:JJ:492:TYR:HA	11:JJ:601:ILE:HG21	1.87	0.56
11:JJ:558:LYS:HA	11:JJ:564:TRP:HA	1.85	0.56
11:JJ:630:LEU:HD13	11:JJ:634:ALA:HA	1.88	0.56
11:JJ:921:VAL:HA	11:JJ:926:ILE:HG22	1.87	0.56
14:MM:588:ASN:ND2	14:MM:912:SER:OG	2.38	0.56
14:MM:810:PRO:O	14:MM:816:ILE:N	2.38	0.56
14:MM:201:ILE:HG22	14:MM:203:ALA:H	1.69	0.56
14:MM:642:ASN:O	14:MM:646:TYR:N	2.33	0.56
6:EE:22:ARG:HD2	6:EE:26:ARG:HB2	1.86	0.56
6:EE:58:CYS:SG	6:EE:59:ILE:N	2.79	0.56
11:JJ:115:GLN:HB2	11:JJ:149:HIS:HA	1.87	0.56
11:JJ:520:GLU:O	11:JJ:524:LYS:N	2.39	0.56
11:JJ:538:LEU:HA	11:JJ:649:ARG:HH21	1.71	0.56
14:MM:194:ARG:HB2	14:MM:256:VAL:HG22	1.87	0.56
9:HH:290:SER:H	9:HH:293:ILE:HD12	1.69	0.56
10:II:228:ASP:OD2	10:II:286:ARG:NH1	2.38	0.56
14:MM:344:GLU:OE2	14:MM:552:ARG:NH1	2.37	0.56
7:FF:86:SER:OG	7:FF:87:PHE:N	2.37	0.56
3:BB:131:GLN:HG3	3:BB:135:ILE:HD13	1.86	0.56
5:DD:26:VAL:HG22	5:DD:94:ILE:HA	1.87	0.56
6:EE:190:LEU:HB2	6:EE:213:LEU:HB2	1.88	0.56
10:II:36:VAL:HB	10:II:107:LEU:HA	1.88	0.56
11:JJ:401:ARG:NH1	11:JJ:402:GLN:O	2.38	0.56
2:AA:50:LYS:HG3	2:AA:55:LYS:HG2	1.88	0.55
5:DD:110:SER:O	5:DD:114:ASN:ND2	2.39	0.55
12:KK:608:SER:O	12:KK:612:ASN:ND2	2.40	0.55
14:MM:293:SER:OG	14:MM:294:ALA:N	2.39	0.55
6:EE:37:PHE:HB2	6:EE:49:ARG:HB3	1.87	0.55
3:BB:162:SER:HA	3:BB:186:THR:HA	1.87	0.55
14:MM:298:ASN:OD1	14:MM:298:ASN:N	2.35	0.55
4:CC:69:ASP:OD2	7:FF:145:LYS:NZ	2.39	0.55
5:DD:66:LEU:HD11	5:DD:105:SER:HB2	1.89	0.55
6:EE:202:ALA:O	6:EE:206:SER:N	2.35	0.55
8:GG:97:LEU:HD13	8:GG:134:ILE:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:JJ:767:ASN:HA	11:JJ:770:LEU:HB2	1.88	0.55
2:AA:82:GLU:OE2	7:FF:6:ARG:NH1	2.34	0.55
14:MM:285:ASP:OD1	14:MM:310:HIS:ND1	2.34	0.55
14:MM:419:CYS:O	14:MM:423:ALA:N	2.37	0.55
14:MM:863:MET:O	14:MM:867:LYS:N	2.37	0.55
7:FF:129:ARG:NH1	7:FF:186:GLU:OE2	2.40	0.55
8:GG:5:ILE:N	8:GG:40:GLY:O	2.38	0.55
8:GG:45:SER:OG	8:GG:54:THR:N	2.39	0.55
11:JJ:852:VAL:HA	11:JJ:855:HIS:HD2	1.70	0.55
7:FF:49:HIS:HD2	7:FF:61:LEU:HD12	1.72	0.55
8:GG:63:ARG:NH1	8:GG:92:SER:OG	2.40	0.55
14:MM:666:HIS:HB3	14:MM:669:ASN:HB2	1.88	0.55
14:MM:325:PRO:HD2	14:MM:552:ARG:HA	1.88	0.55
14:MM:465:LEU:O	14:MM:469:ARG:N	2.39	0.55
11:JJ:109:PHE:HA	11:JJ:143:LYS:HG3	1.89	0.55
11:JJ:181:TYR:HB3	11:JJ:192:VAL:HG11	1.88	0.55
11:JJ:493:ARG:O	11:JJ:590:ARG:NH2	2.33	0.55
14:MM:695:VAL:HA	14:MM:721:VAL:HG22	1.87	0.55
14:MM:960:ALA:O	14:MM:964:LYS:N	2.38	0.55
12:KK:101:CYS:O	12:KK:105:SER:OG	2.23	0.55
14:MM:422:LEU:HD23	14:MM:425:LYS:HD2	1.88	0.55
9:HH:276:SER:OG	9:HH:277:SER:N	2.37	0.54
14:MM:399:LYS:O	14:MM:403:LYS:N	2.38	0.54
14:MM:502:THR:OG1	14:MM:503:GLU:N	2.38	0.54
6:EE:117:THR:OG1	6:EE:120:TYR:N	2.38	0.54
7:FF:93:ILE:HA	7:FF:135:ILE:HB	1.88	0.54
8:GG:204:THR:O	8:GG:208:TYR:N	2.41	0.54
9:HH:307:LEU:HB3	9:HH:312:ILE:HB	1.89	0.54
11:JJ:139:SER:HB3	11:JJ:144:ARG:HA	1.87	0.54
14:MM:351:GLU:O	14:MM:355:LYS:N	2.34	0.54
2:AA:195:CYS:SG	2:AA:238:THR:OG1	2.64	0.54
4:CC:236:TYR:OH	4:CC:388:LEU:O	2.26	0.54
6:EE:78:VAL:HA	6:EE:126:VAL:HB	1.89	0.54
7:FF:101:LEU:O	7:FF:104:LYS:NZ	2.39	0.54
11:JJ:109:PHE:O	11:JJ:144:ARG:N	2.35	0.54
11:JJ:160:ARG:NH1	11:JJ:164:GLU:O	2.40	0.54
4:CC:153:GLN:NE2	5:DD:61:THR:OG1	2.40	0.54
8:GG:63:ARG:HA	8:GG:89:GLN:HE22	1.72	0.54
4:CC:159:ILE:O	4:CC:162:SER:OG	2.25	0.54
10:II:142:ARG:NH2	10:II:154:GLU:OE2	2.40	0.54
11:JJ:328:ALA:HA	11:JJ:386:ILE:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:MM:921:GLU:O	14:MM:925:ASN:N	2.40	0.54
3:BB:47:ASN:ND2	3:BB:133:GLY:O	2.32	0.54
11:JJ:484:LEU:O	11:JJ:488:HIS:ND1	2.38	0.54
12:KK:332:LEU:HA	12:KK:336:ALA:HB3	1.89	0.54
13:LL:44:ARG:O	13:LL:44:ARG:NH1	2.40	0.54
14:MM:86:GLU:HA	14:MM:120:ARG:HA	1.89	0.54
14:MM:325:PRO:O	14:MM:553:GLY:N	2.35	0.54
14:MM:531:TRP:NE1	14:MM:561:GLU:OE2	2.37	0.54
14:MM:540:MET:O	14:MM:543:ARG:NH2	2.41	0.54
7:FF:91:GLY:H	7:FF:127:LEU:HB3	1.73	0.54
14:MM:846:LEU:HA	14:MM:849:LEU:HB3	1.89	0.54
3:BB:5:GLU:OE2	11:JJ:122:ARG:NH2	2.41	0.54
4:CC:158:SER:O	4:CC:162:SER:N	2.39	0.54
4:CC:367:ALA:O	5:DD:176:ASN:ND2	2.40	0.54
6:EE:22:ARG:HH12	6:EE:199:LEU:H	1.53	0.54
11:JJ:542:ILE:HD13	11:JJ:723:THR:HB	1.90	0.54
6:EE:101:LYS:HZ2	6:EE:227:ARG:HH11	1.55	0.54
10:II:146:LEU:HD11	10:II:225:LYS:HA	1.90	0.54
4:CC:129:SER:OG	4:CC:130:VAL:N	2.39	0.54
8:GG:73:ILE:O	8:GG:191:ASN:ND2	2.38	0.54
9:HH:232:TRP:HE1	9:HH:234:ARG:HB3	1.73	0.54
11:JJ:531:ARG:NH1	11:JJ:644:SER:O	2.40	0.54
14:MM:398:VAL:O	14:MM:402:TRP:N	2.34	0.54
14:MM:684:VAL:HA	14:MM:766:SER:HA	1.89	0.54
4:CC:136:VAL:HA	4:CC:219:VAL:HB	1.89	0.53
11:JJ:45:ILE:HG13	11:JJ:153:SER:HA	1.89	0.53
2:AA:168:THR:HB	2:AA:175:ILE:HB	1.90	0.53
3:BB:137:GLY:O	3:BB:141:ASN:ND2	2.42	0.53
4:CC:40:ARG:N	4:CC:44:ARG:O	2.40	0.53
14:MM:489:ILE:O	14:MM:493:GLU:N	2.40	0.53
7:FF:47:SER:HB3	7:FF:63:GLU:HB2	1.90	0.53
14:MM:87:GLN:N	14:MM:119:VAL:O	2.38	0.53
5:DD:139:ILE:HA	5:DD:157:SER:HA	1.91	0.53
11:JJ:318:VAL:HG12	11:JJ:392:VAL:HG12	1.90	0.53
12:KK:585:TYR:HB3	12:KK:589:GLY:HA2	1.91	0.53
14:MM:196:ILE:HB	14:MM:259:VAL:HG13	1.91	0.53
3:BB:154:MET:H	9:HH:83:SER:HG	1.57	0.53
10:II:159:GLU:HA	10:II:188:PHE:HA	1.89	0.53
11:JJ:508:HIS:ND1	11:JJ:611:ASP:OD2	2.41	0.53
11:JJ:753:ARG:HD3	11:JJ:839:TYR:HE2	1.72	0.53
5:DD:54:PRO:HA	5:DD:94:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:DD:106:LEU:HD22	5:DD:160:VAL:HB	1.90	0.53
7:FF:126:ASN:ND2	7:FF:186:GLU:OE1	2.40	0.53
11:JJ:10:ARG:HG3	11:JJ:20:THR:HB	1.89	0.53
2:AA:29:SER:HB3	2:AA:32:GLN:HB2	1.90	0.53
2:AA:207:GLU:O	2:AA:211:LYS:N	2.39	0.53
11:JJ:752:LEU:HD13	11:JJ:821:SER:HB3	1.89	0.53
4:CC:258:THR:HG22	4:CC:267:THR:HG22	1.91	0.53
10:II:46:TYR:N	10:II:53:LEU:O	2.42	0.53
11:JJ:237:GLN:NE2	11:JJ:465:GLY:O	2.42	0.53
11:JJ:557:LYS:HB2	11:JJ:565:GLU:HB3	1.91	0.53
14:MM:328:HIS:HA	14:MM:555:VAL:HB	1.90	0.53
2:AA:31:ASP:OD1	2:AA:31:ASP:N	2.35	0.52
9:HH:128:ILE:HD11	9:HH:134:ALA:HB2	1.91	0.52
11:JJ:61:PRO:HB2	11:JJ:65:ASN:HA	1.91	0.52
11:JJ:97:GLN:OE1	11:JJ:197:ASN:ND2	2.42	0.52
11:JJ:572:ASP:HB3	11:JJ:622:PHE:HB3	1.91	0.52
14:MM:327:GLN:NE2	14:MM:344:GLU:OE2	2.35	0.52
3:BB:67:THR:HG22	3:BB:119:ARG:HE	1.73	0.52
11:JJ:17:LEU:HD11	11:JJ:42:ARG:HA	1.91	0.52
11:JJ:219:VAL:HA	11:JJ:222:ILE:HB	1.91	0.52
12:KK:96:LEU:O	12:KK:100:ASN:N	2.39	0.52
3:BB:23:ARG:N	3:BB:173:ASP:OD2	2.40	0.52
8:GG:232:LYS:O	8:GG:236:THR:N	2.43	0.52
10:II:30:ASP:O	10:II:102:THR:OG1	2.26	0.52
11:JJ:940:ARG:O	11:JJ:944:LEU:N	2.42	0.52
12:KK:31:TYR:HB2	13:LL:7:ILE:HD12	1.91	0.52
4:CC:158:SER:HA	4:CC:161:HIS:HB2	1.90	0.52
6:EE:183:ASN:HD21	6:EE:219:ASN:HA	1.74	0.52
9:HH:72:GLY:HA3	9:HH:97:VAL:HB	1.92	0.52
11:JJ:317:ILE:HB	11:JJ:394:TYR:HB3	1.91	0.52
11:JJ:678:LEU:HA	11:JJ:681:SER:HB3	1.91	0.52
6:EE:242:HIS:O	6:EE:246:GLN:N	2.41	0.52
11:JJ:284:ASN:ND2	11:JJ:287:GLU:OE1	2.43	0.52
11:JJ:411:SER:HB2	11:JJ:422:VAL:HA	1.90	0.52
11:JJ:652:PHE:HZ	11:JJ:660:ARG:HH11	1.58	0.52
14:MM:277:GLU:OE2	14:MM:609:PHE:N	2.42	0.52
4:CC:61:ARG:NH1	4:CC:278:GLN:OE1	2.41	0.52
8:GG:129:GLU:HG3	10:II:225:LYS:HE3	1.90	0.52
11:JJ:440:ARG:NH1	11:JJ:443:GLU:OE2	2.41	0.52
12:KK:238:ASP:N	12:KK:255:GLN:O	2.41	0.52
5:DD:140:LYS:HA	5:DD:158:LEU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:EE:71:VAL:HG23	6:EE:72:GLU:HG2	1.92	0.52
2:AA:198:PHE:HE1	2:AA:221:ILE:HG12	1.75	0.52
4:CC:211:TYR:OH	4:CC:244:PRO:O	2.28	0.52
5:DD:7:ILE:O	5:DD:220:ARG:NH2	2.35	0.52
8:GG:168:PHE:HB3	15:NN:103:ARG:HH21	1.75	0.52
14:MM:925:ASN:O	14:MM:927:ASN:ND2	2.42	0.52
14:MM:966:MET:HA	14:MM:969:ILE:HD12	1.92	0.52
11:JJ:423:PHE:HB3	11:JJ:433:LYS:HB2	1.92	0.52
14:MM:771:GLY:HA2	14:MM:807:VAL:HA	1.91	0.52
1:2:163:U:H5'	14:MM:241:ILE:HD12	1.92	0.51
4:CC:30:SER:O	4:CC:34:HIS:ND1	2.42	0.51
11:JJ:288:GLY:O	11:JJ:301:ILE:N	2.40	0.51
11:JJ:412:VAL:HG11	11:JJ:445:LEU:HD22	1.90	0.51
12:KK:298:ILE:O	12:KK:302:ARG:N	2.43	0.51
14:MM:587:TYR:HA	14:MM:590:ILE:HD12	1.92	0.51
3:BB:76:VAL:HA	3:BB:126:ILE:HB	1.92	0.51
6:EE:60:VAL:HG11	6:EE:145:ILE:HG12	1.92	0.51
6:EE:82:ILE:HD12	6:EE:92:VAL:HG22	1.91	0.51
8:GG:137:PHE:HE1	8:GG:143:ARG:HA	1.75	0.51
14:MM:680:VAL:HG12	14:MM:770:ILE:HG23	1.92	0.51
6:EE:117:THR:HA	6:EE:161:PHE:HB2	1.92	0.51
11:JJ:41:LEU:HD13	11:JJ:154:GLU:HA	1.92	0.51
12:KK:10:LEU:HD11	13:LL:52:ARG:HG3	1.92	0.51
2:AA:74:GLU:HG2	2:AA:121:GLU:HG2	1.90	0.51
6:EE:183:ASN:ND2	6:EE:219:ASN:OD1	2.43	0.51
11:JJ:99:ILE:HD12	11:JJ:102:LEU:HD12	1.93	0.51
11:JJ:217:SER:H	11:JJ:220:GLN:HB3	1.74	0.51
12:KK:103:ILE:HG13	13:LL:93:TYR:HE1	1.75	0.51
14:MM:93:VAL:HG11	14:MM:325:PRO:HG2	1.92	0.51
14:MM:205:SER:O	14:MM:209:TYR:N	2.34	0.51
14:MM:795:ARG:HA	14:MM:798:ASN:HB2	1.93	0.51
14:MM:938:ALA:HB1	14:MM:998:MET:HB3	1.92	0.51
3:BB:43:GLU:HG2	3:BB:48:LYS:HG2	1.92	0.51
8:GG:6:PHE:N	8:GG:9:ASP:OD2	2.40	0.51
11:JJ:378:MET:HB3	11:JJ:382:ARG:HH12	1.74	0.51
11:JJ:825:SER:OG	11:JJ:826:TYR:N	2.43	0.51
4:CC:12:ILE:HG21	10:II:268:TYR:HB3	1.93	0.51
8:GG:70:ASP:OD1	15:NN:100:SER:OG	2.29	0.51
3:BB:136:MET:HB3	3:BB:186:THR:HG21	1.92	0.51
11:JJ:448:ARG:HH12	11:JJ:992:SER:HB3	1.75	0.51
11:JJ:695:ASN:O	11:JJ:806:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AA:142:ASP:OD2	5:DD:11:ASP:N	2.43	0.51
5:DD:167:PHE:HE1	5:DD:174:VAL:HG22	1.76	0.51
11:JJ:636:ILE:HD11	11:JJ:733:LEU:HD11	1.92	0.51
14:MM:169:VAL:HG22	14:MM:317:VAL:HB	1.93	0.51
2:AA:164:LYS:O	2:AA:185:VAL:N	2.35	0.51
4:CC:130:VAL:HG12	4:CC:213:LEU:HB2	1.91	0.51
5:DD:15:GLY:O	5:DD:30:VAL:N	2.41	0.51
11:JJ:592:THR:OG1	11:JJ:593:SER:N	2.44	0.51
11:JJ:596:LEU:HD22	11:JJ:898:SER:HB2	1.91	0.51
14:MM:353:PHE:O	14:MM:357:MET:N	2.42	0.51
3:BB:155:PHE:O	9:HH:74:TYR:OH	2.28	0.51
14:MM:890:ARG:NH2	14:MM:899:ASP:OD1	2.39	0.51
2:AA:250:LYS:NZ	3:BB:197:SER:O	2.36	0.50
4:CC:148:GLU:HA	4:CC:151:ILE:HD12	1.92	0.50
2:AA:81:THR:HA	2:AA:138:VAL:HB	1.93	0.50
3:BB:69:LYS:HD3	3:BB:114:LEU:HD13	1.93	0.50
11:JJ:62:ASP:OD1	11:JJ:66:GLU:N	2.44	0.50
11:JJ:739:ALA:HA	11:JJ:742:ILE:HG12	1.93	0.50
14:MM:326:LEU:HD23	14:MM:553:GLY:HA3	1.92	0.50
14:MM:826:LYS:HA	14:MM:829:ASP:HB2	1.93	0.50
4:CC:239:GLN:HE21	4:CC:291:ILE:HD13	1.76	0.50
4:CC:377:SER:O	4:CC:381:SER:N	2.45	0.50
7:FF:63:GLU:OE2	12:KK:572:LEU:N	2.41	0.50
11:JJ:985:SER:O	11:JJ:994:ARG:NH2	2.45	0.50
9:HH:176:LEU:HA	9:HH:182:ALA:HA	1.94	0.50
14:MM:971:ALA:O	14:MM:975:LYS:N	2.39	0.50
6:EE:29:HIS:HA	6:EE:199:LEU:HD13	1.94	0.50
11:JJ:376:ASP:HA	11:JJ:379:ILE:HD12	1.94	0.50
14:MM:123:VAL:HA	14:MM:315:HIS:HA	1.93	0.50
2:AA:40:PHE:HA	2:AA:47:VAL:HA	1.92	0.50
3:BB:61:LEU:HB2	3:BB:64:GLN:HG2	1.93	0.50
6:EE:99:LEU:HD21	6:EE:138:ILE:HD11	1.94	0.50
10:II:67:GLU:O	10:II:107:LEU:N	2.45	0.50
11:JJ:150:ASN:O	11:JJ:156:THR:OG1	2.29	0.50
11:JJ:173:ALA:O	11:JJ:177:THR:N	2.43	0.50
11:JJ:218:LEU:O	11:JJ:222:ILE:N	2.40	0.50
11:JJ:517:ASP:N	11:JJ:517:ASP:OD1	2.44	0.50
11:JJ:653:SER:H	11:JJ:656:GLN:HB2	1.76	0.50
11:JJ:682:VAL:O	11:JJ:686:GLN:N	2.39	0.50
14:MM:410:ILE:HG12	14:MM:499:LEU:HB3	1.93	0.50
14:MM:793:SER:O	14:MM:797:VAL:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:DD:208:ASN:OD1	5:DD:211:ARG:NH2	2.37	0.50
9:HH:170:ASN:HB2	9:HH:191:TYR:HA	1.94	0.50
10:II:225:LYS:HE2	10:II:261:ASN:HD21	1.77	0.50
11:JJ:222:ILE:HG21	11:JJ:235:ILE:HD11	1.92	0.50
14:MM:223:THR:HB	14:MM:226:ILE:H	1.76	0.50
8:GG:18:PRO:HB2	8:GG:52:VAL:HG22	1.93	0.50
10:II:270:THR:N	10:II:274:MET:O	2.45	0.50
11:JJ:559:LEU:HG	11:JJ:565:GLU:HB2	1.94	0.50
14:MM:434:ASP:HA	14:MM:437:LYS:HB2	1.93	0.50
14:MM:461:ILE:HD11	14:MM:480:LEU:HD12	1.92	0.50
7:FF:63:GLU:OE1	12:KK:570:ILE:N	2.45	0.50
14:MM:352:ASN:O	14:MM:356:ALA:N	2.44	0.50
4:CC:134:VAL:HG11	4:CC:151:ILE:HB	1.92	0.49
6:EE:45:ASN:OD1	6:EE:64:SER:N	2.43	0.49
11:JJ:406:GLN:O	11:JJ:425:ILE:N	2.42	0.49
11:JJ:678:LEU:HB2	11:JJ:726:LEU:HD12	1.93	0.49
14:MM:397:ILE:HG23	14:MM:400:MET:HE1	1.93	0.49
2:AA:166:ASP:OD2	2:AA:182:ARG:NE	2.40	0.49
3:BB:164:GLY:HA2	3:BB:184:THR:HA	1.93	0.49
11:JJ:289:SER:HB3	11:JJ:300:LEU:HD23	1.93	0.49
14:MM:714:HIS:HA	14:MM:764:LEU:HD12	1.94	0.49
8:GG:203:ASN:O	8:GG:207:CYS:N	2.40	0.49
11:JJ:894:ALA:O	11:JJ:898:SER:N	2.45	0.49
12:KK:32:LYS:HG2	12:KK:39:SER:HB2	1.94	0.49
14:MM:306:ILE:HD13	14:MM:309:ILE:HD11	1.95	0.49
14:MM:332:PRO:HB2	14:MM:335:GLY:HA3	1.93	0.49
14:MM:661:ARG:HA	14:MM:664:VAL:HB	1.93	0.49
2:AA:107:ILE:O	2:AA:111:SER:N	2.37	0.49
6:EE:31:PHE:HE1	6:EE:199:LEU:HB3	1.78	0.49
6:EE:37:PHE:O	6:EE:49:ARG:N	2.45	0.49
7:FF:193:ALA:HA	7:FF:202:SER:HA	1.94	0.49
11:JJ:780:LEU:HA	11:JJ:786:LEU:HD12	1.93	0.49
12:KK:96:LEU:HA	12:KK:99:LEU:HB2	1.95	0.49
14:MM:93:VAL:N	14:MM:113:VAL:O	2.42	0.49
14:MM:1022:GLY:O	14:MM:1026:ARG:N	2.42	0.49
4:CC:243:LEU:N	4:CC:282:VAL:O	2.37	0.49
8:GG:101:ALA:HB1	8:GG:135:GLU:HG2	1.94	0.49
9:HH:213:HIS:ND1	14:MM:597:GLU:OE2	2.35	0.49
11:JJ:73:SER:O	11:JJ:87:TYR:OH	2.23	0.49
11:JJ:422:VAL:O	11:JJ:436:ILE:N	2.38	0.49
11:JJ:572:ASP:H	11:JJ:623:ALA:HA	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:MM:712:THR:HB	14:MM:715:GLU:H	1.76	0.49
5:DD:132:ALA:HB1	5:DD:205:LEU:HD23	1.95	0.49
5:DD:168:VAL:O	5:DD:172:LYS:N	2.45	0.49
6:EE:97:SER:HB2	7:FF:108:ASN:HB3	1.93	0.49
11:JJ:911:GLU:OE1	11:JJ:982:GLN:NE2	2.41	0.49
8:GG:206:ALA:HB2	8:GG:234:ILE:HG13	1.95	0.49
9:HH:143:LEU:HD13	9:HH:149:ARG:HH21	1.77	0.49
14:MM:985:VAL:HG12	14:MM:988:ASP:H	1.78	0.49
10:II:23:THR:HG21	12:KK:539:VAL:HG13	1.95	0.49
11:JJ:899:ILE:O	11:JJ:903:VAL:N	2.44	0.49
14:MM:903:LEU:HA	14:MM:906:ARG:HD2	1.95	0.49
4:CC:350:LEU:HB2	4:CC:359:GLN:H	1.78	0.49
11:JJ:73:SER:OG	11:JJ:74:ASP:OD1	2.30	0.49
13:LL:16:LYS:O	13:LL:20:GLU:N	2.46	0.49
2:AA:198:PHE:CE2	2:AA:264:CYS:HB3	2.48	0.49
3:BB:47:ASN:OD1	3:BB:132:ASP:N	2.43	0.49
5:DD:76:PRO:O	5:DD:128:ASN:ND2	2.35	0.49
11:JJ:903:VAL:HG11	11:JJ:935:VAL:HG21	1.95	0.49
12:KK:16:VAL:HG22	13:LL:17:ALA:HB1	1.94	0.49
2:AA:286:ASP:O	2:AA:290:ARG:N	2.43	0.48
11:JJ:10:ARG:HD3	11:JJ:18:SER:HB3	1.93	0.48
12:KK:48:LYS:O	12:KK:52:MET:N	2.40	0.48
14:MM:187:GLN:O	14:MM:191:ASN:ND2	2.46	0.48
2:AA:126:VAL:HG23	2:AA:130:LYS:H	1.78	0.48
8:GG:187:ALA:HB3	8:GG:195:TRP:HB3	1.96	0.48
9:HH:174:GLN:HB2	9:HH:185:HIS:HD2	1.78	0.48
10:II:211:ARG:NE	10:II:213:THR:O	2.47	0.48
10:II:211:ARG:HH11	10:II:214:ASP:HB3	1.79	0.48
11:JJ:12:ARG:NH2	11:JJ:18:SER:OG	2.46	0.48
11:JJ:227:ASN:OD1	11:JJ:227:ASN:N	2.46	0.48
12:KK:551:VAL:O	12:KK:555:SER:N	2.46	0.48
12:KK:584:ALA:O	12:KK:592:ASN:N	2.43	0.48
4:CC:362:LEU:HB2	5:DD:180:LEU:HB3	1.96	0.48
5:DD:190:GLN:O	5:DD:194:LEU:N	2.46	0.48
5:DD:217:ILE:O	5:DD:221:LEU:N	2.45	0.48
8:GG:84:TYR:N	8:GG:97:LEU:O	2.36	0.48
11:JJ:59:VAL:HG13	11:JJ:67:LEU:HD23	1.95	0.48
11:JJ:161:LEU:N	11:JJ:164:GLU:OE1	2.42	0.48
11:JJ:136:CYS:HA	11:JJ:145:PHE:HB2	1.96	0.48
11:JJ:316:VAL:HA	11:JJ:395:ILE:HA	1.96	0.48
11:JJ:317:ILE:HD12	11:JJ:394:TYR:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:JJ:689:LEU:HD23	11:JJ:693:ALA:HB3	1.95	0.48
11:JJ:830:ARG:NH2	11:JJ:837:ASP:OD1	2.46	0.48
12:KK:39:SER:O	12:KK:43:LYS:N	2.40	0.48
3:BB:5:GLU:OE2	11:JJ:129:TYR:OH	2.26	0.48
11:JJ:561:ASN:ND2	11:JJ:629:GLU:OE2	2.41	0.48
11:JJ:953:PHE:HB2	11:JJ:960:LEU:HD13	1.95	0.48
13:LL:74:SER:HA	13:LL:77:LEU:HB3	1.95	0.48
2:AA:250:LYS:N	3:BB:199:LEU:O	2.43	0.48
4:CC:131:TYR:CZ	7:FF:11:GLY:HA2	2.49	0.48
10:II:254:VAL:HB	10:II:288:CYS:HA	1.94	0.48
11:JJ:130:THR:O	11:JJ:134:THR:N	2.45	0.48
12:KK:569:SER:HB2	12:KK:574:LYS:HG3	1.96	0.48
14:MM:411:VAL:HB	14:MM:500:PHE:HA	1.96	0.48
14:MM:646:TYR:O	14:MM:650:GLU:N	2.40	0.48
3:BB:105:VAL:O	3:BB:109:GLU:N	2.47	0.48
8:GG:161:ASN:HA	8:GG:164:ARG:HD3	1.96	0.48
9:HH:137:MET:HB2	9:HH:140:SER:HB3	1.96	0.48
11:JJ:879:MET:SD	11:JJ:882:ARG:NH2	2.87	0.48
14:MM:94:ASP:O	14:MM:552:ARG:NH2	2.35	0.48
14:MM:504:THR:O	14:MM:508:GLY:N	2.35	0.48
3:BB:176:SER:HA	3:BB:179:GLU:HB2	1.96	0.48
14:MM:242:LEU:O	14:MM:246:LEU:N	2.47	0.48
14:MM:506:SER:O	14:MM:539:GLN:NE2	2.47	0.48
8:GG:18:PRO:HD3	15:NN:92:LEU:HD22	1.96	0.47
11:JJ:250:PHE:HE2	11:JJ:462:TYR:H	1.62	0.47
12:KK:588:ASP:OD1	12:KK:589:GLY:N	2.47	0.47
14:MM:100:THR:HG23	14:MM:329:TYR:HE1	1.79	0.47
14:MM:343:ASP:N	14:MM:343:ASP:OD1	2.47	0.47
6:EE:249:ALA:HA	6:EE:252:GLU:HB3	1.96	0.47
11:JJ:512:ALA:HB3	11:JJ:620:ASP:HB3	1.97	0.47
14:MM:516:VAL:HG23	14:MM:544:ALA:HB2	1.96	0.47
14:MM:699:ALA:O	14:MM:718:ILE:N	2.43	0.47
2:AA:68:TYR:HB3	2:AA:70:ASP:H	1.79	0.47
10:II:48:HIS:CG	12:KK:552:LEU:HD13	2.49	0.47
11:JJ:316:VAL:HA	11:JJ:396:GLN:H	1.79	0.47
14:MM:92:GLU:HA	14:MM:114:ARG:HA	1.96	0.47
14:MM:722:VAL:HG22	14:MM:759:VAL:HG22	1.95	0.47
5:DD:138:ILE:O	5:DD:158:LEU:N	2.36	0.47
6:EE:207:GLU:O	6:EE:232:ASN:ND2	2.47	0.47
7:FF:83:ILE:HG22	7:FF:85:GLY:H	1.80	0.47
7:FF:118:MET:O	7:FF:122:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:JJ:615:LEU:HD22	11:JJ:646:ILE:HD11	1.96	0.47
11:JJ:941:LEU:HD13	11:JJ:960:LEU:HD21	1.97	0.47
12:KK:31:TYR:HB3	12:KK:38:PHE:CG	2.49	0.47
14:MM:537:TYR:HA	14:MM:540:MET:HB2	1.97	0.47
9:HH:79:MET:HB3	9:HH:81:TYR:CZ	2.50	0.47
12:KK:368:PHE:O	12:KK:372:ILE:N	2.46	0.47
12:KK:540:PRO:HA	12:KK:543:ARG:HB3	1.96	0.47
14:MM:622:GLU:O	14:MM:626:ALA:N	2.40	0.47
2:AA:34:ARG:NE	2:AA:222:ASP:OD2	2.41	0.47
4:CC:81:LYS:NZ	12:KK:578:ARG:O	2.40	0.47
5:DD:209[A]:ILE:HA	5:DD:212:ILE:HD12	1.97	0.47
5:DD:209[B]:ILE:HA	5:DD:212:ILE:HD12	1.97	0.47
7:FF:70:GLN:H	7:FF:145:LYS:HB3	1.80	0.47
8:GG:200:GLU:OE1	8:GG:202:SER:OG	2.32	0.47
9:HH:63:ASP:N	9:HH:63:ASP:OD1	2.48	0.47
11:JJ:225:LEU:HB2	11:JJ:228:ALA:HB2	1.97	0.47
11:JJ:883:ASN:OD1	11:JJ:886:ARG:NH1	2.47	0.47
14:MM:588:ASN:ND2	14:MM:911:ILE:O	2.47	0.47
14:MM:1032:GLU:OE2	14:MM:1062:HIS:ND1	2.35	0.47
9:HH:118:GLU:HB2	9:HH:125:LYS:HB2	1.95	0.47
10:II:254:VAL:HG21	10:II:286:ARG:HB3	1.96	0.47
14:MM:1035:VAL:HA	14:MM:1038:LEU:HD12	1.97	0.47
9:HH:348:ILE:O	9:HH:352:GLU:N	2.47	0.47
12:KK:31:TYR:CD2	13:LL:7:ILE:HB	2.49	0.47
14:MM:1050:LEU:O	14:MM:1054:MET:N	2.45	0.47
3:BB:166:TYR:O	3:BB:169:THR:N	2.39	0.47
3:BB:185:VAL:HG22	3:BB:201:VAL:HG22	1.97	0.47
4:CC:360:LEU:HB3	5:DD:182:SER:HB2	1.96	0.47
5:DD:74:LEU:HD23	5:DD:77:LEU:HD12	1.97	0.47
11:JJ:766:LEU:O	11:JJ:770:LEU:N	2.48	0.47
12:KK:237:VAL:N	12:KK:289:VAL:O	2.41	0.47
14:MM:864:LYS:O	14:MM:868:ARG:N	2.38	0.47
4:CC:297:TYR:N	4:CC:347:ILE:O	2.49	0.46
9:HH:176:LEU:HG	9:HH:182:ALA:HB2	1.97	0.46
11:JJ:364:VAL:HG21	11:JJ:369:GLN:HB2	1.97	0.46
13:LL:84:LYS:O	13:LL:88:ASP:N	2.48	0.46
14:MM:475:HIS:HB2	14:MM:499:LEU:HD11	1.97	0.46
6:EE:9:SER:O	6:EE:13:ASP:N	2.45	0.46
11:JJ:705:MET:HG2	11:JJ:712:PRO:HB3	1.97	0.46
14:MM:699:ALA:N	14:MM:718:ILE:O	2.48	0.46
10:II:45:GLN:HE21	10:II:52:THR:HB	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:MM:433:SER:O	14:MM:437:LYS:N	2.40	0.46
14:MM:946:GLN:HE21	14:MM:1030:ARG:HH12	1.63	0.46
2:AA:58:CYS:SG	2:AA:59:ARG:N	2.89	0.46
6:EE:138:ILE:HA	6:EE:141:ILE:HD12	1.96	0.46
6:EE:204:ASN:OD1	6:EE:205:GLU:N	2.47	0.46
8:GG:80:PHE:HB2	8:GG:85:LYS:HG2	1.97	0.46
14:MM:153:PHE:O	14:MM:157:ALA:N	2.49	0.46
14:MM:778:PRO:HG2	14:MM:786:GLN:HB3	1.97	0.46
14:MM:889:LEU:HB3	14:MM:894:PHE:HB2	1.98	0.46
14:MM:941:SER:HB3	14:MM:1001:VAL:HG21	1.98	0.46
2:AA:16:LEU:HD11	2:AA:203:PRO:HA	1.96	0.46
3:BB:8:SER:OG	3:BB:12:LEU:N	2.37	0.46
4:CC:147:GLU:O	4:CC:150:THR:OG1	2.33	0.46
11:JJ:42:ARG:HB2	11:JJ:45:ILE:HD11	1.97	0.46
11:JJ:62:ASP:OD1	11:JJ:62:ASP:N	2.48	0.46
11:JJ:908:ARG:HA	11:JJ:994:ARG:HH21	1.79	0.46
12:KK:84:ILE:O	12:KK:88:LEU:N	2.43	0.46
14:MM:80:MET:N	14:MM:125:LEU:H	2.14	0.46
2:AA:130:LYS:HD2	2:AA:174:ILE:HG13	1.97	0.46
2:AA:216:SER:N	2:AA:217:GLU:OE1	2.44	0.46
11:JJ:669:GLU:HA	11:JJ:672:MET:HB2	1.98	0.46
11:JJ:712:PRO:HG2	11:JJ:905:GLN:HB2	1.98	0.46
11:JJ:941:LEU:O	11:JJ:945:THR:N	2.47	0.46
14:MM:719:VAL:HB	14:MM:762:ILE:HG13	1.96	0.46
14:MM:719:VAL:N	14:MM:762:ILE:O	2.39	0.46
10:II:256:PHE:HZ	10:II:266:LEU:HD22	1.81	0.46
11:JJ:52:CYS:HG	11:JJ:184:HIS:CE1	2.32	0.46
11:JJ:678:LEU:HD12	11:JJ:726:LEU:HB2	1.98	0.46
3:BB:156:ASP:OD1	3:BB:157:TYR:N	2.48	0.46
13:LL:51:ASN:O	13:LL:55:TYR:N	2.49	0.46
14:MM:503:GLU:O	14:MM:506:SER:OG	2.27	0.46
15:NN:5:UNK:O	15:NN:9:UNK:N	2.48	0.46
11:JJ:110:ASP:OD2	11:JJ:144:ARG:NH1	2.49	0.46
11:JJ:406:GLN:HG2	11:JJ:425:ILE:HB	1.97	0.46
12:KK:46:ALA:HB2	13:LL:67:VAL:HG11	1.98	0.46
2:AA:101:GLU:OE1	2:AA:101:GLU:N	2.38	0.46
3:BB:72:LEU:HD23	3:BB:105:VAL:HA	1.97	0.46
3:BB:140:ILE:HA	3:BB:143:ILE:HD12	1.98	0.46
7:FF:205:LYS:HE3	10:II:46:TYR:HE1	1.80	0.46
14:MM:166:SER:OG	14:MM:289:TYR:N	2.46	0.46
5:DD:3:VAL:HG12	5:DD:21:SER:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:HH:117:ALA:H	9:HH:126:VAL:HA	1.81	0.45
11:JJ:314:ASP:OD1	11:JJ:399:SER:OG	2.31	0.45
14:MM:891:ARG:HE	14:MM:976:ILE:HG21	1.80	0.45
2:AA:144:ASP:OD1	2:AA:225:LEU:N	2.45	0.45
4:CC:387:ASP:O	4:CC:391:ARG:N	2.49	0.45
7:FF:71:THR:OG1	7:FF:144:ASP:OD1	2.23	0.45
11:JJ:773:ARG:HG2	11:JJ:975:VAL:HG12	1.98	0.45
14:MM:518:PHE:HB2	14:MM:557:MET:HA	1.98	0.45
14:MM:533:SER:N	14:MM:536:GLU:OE1	2.48	0.45
4:CC:44:ARG:HB3	4:CC:48:GLU:HB2	1.98	0.45
4:CC:360:LEU:HD21	4:CC:362:LEU:HD13	1.98	0.45
10:II:149:GLN:HG2	10:II:150:ARG:HH11	1.81	0.45
14:MM:583:PHE:HB3	14:MM:610:PHE:HB2	1.99	0.45
3:BB:66:ASP:OD2	3:BB:68:SER:OG	2.32	0.45
4:CC:221:SER:HB2	7:FF:53:ILE:HG23	1.98	0.45
10:II:223:CYS:HA	10:II:286:ARG:HA	1.99	0.45
11:JJ:413:ASP:OD2	11:JJ:416:SER:N	2.50	0.45
13:LL:74:SER:O	13:LL:78:GLY:N	2.37	0.45
13:LL:79:GLU:OE1	13:LL:82:ARG:NH1	2.43	0.45
13:LL:109:GLU:O	13:LL:113:ASN:ND2	2.48	0.45
14:MM:882:LEU:HG	14:MM:886:LYS:HE3	1.97	0.45
2:AA:163:LYS:HA	2:AA:186:PRO:HA	1.98	0.45
9:HH:347:ASP:O	9:HH:350:THR:OG1	2.31	0.45
14:MM:938:ALA:O	14:MM:941:SER:OG	2.25	0.45
10:II:259:ALA:O	10:II:264:GLY:N	2.44	0.45
11:JJ:377:ALA:O	11:JJ:381:GLN:N	2.45	0.45
14:MM:419:CYS:HB3	14:MM:500:PHE:HB3	1.99	0.45
14:MM:892:LEU:HD13	14:MM:892:LEU:HA	1.83	0.45
14:MM:940:LEU:HD22	14:MM:1034:LEU:HD21	1.98	0.45
8:GG:67:SER:OG	8:GG:70:ASP:OD2	2.30	0.45
11:JJ:692:GLY:O	11:JJ:783:SER:OG	2.22	0.45
11:JJ:767:ASN:O	11:JJ:771:ASN:N	2.50	0.45
14:MM:445:ASN:O	14:MM:449:ALA:N	2.50	0.45
14:MM:640:GLU:HG2	14:MM:642:ASN:H	1.80	0.45
14:MM:731:PRO:HB3	14:MM:734:LEU:HD12	1.98	0.45
2:AA:43:GLU:HB2	2:AA:46:ASP:HB2	1.98	0.45
3:BB:164:GLY:O	3:BB:171:LEU:N	2.43	0.45
4:CC:378:LEU:HB3	4:CC:382:ARG:HH12	1.82	0.45
9:HH:291:ASN:HA	9:HH:294:ARG:HD2	1.98	0.45
10:II:34:ASN:N	10:II:104:LYS:O	2.48	0.45
13:LL:92:GLN:HA	13:LL:95:ASN:HD22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:HH:183:SER:OG	9:HH:184:LEU:N	2.49	0.45
14:MM:177:LYS:HB3	14:MM:292:LEU:HD13	1.99	0.45
14:MM:757:CYS:HB2	14:MM:788:GLU:HG3	1.98	0.45
10:II:141:THR:HG22	10:II:155:ILE:HA	1.99	0.45
14:MM:1039:VAL:O	14:MM:1043:ASN:ND2	2.50	0.45
4:CC:61:ARG:HB3	4:CC:72:ASN:HB3	1.99	0.44
11:JJ:736:ILE:HG23	11:JJ:838:ILE:HG23	1.99	0.44
2:AA:102:VAL:HA	2:AA:105:SER:HB3	1.99	0.44
3:BB:171:LEU:HD23	3:BB:171:LEU:HA	1.82	0.44
11:JJ:760:SER:O	11:JJ:764:GLU:N	2.46	0.44
4:CC:78:ASN:ND2	4:CC:236:TYR:HB2	2.33	0.44
4:CC:93:GLY:HA2	4:CC:213:LEU:HA	1.98	0.44
8:GG:183:LYS:HE3	15:NN:118:ASN:H	1.82	0.44
9:HH:323:TYR:O	9:HH:326:SER:OG	2.30	0.44
10:II:139:VAL:HG22	10:II:158:VAL:HG22	1.97	0.44
11:JJ:318:VAL:HA	11:JJ:392:VAL:HA	1.99	0.44
11:JJ:539:ILE:HD13	11:JJ:555:HIS:HB3	2.00	0.44
11:JJ:764:GLU:HA	11:JJ:767:ASN:HB2	2.00	0.44
11:JJ:764:GLU:HA	11:JJ:767:ASN:HD22	1.82	0.44
12:KK:46:ALA:O	12:KK:50:ALA:N	2.47	0.44
14:MM:407:ASN:OD1	14:MM:407:ASN:N	2.49	0.44
5:DD:187:ASN:OD1	5:DD:189:ASP:N	2.51	0.44
6:EE:223:THR:OG1	6:EE:224:SER:N	2.51	0.44
14:MM:171:ALA:H	14:MM:177:LYS:HD3	1.81	0.44
14:MM:400:MET:O	14:MM:404:LYS:N	2.44	0.44
14:MM:222:MET:HB2	14:MM:237:MET:HB3	1.99	0.44
6:EE:31:PHE:HD2	9:HH:5:ILE:HD12	1.82	0.44
6:EE:256:PRO:HA	6:EE:259:VAL:HB	2.00	0.44
10:II:17:ILE:HD11	10:II:58:ALA:HB2	2.00	0.44
11:JJ:627:ILE:HB	11:JJ:640:ASN:HB2	1.99	0.44
14:MM:246:LEU:HA	14:MM:246:LEU:HD23	1.83	0.44
14:MM:486:VAL:HA	14:MM:489:ILE:HD12	1.99	0.44
1:2:176:U:OP2	2:AA:113:ARG:NH2	2.51	0.44
6:EE:213:LEU:HD23	6:EE:228:SER:HA	1.99	0.44
9:HH:127:ASP:OD1	9:HH:129:GLY:N	2.47	0.44
14:MM:401:ILE:O	14:MM:405:LYS:N	2.50	0.44
14:MM:449:ALA:HA	14:MM:456:ARG:HH21	1.82	0.44
14:MM:683:SER:HA	14:MM:689:ASN:HA	2.00	0.44
2:AA:120:VAL:HA	2:AA:123:LEU:HD13	2.00	0.44
6:EE:189:ILE:HG23	6:EE:201:PRO:HD2	1.99	0.44
7:FF:169:ILE:HB	7:FF:200:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:GG:150:LEU:HD13	8:GG:195:TRP:CD2	2.53	0.44
9:HH:173:VAL:HA	9:HH:184:LEU:HD23	1.99	0.44
12:KK:36:ARG:O	12:KK:40:LYS:N	2.43	0.44
13:LL:111:ALA:HA	13:LL:114:ILE:HD12	2.00	0.44
14:MM:93:VAL:O	14:MM:113:VAL:N	2.43	0.44
14:MM:724:ASN:HB3	14:MM:791:GLY:HA3	2.00	0.44
6:EE:17:SER:HB3	6:EE:20:SER:HA	1.99	0.44
11:JJ:167:ASN:HA	11:JJ:170:ASN:HD22	1.83	0.44
5:DD:36:PRO:HB3	5:DD:87:LEU:HB2	2.00	0.43
8:GG:231:PHE:O	8:GG:235:LEU:N	2.35	0.43
11:JJ:178:CYS:HB2	11:JJ:213:ILE:HD11	1.99	0.43
11:JJ:525:ASP:HB3	11:JJ:528:LEU:HB2	1.99	0.43
14:MM:792:LYS:O	14:MM:796:GLU:N	2.49	0.43
14:MM:1023:SER:HA	14:MM:1026:ARG:HB2	1.99	0.43
2:AA:240:ASN:ND2	2:AA:244:GLU:HG2	2.33	0.43
5:DD:14:ASP:OD2	5:DD:32:GLY:N	2.49	0.43
6:EE:86:ARG:HG2	6:EE:88:ASP:H	1.81	0.43
10:II:32:ILE:HB	10:II:103:VAL:HG12	2.00	0.43
11:JJ:87:TYR:N	11:JJ:191:ASN:O	2.41	0.43
11:JJ:370:ARG:O	11:JJ:374:ALA:N	2.49	0.43
11:JJ:763:PHE:HB3	11:JJ:778:ILE:HD12	2.00	0.43
11:JJ:959:LYS:HD3	11:JJ:974:TYR:CZ	2.53	0.43
14:MM:220:GLY:N	14:MM:234:CYS:O	2.37	0.43
10:II:40:GLY:HA3	10:II:110:VAL:HB	1.99	0.43
11:JJ:681:SER:O	11:JJ:685:LYS:N	2.48	0.43
12:KK:362:ALA:O	12:KK:366:THR:N	2.49	0.43
4:CC:298:GLY:N	4:CC:331:ILE:O	2.39	0.43
8:GG:119:VAL:HA	8:GG:149:ILE:HA	2.00	0.43
11:JJ:755:HIS:HD2	11:JJ:816:ALA:HB2	1.84	0.43
14:MM:186:ALA:HA	14:MM:189:LEU:HB2	2.00	0.43
14:MM:405:LYS:O	14:MM:514:LYS:NZ	2.50	0.43
5:DD:70:LEU:HD13	5:DD:113:ILE:HG12	1.99	0.43
8:GG:183:LYS:HA	8:GG:183:LYS:HD3	1.72	0.43
11:JJ:237:GLN:HG3	11:JJ:464:LEU:HB3	1.99	0.43
11:JJ:454:ASP:H	11:JJ:465:GLY:HA2	1.83	0.43
11:JJ:653:SER:OG	11:JJ:654:TYR:N	2.51	0.43
11:JJ:655:GLU:HG2	11:JJ:659:LEU:HD23	2.00	0.43
14:MM:394:ILE:HA	14:MM:397:ILE:HD12	2.00	0.43
14:MM:399:LYS:HA	14:MM:402:TRP:HB3	2.00	0.43
2:AA:101:GLU:O	2:AA:105:SER:N	2.51	0.43
6:EE:261:SER:HB3	9:HH:7:ILE:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:KK:96:LEU:HA	12:KK:99:LEU:HD12	2.00	0.43
14:MM:268:ARG:HB3	14:MM:579:LEU:HD12	1.99	0.43
14:MM:459:PRO:O	14:MM:463:HIS:ND1	2.52	0.43
14:MM:645:GLU:HA	14:MM:648:GLU:HB2	2.00	0.43
14:MM:670:ALA:HB3	14:MM:764:LEU:HD22	2.00	0.43
3:BB:225:ARG:H	3:BB:225:ARG:HG3	1.64	0.43
4:CC:21:VAL:HA	10:II:190:VAL:HG11	2.01	0.43
5:DD:163:LEU:HD13	5:DD:180:LEU:HD13	2.01	0.43
6:EE:258:VAL:HG13	9:HH:5:ILE:HG21	2.00	0.43
11:JJ:13:LEU:N	11:JJ:17:LEU:O	2.39	0.43
11:JJ:419:THR:HA	11:JJ:439:ARG:HA	2.01	0.43
14:MM:296:ILE:HD11	14:MM:299:ALA:HA	2.00	0.43
14:MM:727:TYR:CE2	14:MM:729:ASP:HB2	2.53	0.43
2:AA:162:PHE:HD2	2:AA:187:LEU:HD11	1.82	0.43
3:BB:24:ARG:HG3	11:JJ:13:LEU:HD21	2.00	0.43
3:BB:110:LYS:HA	3:BB:110:LYS:HD3	1.84	0.43
4:CC:308:LEU:HD13	12:KK:610:LEU:HA	2.00	0.43
8:GG:172:PHE:HA	8:GG:173:PRO:HD3	1.87	0.43
10:II:211:ARG:HA	10:II:248:ALA:HA	2.00	0.43
3:BB:168:THR:HG22	3:BB:209:ARG:HH21	1.84	0.43
11:JJ:193:VAL:HG22	11:JJ:214:ILE:HG21	1.99	0.43
11:JJ:777:SER:OG	11:JJ:778:ILE:N	2.49	0.43
14:MM:407:ASN:HB2	14:MM:497:LYS:HD2	2.01	0.43
3:BB:22:LEU:HD23	3:BB:173:ASP:HB2	2.01	0.43
5:DD:28:CYS:SG	5:DD:29:SER:N	2.91	0.43
10:II:38:GLY:O	10:II:41:THR:OG1	2.27	0.43
14:MM:240:GLU:HG3	14:MM:275:VAL:HG11	2.00	0.43
14:MM:619:PRO:HA	14:MM:622:GLU:HB2	2.00	0.43
2:AA:137:ASP:OD2	5:DD:57:GLY:N	2.52	0.42
4:CC:257:MET:HA	11:JJ:294:ARG:HH11	1.85	0.42
7:FF:106:ASN:OD1	7:FF:107:THR:N	2.51	0.42
9:HH:339:ASN:O	9:HH:343:SER:N	2.50	0.42
11:JJ:23:VAL:HB	11:JJ:36:VAL:HG23	2.01	0.42
11:JJ:519:PRO:O	11:JJ:523:SER:N	2.45	0.42
11:JJ:555:HIS:HD2	11:JJ:557:LYS:HG3	1.82	0.42
11:JJ:783:SER:HB3	11:JJ:832:TYR:CZ	2.53	0.42
12:KK:29:ASP:HA	12:KK:32:LYS:HD2	2.01	0.42
12:KK:46:ALA:HA	12:KK:49:LEU:HD12	2.01	0.42
14:MM:329:TYR:N	14:MM:555:VAL:O	2.51	0.42
14:MM:449:ALA:O	14:MM:456:ARG:NH2	2.52	0.42
14:MM:678:ARG:HA	14:MM:774:ARG:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AA:262:MET:HE1	3:BB:210:LEU:HB3	2.01	0.42
7:FF:195:GLU:OE2	7:FF:198:GLY:N	2.52	0.42
8:GG:76:ILE:O	8:GG:116:GLY:N	2.50	0.42
9:HH:90:ARG:HG2	9:HH:95:LEU:HD12	2.01	0.42
9:HH:107:GLU:HB3	14:MM:906:ARG:HH12	1.84	0.42
14:MM:883:ARG:HA	14:MM:886:LYS:HD2	2.01	0.42
5:DD:13:VAL:HG11	5:DD:29:SER:HB2	2.01	0.42
6:EE:57:GLU:HB3	6:EE:131:ILE:HB	2.01	0.42
6:EE:65:LYS:O	6:EE:123:LYS:N	2.52	0.42
9:HH:176:LEU:HD23	9:HH:180:GLY:HA2	2.00	0.42
11:JJ:735:ASN:OD1	11:JJ:842:PHE:N	2.51	0.42
11:JJ:987:MET:HA	11:JJ:994:ARG:HA	2.01	0.42
12:KK:31:TYR:HA	12:KK:34:LEU:HB2	2.01	0.42
14:MM:592:ASN:HA	14:MM:595:ARG:HB3	2.00	0.42
3:BB:23:ARG:HD2	3:BB:45:GLY:HA3	2.02	0.42
11:JJ:967:SER:OG	11:JJ:968:ASP:N	2.52	0.42
11:JJ:968:ASP:N	11:JJ:968:ASP:OD1	2.51	0.42
14:MM:87:GLN:HB3	14:MM:119:VAL:HB	2.01	0.42
14:MM:139:ARG:HH22	14:MM:155:ASP:HA	1.83	0.42
14:MM:461:ILE:HA	14:MM:464:ILE:HG22	2.02	0.42
14:MM:876:VAL:HB	14:MM:879:LEU:HG	2.01	0.42
2:AA:229:LEU:HA	2:AA:229:LEU:HD23	1.84	0.42
11:JJ:52:CYS:SG	11:JJ:184:HIS:NE2	2.73	0.42
14:MM:466:PRO:HA	14:MM:469:ARG:HB2	2.01	0.42
2:AA:238:THR:HB	2:AA:246:VAL:HB	2.02	0.42
4:CC:261:THR:HG22	4:CC:262:ARG:H	1.84	0.42
4:CC:345:SER:HA	4:CC:365:GLY:H	1.84	0.42
4:CC:348:SER:HB2	4:CC:361:THR:HB	2.02	0.42
11:JJ:88:VAL:HB	11:JJ:111:VAL:HG22	2.00	0.42
11:JJ:632:ASP:OD1	11:JJ:679:LYS:NZ	2.52	0.42
11:JJ:667:ASN:OD1	11:JJ:675:ARG:NH2	2.50	0.42
12:KK:81:PHE:CE1	13:LL:61:MET:HG3	2.54	0.42
14:MM:696:VAL:HB	14:MM:720:ASN:HB2	2.02	0.42
14:MM:793:SER:HA	14:MM:796:GLU:HB2	2.02	0.42
14:MM:842:ASN:N	14:MM:842:ASN:OD1	2.52	0.42
14:MM:931:LEU:HD23	14:MM:931:LEU:HA	1.83	0.42
2:AA:44:PHE:HA	2:AA:161:HIS:CE1	2.53	0.42
4:CC:357:TYR:OH	4:CC:382:ARG:NH1	2.51	0.42
6:EE:68:ASP:HB3	6:EE:71:VAL:HG22	2.01	0.42
11:JJ:212:ASN:OD1	11:JJ:212:ASN:N	2.52	0.42
12:KK:103:ILE:HG13	13:LL:93:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:MM:170:SER:OG	14:MM:294:ALA:O	2.37	0.42
14:MM:747:ARG:NH1	14:MM:753:GLU:OE1	2.51	0.42
3:BB:157:TYR:OH	3:BB:229:ASP:OD1	2.28	0.42
3:BB:218:ILE:H	3:BB:218:ILE:HG13	1.66	0.42
4:CC:86:ILE:HD13	12:KK:576:LEU:HG	2.01	0.42
4:CC:97:GLU:HA	4:CC:209:TRP:CD1	2.55	0.42
8:GG:191:ASN:OD1	8:GG:191:ASN:N	2.50	0.42
14:MM:153:PHE:HB2	14:MM:317:VAL:HG11	2.01	0.42
4:CC:40:ARG:HD3	4:CC:44:ARG:HB2	2.02	0.42
11:JJ:894:ALA:HA	11:JJ:897:ALA:HB3	2.01	0.42
14:MM:587:TYR:CG	14:MM:917:LEU:HD21	2.55	0.42
14:MM:703:ASN:HB2	14:MM:711:TYR:HE2	1.85	0.42
14:MM:791:GLY:HA2	14:MM:794:LEU:HD12	2.02	0.42
4:CC:348:SER:O	4:CC:361:THR:N	2.51	0.42
5:DD:4:GLN:HG3	5:DD:20:VAL:HB	2.02	0.42
6:EE:29:HIS:HD2	9:HH:4:VAL:HG22	1.85	0.42
11:JJ:104:ASN:HD21	11:JJ:106:ASN:HB2	1.84	0.42
14:MM:137:HIS:NE2	14:MM:162:ASP:OD2	2.37	0.42
14:MM:781:ILE:HG13	14:MM:782:ARG:H	1.85	0.42
3:BB:200:LEU:HD12	3:BB:200:LEU:HA	1.91	0.41
4:CC:350:LEU:HA	4:CC:350:LEU:HD23	1.86	0.41
11:JJ:229:ASP:HA	11:JJ:232:ARG:HE	1.84	0.41
11:JJ:507:GLY:HA2	11:JJ:607:LEU:HD11	2.01	0.41
14:MM:158:ILE:HG23	14:MM:183:TYR:CE2	2.55	0.41
14:MM:680:VAL:HG12	14:MM:770:ILE:HG12	2.02	0.41
14:MM:846:LEU:O	14:MM:850:TYR:N	2.51	0.41
14:MM:895:CYS:HA	14:MM:902:GLU:HG2	2.01	0.41
3:BB:23:ARG:HH22	3:BB:47:ASN:HD22	1.67	0.41
5:DD:51:ILE:HB	5:DD:91:THR:HG23	2.01	0.41
9:HH:342:GLU:O	9:HH:346:SER:N	2.48	0.41
11:JJ:26:ARG:HB3	11:JJ:33:THR:HB	2.02	0.41
14:MM:650:GLU:HA	14:MM:653:ILE:HB	2.01	0.41
14:MM:777:MET:HA	14:MM:778:PRO:HD3	1.93	0.41
2:AA:5:ILE:HD11	2:AA:90:GLN:HE21	1.85	0.41
6:EE:26:ARG:HD2	6:EE:30:GLN:HB2	2.01	0.41
14:MM:83:ASP:OD2	14:MM:131:TYR:OH	2.38	0.41
14:MM:327:GLN:HE21	14:MM:552:ARG:HH11	1.69	0.41
14:MM:339:TYR:HB3	14:MM:352:ASN:HB3	2.02	0.41
14:MM:903:LEU:HA	14:MM:906:ARG:HB2	2.02	0.41
2:AA:239:LEU:HB3	2:AA:240:ASN:H	1.73	0.41
4:CC:72:ASN:OD1	4:CC:73:ASN:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CC:150:THR:HB	4:CC:154:LYS:HE3	2.01	0.41
6:EE:15:LEU:HD21	6:EE:205:GLU:HG2	2.01	0.41
9:HH:9:LYS:HE2	9:HH:9:LYS:HB2	1.81	0.41
11:JJ:703:VAL:HG11	11:JJ:902:TYR:HB3	2.03	0.41
11:JJ:857:GLN:HG2	11:JJ:867:LEU:HD11	2.02	0.41
12:KK:584:ALA:N	12:KK:592:ASN:O	2.54	0.41
14:MM:245:MET:HB3	14:MM:250:SER:HB3	2.01	0.41
14:MM:343:ASP:OD1	14:MM:347:THR:N	2.33	0.41
14:MM:840:LEU:HA	14:MM:843:SER:HB3	2.02	0.41
9:HH:70:GLY:O	9:HH:73:THR:OG1	2.29	0.41
11:JJ:555:HIS:CD2	11:JJ:557:LYS:HG3	2.55	0.41
11:JJ:557:LYS:O	11:JJ:565:GLU:N	2.36	0.41
12:KK:288:LYS:H	12:KK:311:LEU:HA	1.85	0.41
12:KK:294:PHE:O	12:KK:298:ILE:N	2.42	0.41
14:MM:105:LEU:HD11	14:MM:344:GLU:HB2	2.03	0.41
2:AA:28:ARG:HB3	2:AA:32:GLN:HB3	2.03	0.41
6:EE:146:TYR:O	6:EE:150:ASN:ND2	2.54	0.41
8:GG:190:LEU:HD23	8:GG:190:LEU:HA	1.90	0.41
11:JJ:50:ARG:HG3	11:JJ:73:SER:HA	2.03	0.41
11:JJ:217:SER:N	11:JJ:220:GLN:HB3	2.34	0.41
11:JJ:268:LEU:HD23	11:JJ:268:LEU:HA	1.92	0.41
12:KK:27:ASP:OD1	12:KK:27:ASP:N	2.49	0.41
14:MM:956:LYS:HA	14:MM:957:PRO:HD3	1.82	0.41
2:AA:55:LYS:HB3	2:AA:141:LEU:HD12	2.02	0.41
4:CC:22:LEU:HG	4:CC:30:SER:HB2	2.02	0.41
7:FF:203:PHE:HB3	7:FF:207:GLY:HA2	2.02	0.41
9:HH:170:ASN:HB2	9:HH:192:GLY:H	1.86	0.41
11:JJ:198:ASP:O	11:JJ:202:ARG:N	2.53	0.41
11:JJ:715:VAL:HG23	11:JJ:906:VAL:HG11	2.02	0.41
14:MM:957:PRO:HA	14:MM:960:ALA:HB3	2.02	0.41
3:BB:157:TYR:HD2	3:BB:225:ARG:HB2	1.86	0.41
4:CC:40:ARG:NH2	4:CC:333:ASP:O	2.38	0.41
6:EE:48:SER:HB3	6:EE:148:ALA:HB2	2.02	0.41
7:FF:47:SER:HG	7:FF:49:HIS:CE1	2.39	0.41
11:JJ:26:ARG:N	11:JJ:33:THR:O	2.43	0.41
11:JJ:630:LEU:HB3	11:JJ:636:ILE:HA	2.03	0.41
13:LL:40:LEU:HD23	13:LL:45:ALA:HB1	2.02	0.41
14:MM:475:HIS:CE1	14:MM:505:PHE:HB2	2.56	0.41
14:MM:778:PRO:HB3	14:MM:786:GLN:HE21	1.86	0.41
14:MM:833:THR:OG1	14:MM:834:LYS:N	2.54	0.41
5:DD:81:HIS:CD2	10:II:263:ALA:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:FF:46:LEU:HD13	7:FF:48:LEU:HD11	2.02	0.41
11:JJ:539:ILE:HB	11:JJ:648:SER:HA	2.03	0.41
11:JJ:681:SER:OG	11:JJ:725:SER:O	2.33	0.41
11:JJ:826:TYR:HA	11:JJ:829:PHE:CD2	2.55	0.41
11:JJ:930:VAL:HB	11:JJ:933:PHE:HB2	2.02	0.41
14:MM:138:LYS:HA	14:MM:138:LYS:HD3	1.87	0.41
14:MM:168:LEU:HA	14:MM:291:PHE:HB2	2.02	0.41
14:MM:212:LEU:HA	14:MM:215:GLU:HB3	2.03	0.41
2:AA:29:SER:OG	2:AA:30:PHE:N	2.53	0.40
2:AA:79:ILE:HA	2:AA:136:ALA:HB3	2.03	0.40
2:AA:164:LYS:N	2:AA:185:VAL:O	2.35	0.40
3:BB:18:ARG:NH2	11:JJ:44:ASP:OD2	2.54	0.40
3:BB:41:TYR:CE2	3:BB:43:GLU:HG3	2.56	0.40
5:DD:168:VAL:HG23	5:DD:173:VAL:HB	2.03	0.40
8:GG:73:ILE:H	8:GG:191:ASN:HD21	1.69	0.40
11:JJ:20:THR:O	11:JJ:39:HIS:N	2.49	0.40
11:JJ:921:VAL:HG12	11:JJ:953:PHE:HE1	1.86	0.40
14:MM:139:ARG:NH2	14:MM:155:ASP:OD1	2.54	0.40
14:MM:332:PRO:HB3	14:MM:360:ILE:HG12	2.03	0.40
3:BB:15:ASP:OD1	3:BB:15:ASP:N	2.54	0.40
3:BB:163:VAL:HG22	3:BB:172:LEU:HA	2.03	0.40
5:DD:132:ALA:HB3	5:DD:202:CYS:HB3	2.02	0.40
6:EE:169:LEU:HA	6:EE:170:PRO:HD3	1.94	0.40
8:GG:220:THR:HA	8:GG:223:PHE:CD2	2.55	0.40
11:JJ:91:ASP:HB3	11:JJ:94:VAL:HG13	2.03	0.40
11:JJ:310:ALA:HA	11:JJ:398:ARG:HH12	1.87	0.40
11:JJ:323:GLN:HA	11:JJ:326:TRP:CG	2.56	0.40
11:JJ:591:GLY:HA3	11:JJ:887:LYS:HG3	2.03	0.40
12:KK:332:LEU:O	12:KK:338:PHE:N	2.42	0.40
12:KK:598:ASP:OD2	12:KK:602:ARG:NE	2.54	0.40
14:MM:889:LEU:O	14:MM:893:GLY:N	2.54	0.40
2:AA:203:PRO:HG2	2:AA:204:GLN:HG2	2.04	0.40
4:CC:51:ASP:OD1	4:CC:52:VAL:N	2.52	0.40
4:CC:62:TYR:HB3	4:CC:242:LYS:NZ	2.37	0.40
5:DD:164:ALA:HB3	5:DD:179:LEU:H	1.86	0.40
6:EE:36:ILE:HD12	9:HH:7:ILE:HG23	2.03	0.40
6:EE:154:LEU:HA	6:EE:155:PRO:HD3	1.93	0.40
7:FF:231:LYS:HG2	7:FF:235:ASN:HD21	1.86	0.40
14:MM:90:SER:OG	14:MM:115:LEU:O	2.33	0.40
14:MM:522:ARG:HB2	14:MM:529:PHE:CZ	2.57	0.40
2:AA:100:ASP:OD1	2:AA:100:ASP:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AA:236:THR:HG22	2:AA:247:GLN:HE22	1.86	0.40
2:AA:243:ARG:HA	2:AA:269:TYR:HE1	1.86	0.40
4:CC:345:SER:OG	4:CC:366:GLY:N	2.48	0.40
5:DD:206:VAL:HA	5:DD:209[A]:ILE:HD12	2.03	0.40
5:DD:206:VAL:HA	5:DD:209[B]:ILE:HD12	2.03	0.40
11:JJ:736:ILE:O	11:JJ:740:ARG:N	2.45	0.40
12:KK:364:ALA:O	12:KK:368:PHE:N	2.55	0.40
2:AA:24:ARG:HH11	2:AA:30:PHE:HA	1.87	0.40
7:FF:189:ASP:OD1	7:FF:190:MET:N	2.54	0.40
9:HH:64:ASP:HB3	9:HH:67:TRP:HD1	1.87	0.40
9:HH:112:VAL:HG12	9:HH:228:ASN:H	1.86	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	
2	AA	297/303 (98%)	276 (93%)	21 (7%)	0	100	100
3	BB	242/248 (98%)	224 (93%)	18 (7%)	0	100	100
4	CC	332/393 (84%)	304 (92%)	27 (8%)	1 (0%)	41	76
5	DD	222/245 (91%)	209 (94%)	13 (6%)	0	100	100
6	EE	266/267 (100%)	252 (95%)	14 (5%)	0	100	100
7	FF	209/250 (84%)	191 (91%)	18 (9%)	0	100	100
8	GG	235/242 (97%)	216 (92%)	19 (8%)	0	100	100
9	HH	287/361 (80%)	262 (91%)	25 (9%)	0	100	100
10	II	214/301 (71%)	198 (92%)	16 (8%)	0	100	100
11	JJ	942/1003 (94%)	875 (93%)	67 (7%)	0	100	100
12	KK	404/733 (55%)	366 (91%)	38 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	LL	111/184 (60%)	108 (97%)	3 (3%)	0	100	100
14	MM	972/1073 (91%)	909 (94%)	63 (6%)	0	100	100
15	NN	27/40 (68%)	23 (85%)	4 (15%)	0	100	100
All	All	4760/5643 (84%)	4413 (93%)	346 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	CC	337	GLU

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	
2	AA	255/265 (96%)	255 (100%)	0	100	100
3	BB	210/219 (96%)	207 (99%)	3 (1%)	67	81
4	CC	282/349 (81%)	281 (100%)	1 (0%)	91	94
5	DD	196/216 (91%)	196 (100%)	0	100	100
6	EE	238/241 (99%)	238 (100%)	0	100	100
7	FF	181/219 (83%)	180 (99%)	1 (1%)	86	92
8	GG	194/210 (92%)	194 (100%)	0	100	100
9	HH	243/313 (78%)	242 (100%)	1 (0%)	91	94
10	II	174/249 (70%)	172 (99%)	2 (1%)	73	85
11	JJ	812/901 (90%)	808 (100%)	4 (0%)	88	93
12	KK	150/671 (22%)	150 (100%)	0	100	100
13	LL	99/168 (59%)	98 (99%)	1 (1%)	76	86
14	MM	810/953 (85%)	804 (99%)	6 (1%)	84	90
15	NN	25/25 (100%)	25 (100%)	0	100	100
All	All	3869/4999 (77%)	3850 (100%)	19 (0%)	89	93

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	BB	77	ASN
3	BB	86	ARG
3	BB	225	ARG
4	CC	73	ASN
7	FF	55	ASN
9	HH	212	ASN
10	II	51	ARG
10	II	130	ASN
11	JJ	29	ASN
11	JJ	144	ARG
11	JJ	169	ARG
11	JJ	775	ASN
13	LL	64	ASN
14	MM	470	ARG
14	MM	530	ARG
14	MM	543	ARG
14	MM	614	ASN
14	MM	642	ASN
14	MM	844	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
3	BB	30	ASN
3	BB	64	GLN
3	BB	77	ASN
4	CC	73	ASN
4	CC	153	GLN
4	CC	239	GLN
4	CC	287	ASN
5	DD	81	HIS
5	DD	216	ASN
6	EE	150	ASN
6	EE	183	ASN
6	EE	219	ASN
7	FF	55	ASN
7	FF	235	ASN
9	HH	212	ASN
11	JJ	29	ASN
11	JJ	170	ASN
11	JJ	197	ASN

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Mol	Chain	Res	Type
11	JJ	201	ASN
11	JJ	555	HIS
11	JJ	775	ASN
11	JJ	855	HIS
11	JJ	857	GLN
12	KK	83	ASN
12	KK	604	GLN
12	KK	612	ASN
13	LL	64	ASN
13	LL	95	ASN
13	LL	113	ASN
14	MM	117	HIS
14	MM	191	ASN
14	MM	445	ASN
14	MM	475	HIS
14	MM	539	GLN
14	MM	588	ASN
14	MM	614	ASN
14	MM	669	ASN
14	MM	786	GLN
14	MM	832	ASN
14	MM	874	GLN
14	MM	929	ASN
14	MM	946	GLN
14	MM	1043	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	22/23 (95%)	15 (68%)	0

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	161	U
1	2	162	U
1	2	163	U
1	2	164	A
1	2	165	A
1	2	166	A
1	2	167	U

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Mol	Chain	Res	Type
1	2	169	U
1	2	170	U
1	2	171	U
1	2	172	U
1	2	175	U
1	2	176	U
1	2	177	U
1	2	178	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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
15	NN	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	NN	11:UNK	C	90:PRO	N	57.41

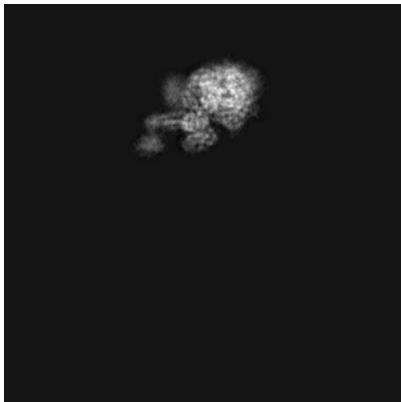
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4301. These allow visual inspection of the internal detail of the map and identification of artifacts.

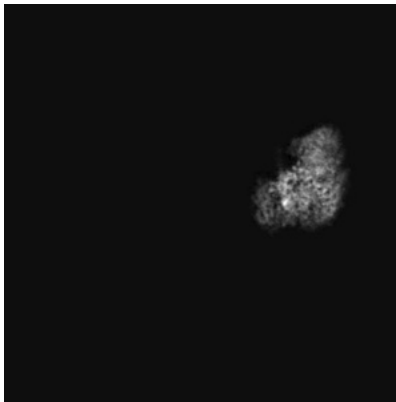
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

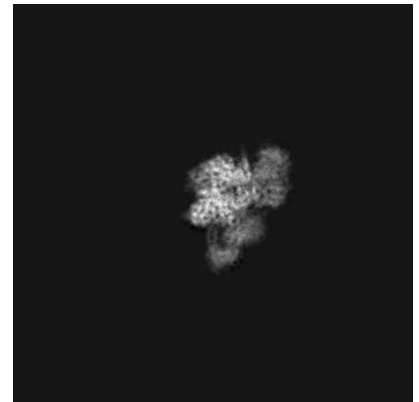
6.1.1 Primary map



X



Y

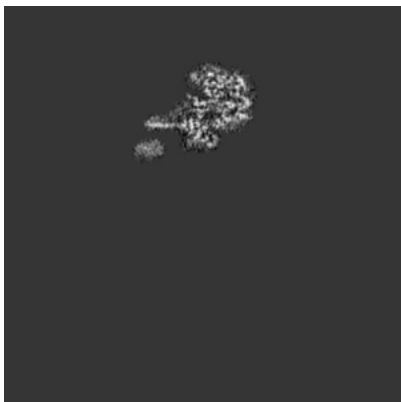


Z

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

6.2 Central slices [i](#)

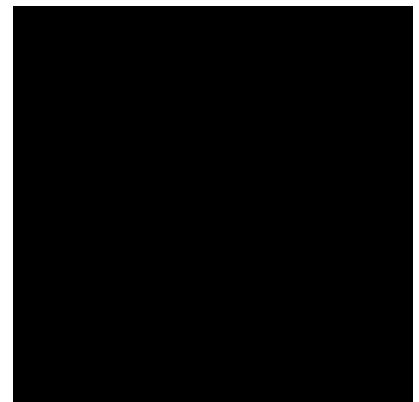
6.2.1 Primary map



X Index: 220



Y Index: 220

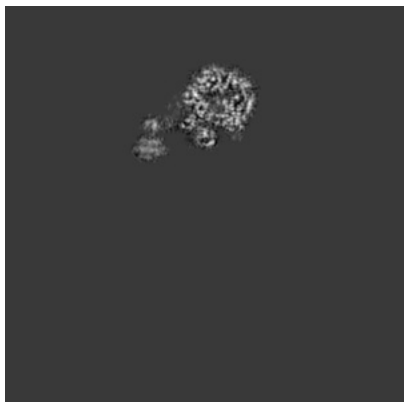


Z Index: 220

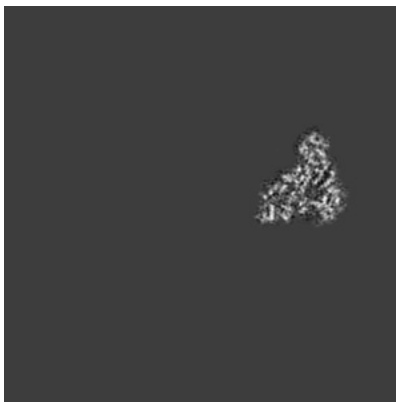
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

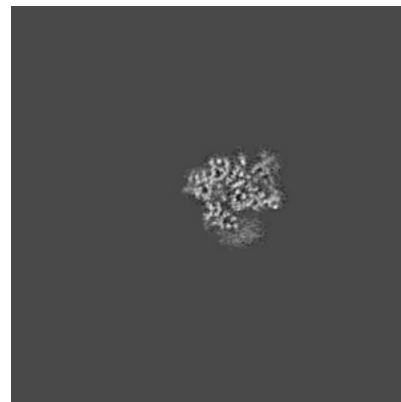
6.3.1 Primary map



X Index: 228



Y Index: 223

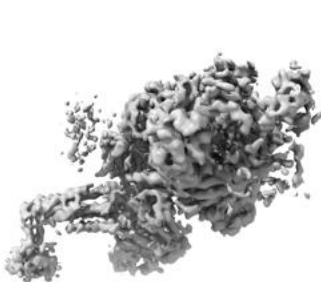


Z Index: 332

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

6.4 Orthogonal surface views [i](#)

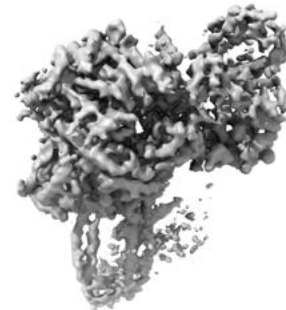
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

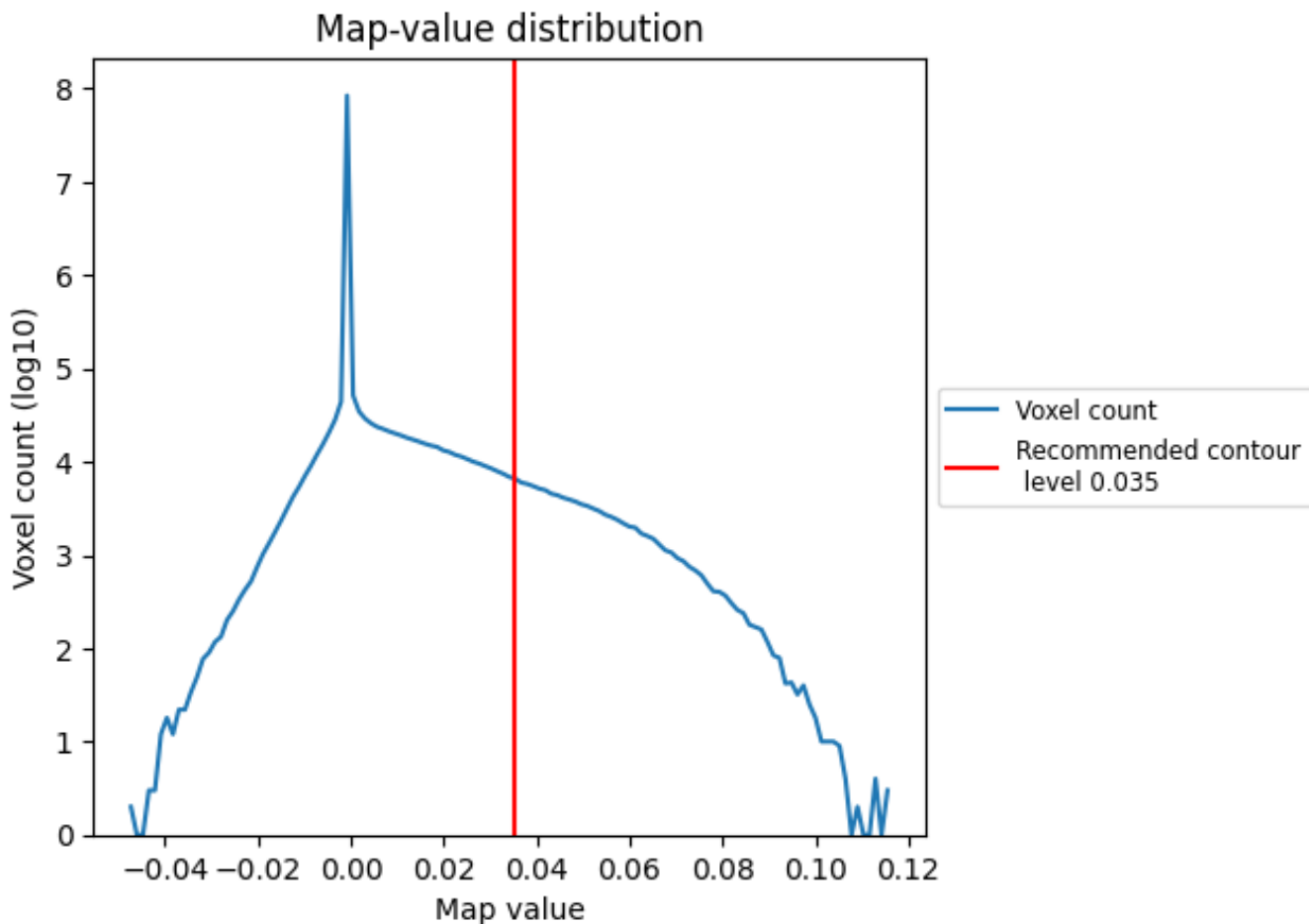
6.5 Mask visualisation

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

7 Map analysis [i](#)

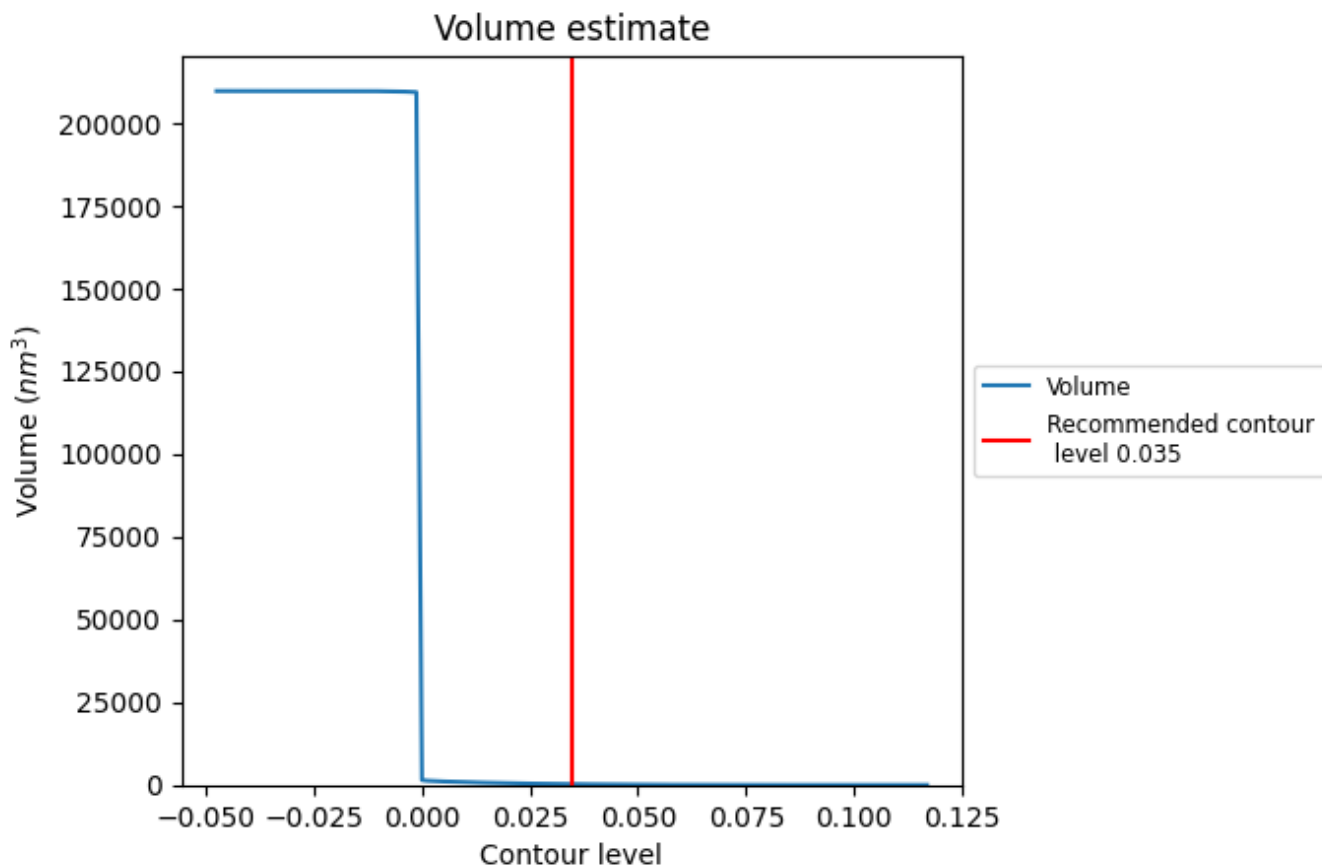
This section contains the results of statistical analysis of the map.

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.

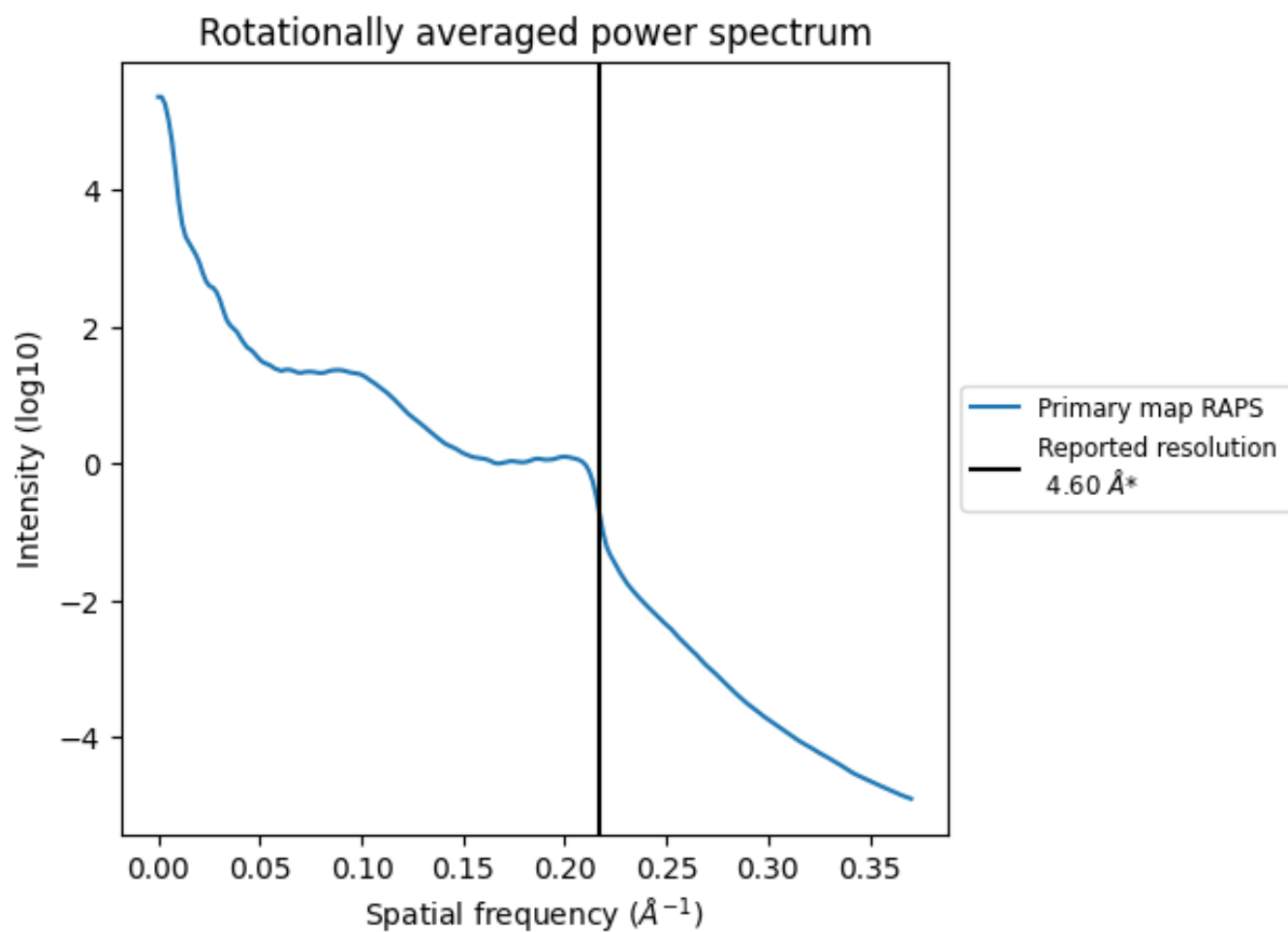
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 244 nm³; this corresponds to an approximate mass of 220 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 0.217\AA^{-1}

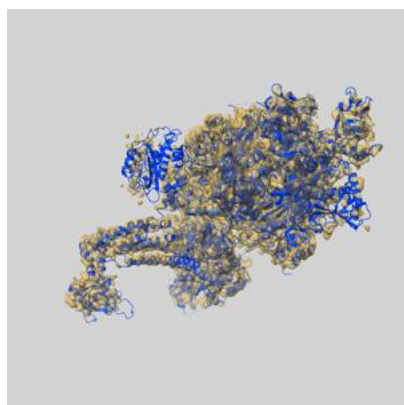
8 Fourier-Shell correlation

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

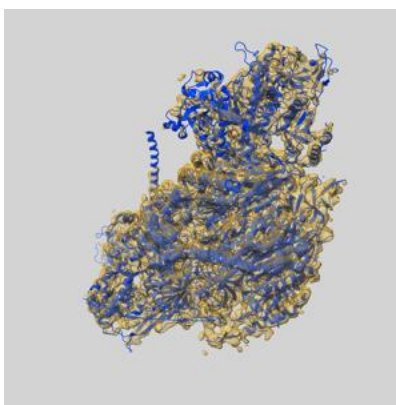
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4301 and PDB model 6FSZ. Per-residue inclusion information can be found in section 3 on page 9.

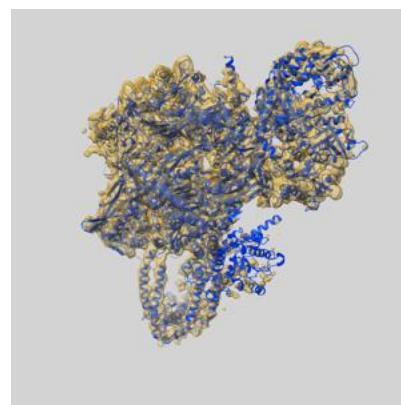
9.1 Map-model overlay [i](#)



X



Y



Z

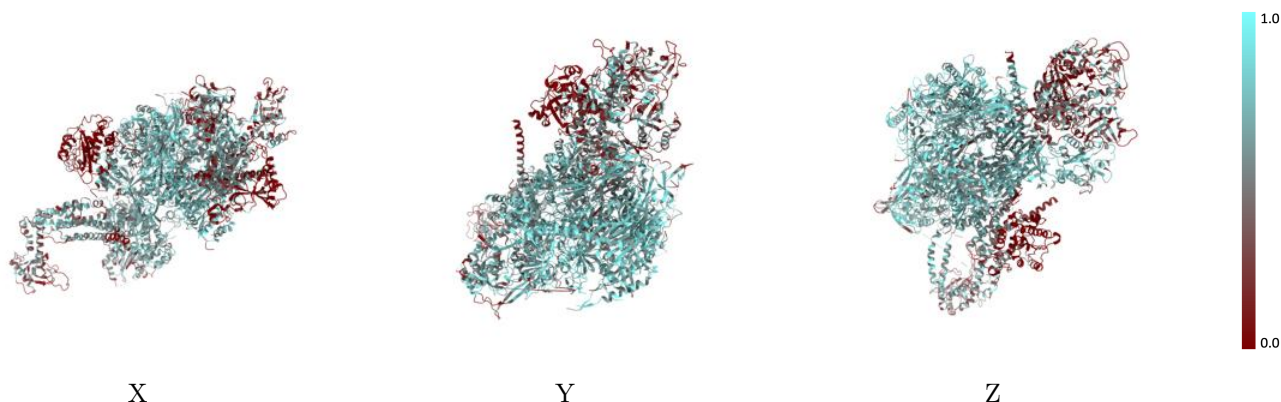
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



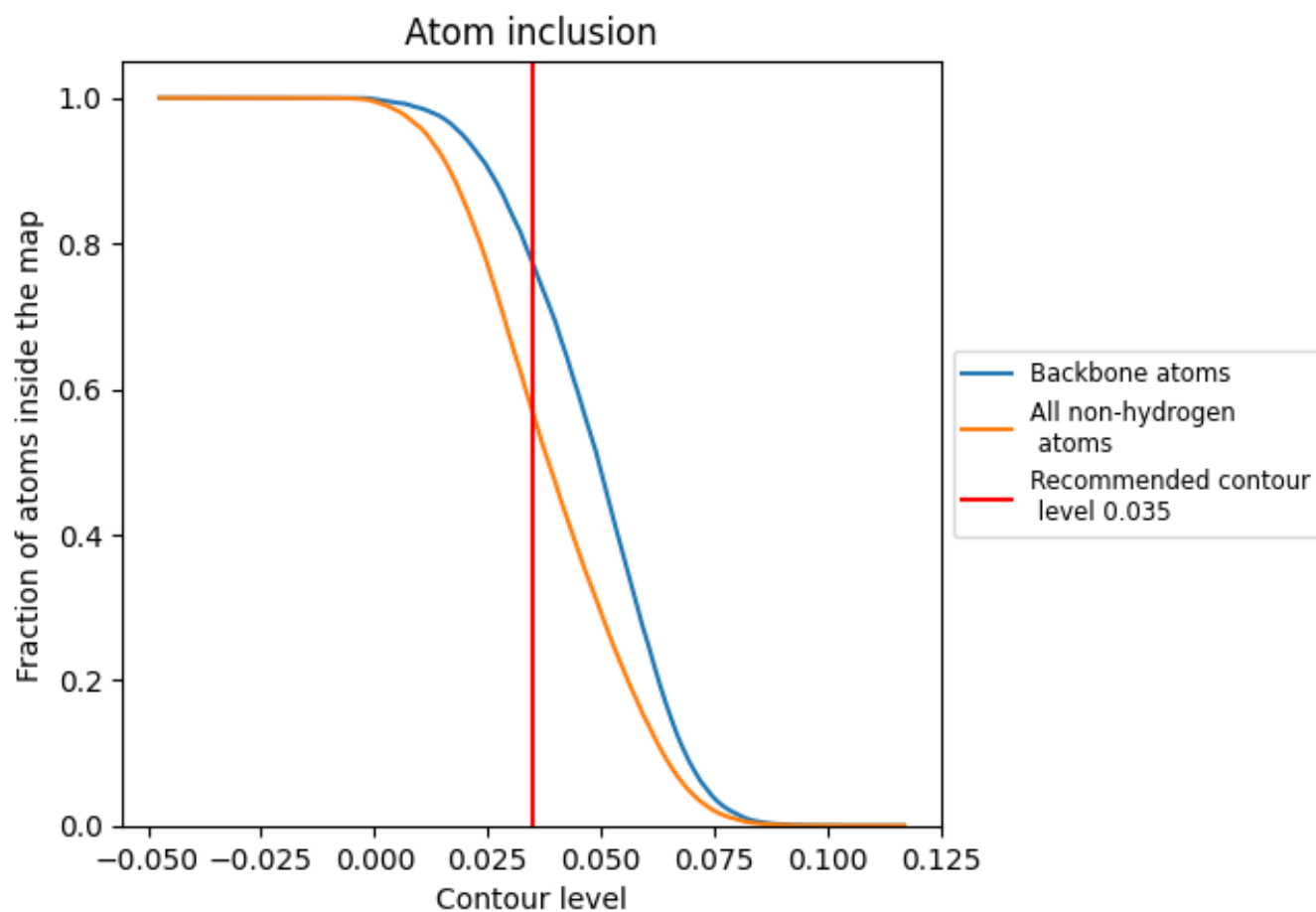
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 57% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5659	 0.2830
2	 0.6217	 0.3030
AA	 0.6860	 0.3290
BB	 0.6759	 0.3310
CC	 0.6773	 0.3090
DD	 0.7114	 0.3230
EE	 0.6841	 0.3220
FF	 0.6912	 0.3140
GG	 0.7038	 0.3170
HH	 0.6394	 0.3220
II	 0.7064	 0.3230
JJ	 0.3907	 0.2410
KK	 0.3268	 0.2140
LL	 0.4243	 0.2320
MM	 0.5551	 0.2630
NN	 0.4853	 0.3000

