Full wwPDB EM Validation Report (i)

Sep 9, 2026 – 09:44 pm BST

PDB ID	:	6GEN / pdb_00006gen
EMDB ID	:	EMD-4396
Title	:	Chromatin remodeller-nucleosome complex at 4.5 A resolution.
Authors	:	Willhoft, O.; Chua, E.Y.D.; Wilkinson, M.; Wigley, D.B.
Deposited on	:	2018-04-27
Resolution	:	3.60 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 (i) 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 (i)) were used in the production of this report:

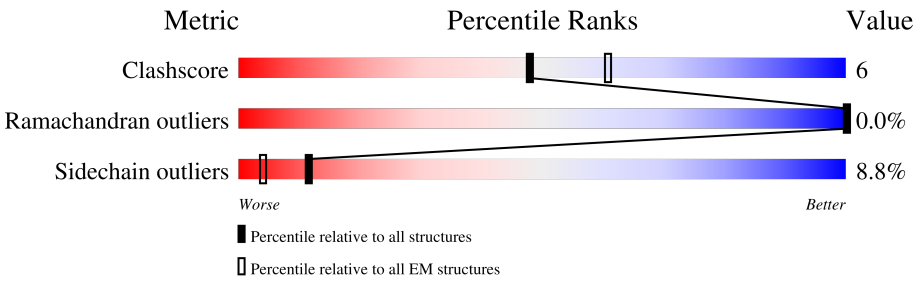
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

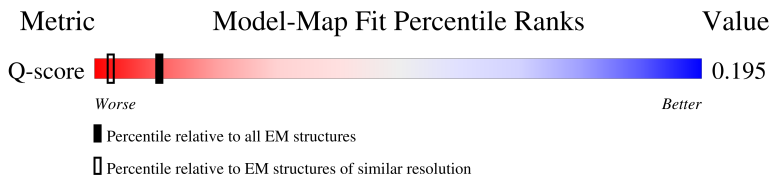
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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 <=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	Z	131	8% / 100%
2	A	136	59% / 12% / • / 29%
2	B	136	• / 60% / 11% / • / 29%
3	C	103	• / 66% / 12% / • / 20%

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Mol	Chain	Length	Quality of chain
3	D	103	66% 10% 22%
4	E	132	69% 8% 22%
4	F	132	70% 6% 23%
5	G	131	61% 11% 27%
5	H	131	57% 11% 31%
6	I	173	92% 8%
7	J	173	9% 83% 17%
8	M	1514	34% 10% 55%
9	R	438	78% 15% 6%
10	S	280	60% 14% 26%
11	T	463	13% 76% 18%
11	V	463	76% 16% 6%
11	X	463	24% 74% 18% 5%
12	U	471	67% 22% 9%
12	W	471	67% 21% 8%
12	Y	471	21% 70% 21% 5%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 44481 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 Vacuolar protein sorting-associated protein 72.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	Z	131	655	393	131	131	0	0

- Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	A	97	796	506	152	138	0	0
2	B	97	796	506	152	138	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLU	ASP	conflict	UNP P61830
B	123	GLU	ASP	conflict	UNP P61830

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	82	651	410	126	115	0	0
3	D	80	638	401	124	113	0	0

- Molecule 4 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	103	795	499	156	140	0	0
4	F	101	779	489	153	137	0	0

- Molecule 5 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	96	746	468	131	146	1	0	0
5	H	91	712	449	125	137	1	0	0

- Molecule 6 is a DNA chain called DNA (173-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	I	173	3525	1673	640	1039	173	0	0

- Molecule 7 is a DNA chain called DNA (173-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	J	173	3568	1687	671	1037	173	0	0

- Molecule 8 is a protein called Helicase SWR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	M	688	5398	3438	960	974	26	0	0

- Molecule 9 is a protein called Actin-like protein ARP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	R	411	3335	2156	544	619	16	0	0

- Molecule 10 is a protein called Vacuolar protein sorting-associated protein 71.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	S	208	1695	1071	302	312	10	0	0

- Molecule 11 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	T	443	3391	2140	584	657	10	0	0

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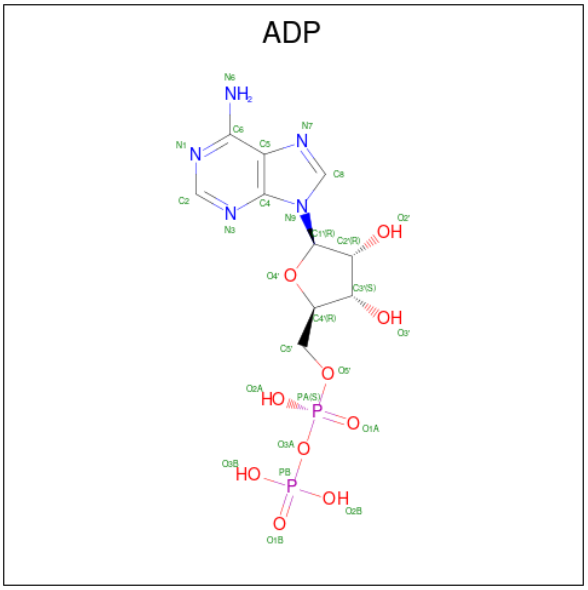
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	V	434	3336	2107	574	645	10	0	0
11	X	442	3397	2144	584	659	10	0	0

- Molecule 12 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	U	430	3299	2063	570	655	11	0	0
12	W	433	3325	2085	572	657	11	0	0
12	Y	447	3410	2133	590	675	12	0	0

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	M	1	27	10	5	10	2	0
13	R	1	27	10	5	10	2	0
13	T	1	27	10	5	10	2	0
13	U	1	27	10	5	10	2	0

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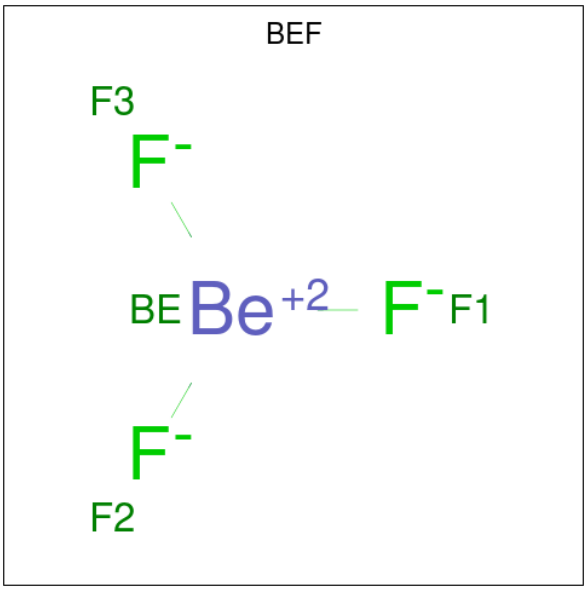
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	V	1	27	10	5	10	2	0
13	W	1	27	10	5	10	2	0
13	X	1	27	10	5	10	2	0
13	Y	1	27	10	5	10	2	0

- Molecule 14 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
14	M	1	4	1	3	0
14	R	1	4	1	3	0

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
15	M	1	1	1	0
15	R	1	1	1	0
15	U	2	2	2	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
15	V	1	1	1	0
			Total	Mg	
15	W	1	1	1	0
			Total	Mg	
15	Y	2	2	2	0

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

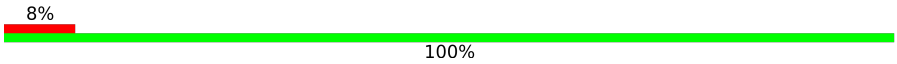
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
16	S	2	2	2	0

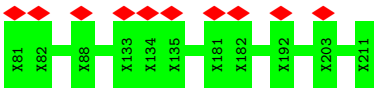
3 Residue-property plots (i)

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: Vacuolar protein sorting-associated protein 72

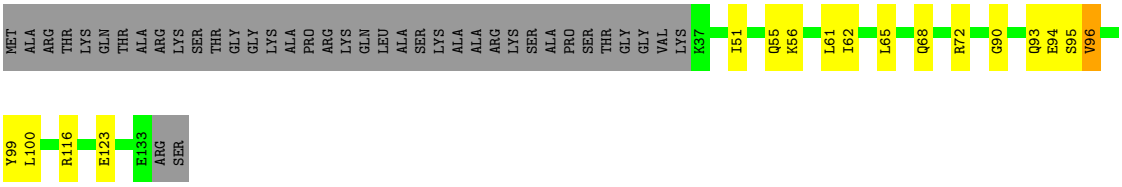
Chain Z:





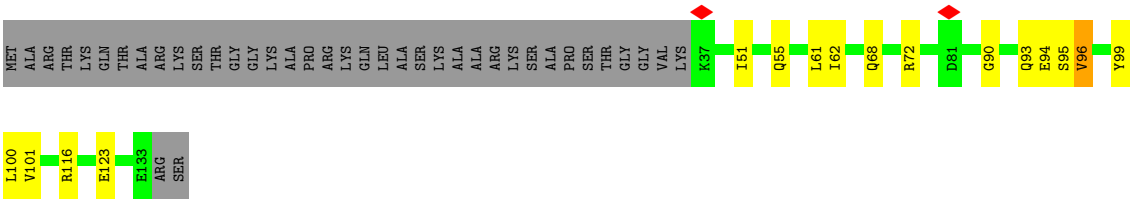
• Molecule 2: Histone H3

Chain A:



• Molecule 2: Histone H3

Chain B:

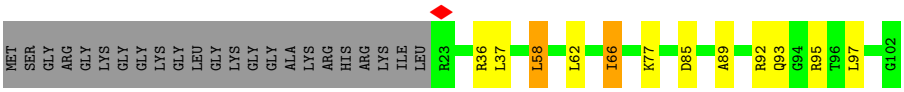


• Molecule 3: Histone H4

Chain C:

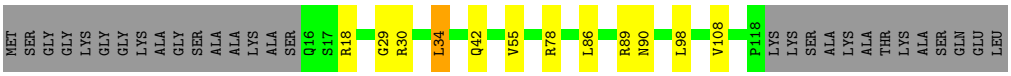
• Molecule 3: Histone H4

Chain D:



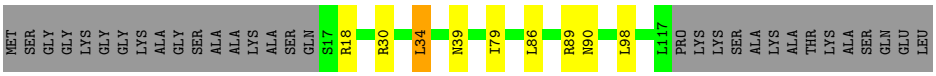
• Molecule 4: Histone H2A.1

Chain E:



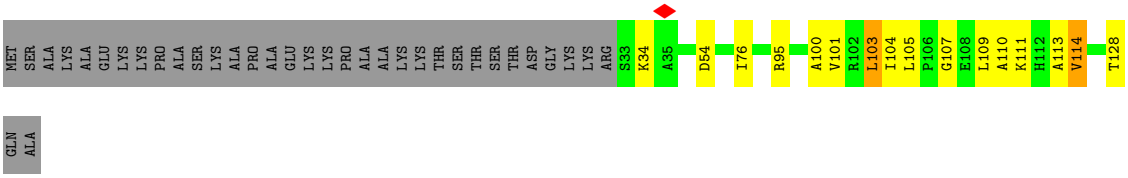
• Molecule 4: Histone H2A.1

Chain F:



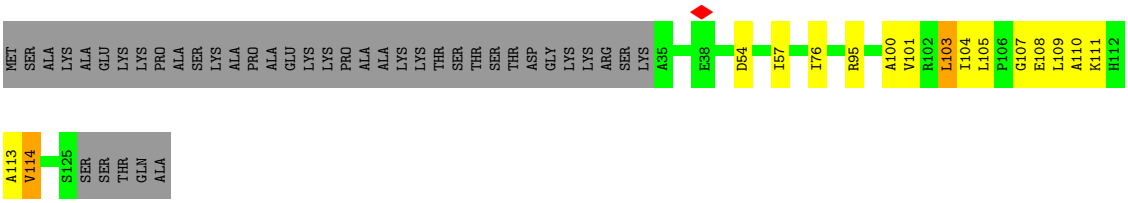
• Molecule 5: Histone H2B.1

Chain G:



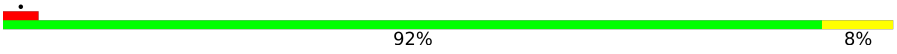
• Molecule 5: Histone H2B.1

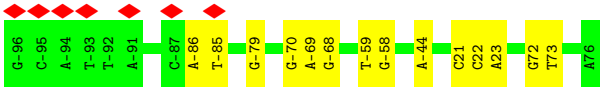
Chain H:



• Molecule 6: DNA (173-MER)

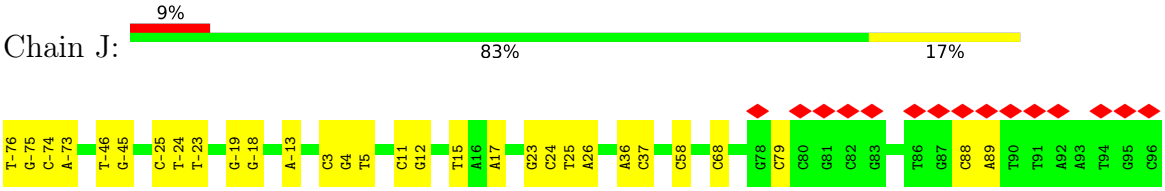
Chain I:





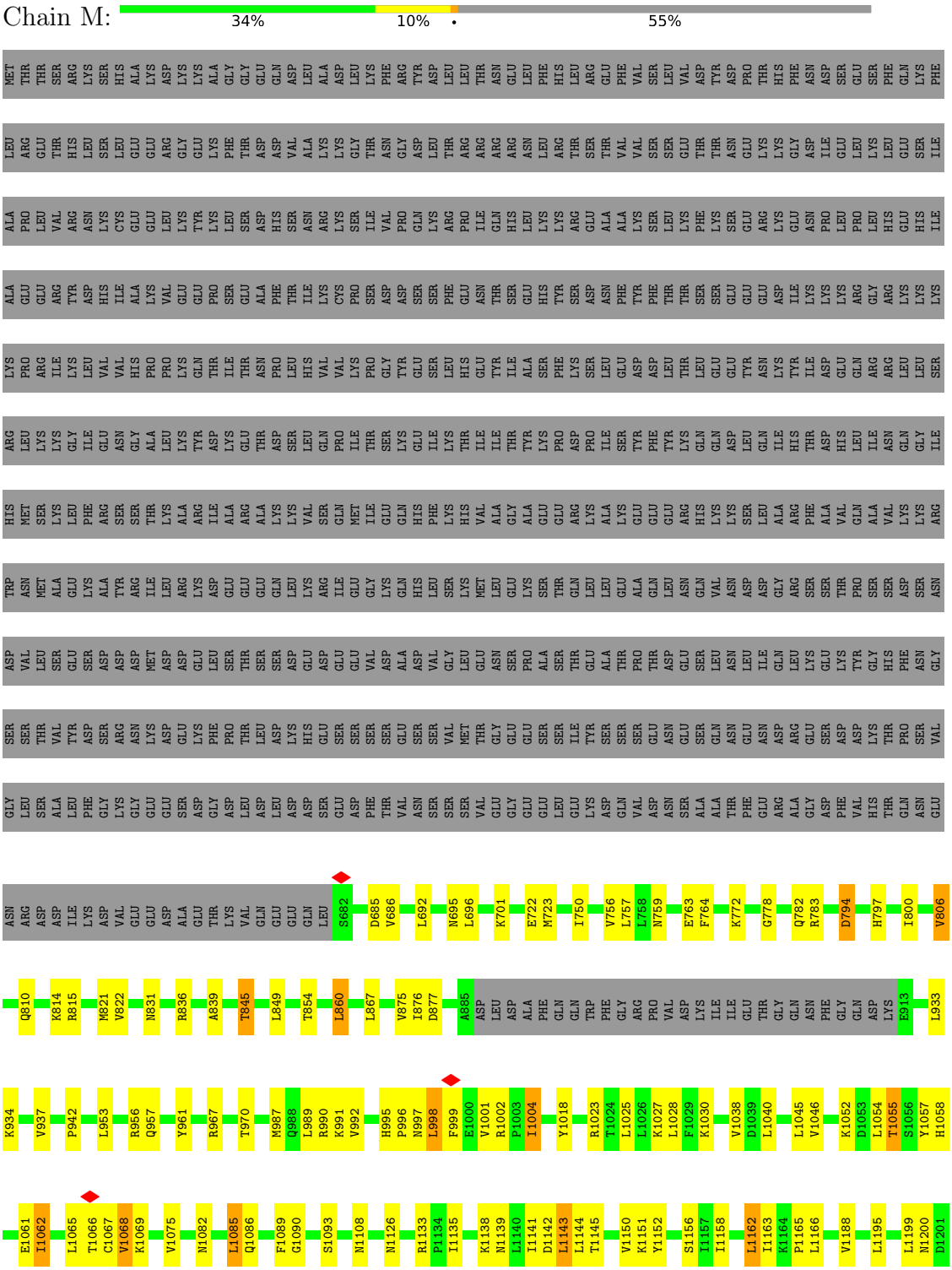
• Molecule 7: DNA (173-MER)

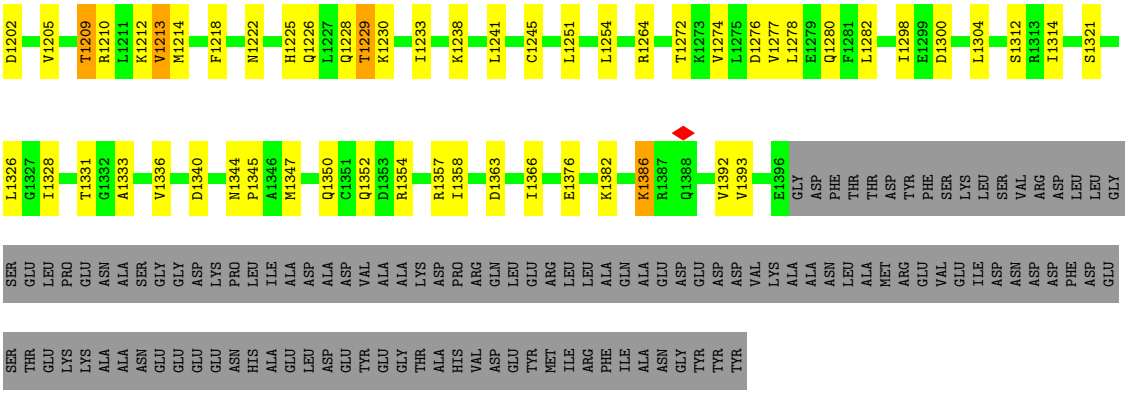
Chain J:



• Molecule 8: Helicase SWR1

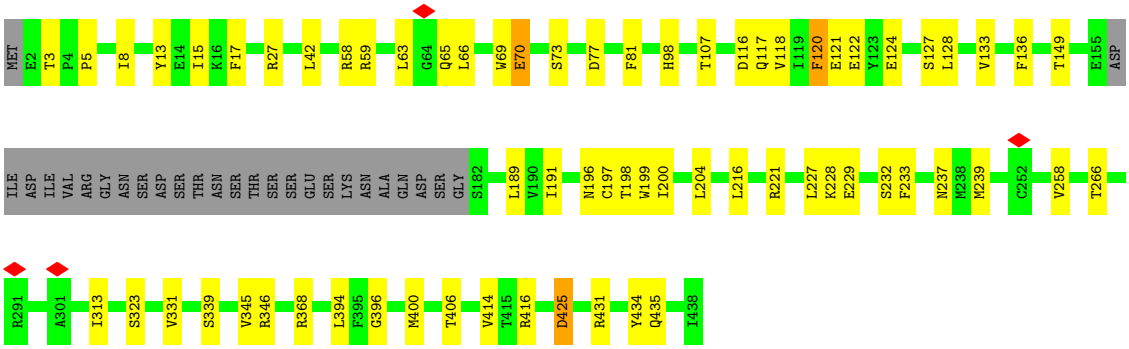
Chain M:





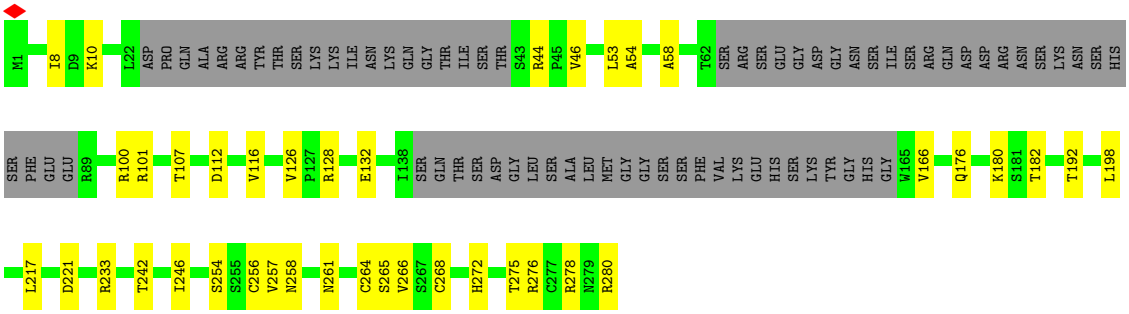
• Molecule 9: Actin-like protein ARP6

Chain R:



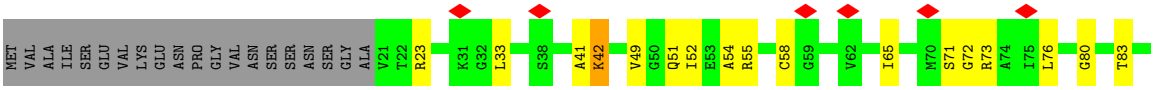
• Molecule 10: Vacuolar protein sorting-associated protein 71

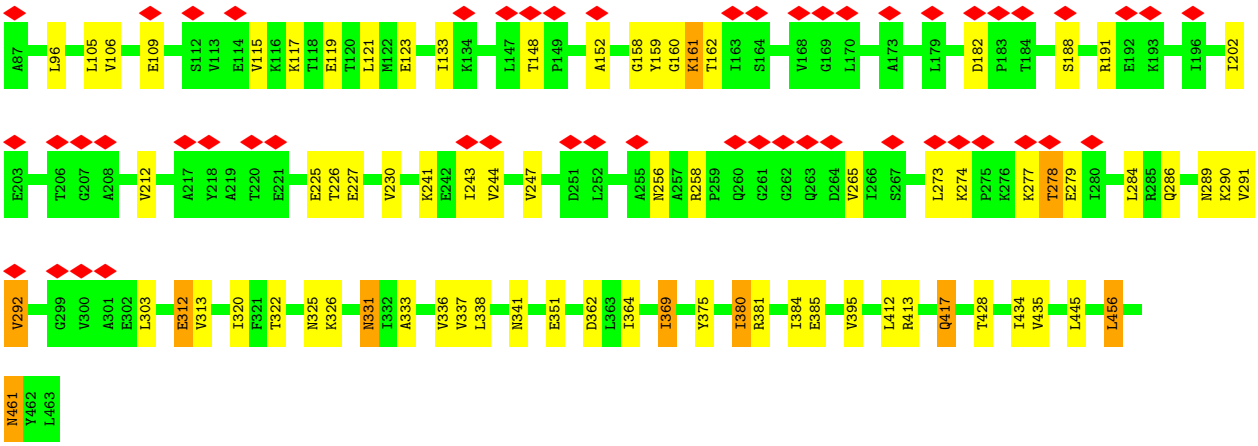
Chain S:



• Molecule 11: RuvB-like protein 1

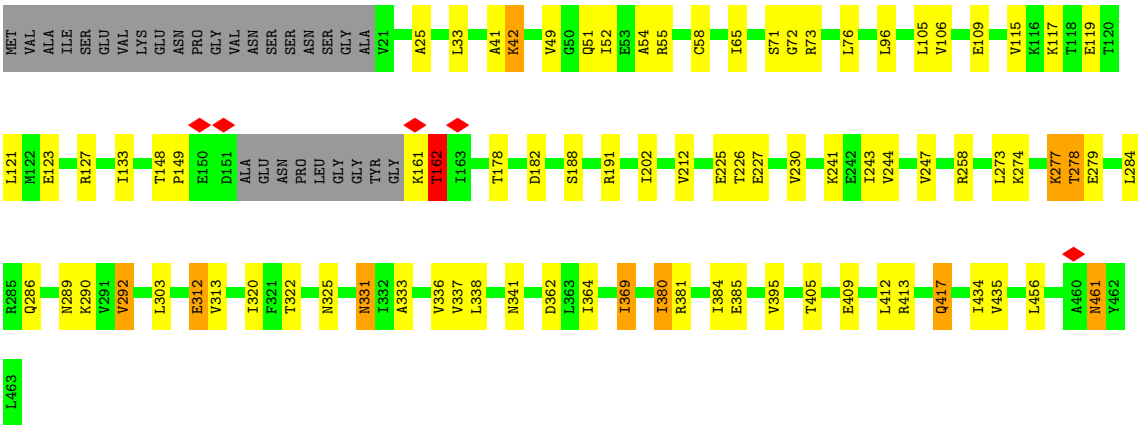
Chain T:





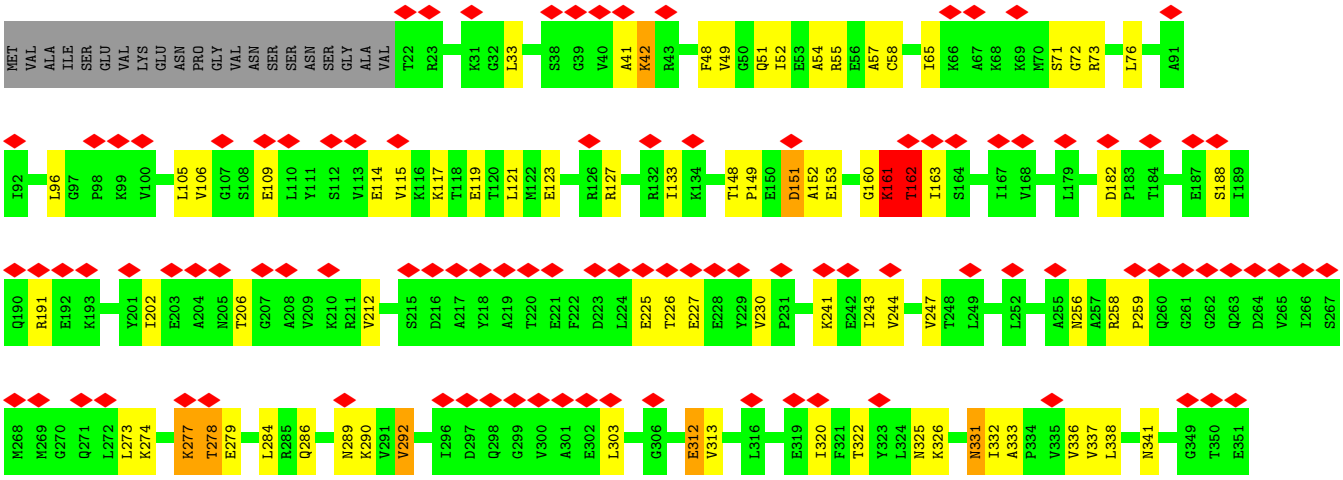
• Molecule 11: RuvB-like protein 1

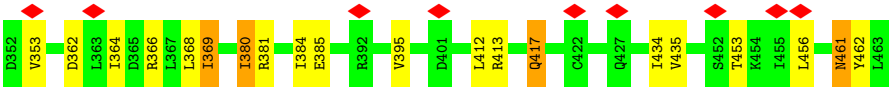
Chain V:



• Molecule 11: RuvB-like protein 1

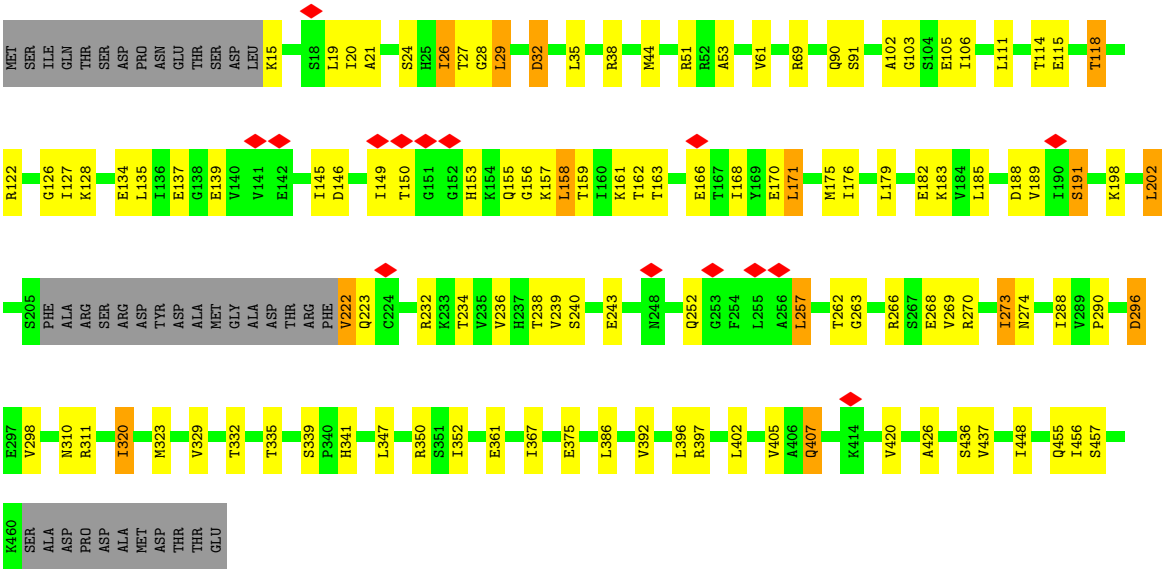
Chain X:





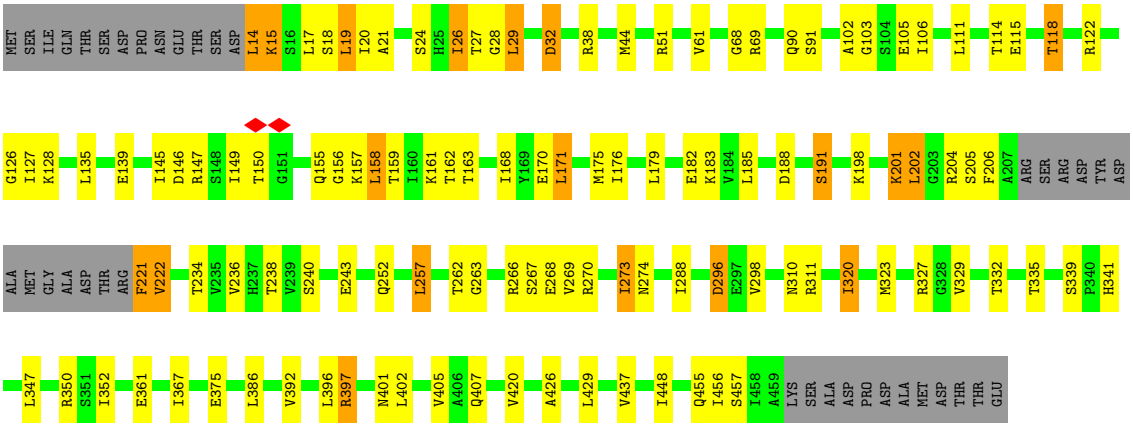
• Molecule 12: RuvB-like protein 2

Chain U:



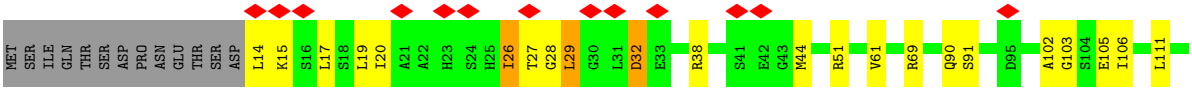
• Molecule 12: RuvB-like protein 2

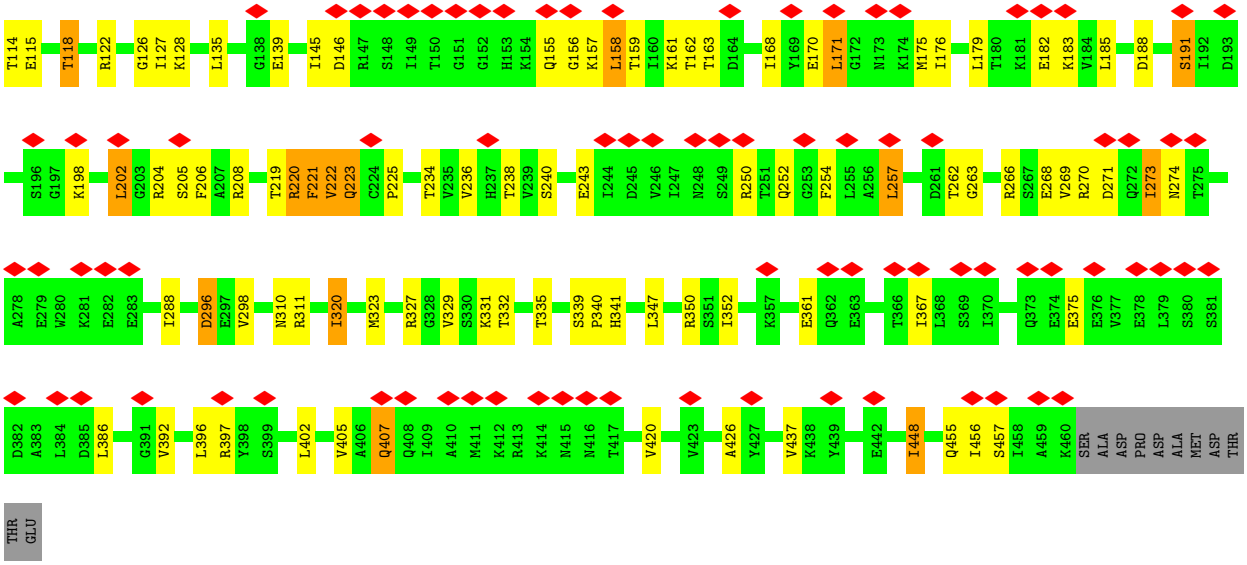
Chain W:



• Molecule 12: RuvB-like protein 2

Chain Y:




T114 E115 T118 R122 G126 I127 K128 L135 G138 E139 I145 D146 R147 S148 I149 T150 G151 G152 H153 K154 Q155 G156 K157 L158 T159 I160 K161 T162 T163 D164 I168 Y169 E170 L171 G172 N173 K174 M175 I176 L179 T180 K181 E182 K183 V184 L185 D188 S191 I192 D193
S196 G197 K198 L202 G203 R204 S205 F206 A207 R208 T219 R220 F221 V222 Q223 C224 P225 T234 V235 V236 H237 T238 V239 S240 E243 I244 D245 V246 I247 N248 S249 R250 T251 Q252 G253 F254 L255 A256 L257 D261 T262 G263 R266 S267 E268 V269 R270 D271 Q272 I273 N274 T275
A278 E279 W280 K281 E282 E283 I288 D296 E297 V298 N310 R311 I320 M323 R327 G328 V329 S330 K331 T332 T335 S339 P340 H341 L347 R350 S351 I352 K357 E361 Q362 E363 T366 I367 L368 S369 I370 Q373 E374 E375 E376 V377 E378 L379 S380 S381
D382 A383 L384 D385 L386 G391 V392 L396 R397 Y398 S399 L402 V405 A406 Q407 Q408 I409 A410 M411 K412 R413 K414 N415 N416 T417 V420 V423 A426 Y427 V437 K438 Y439 E442 I448 Q455 I456 S457 I458 A459 K460 SER ALA ASP PRO ASP ALA MET ASP THR
THR GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98529	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 ($e^-/Å^2$)	1.71794871794872	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.207	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0359	Depositor
Map size (Å)	426.24, 426.24, 426.24	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	$\#\|Z\|>5$
2	A	0.16	0/807	0.41	0/1081
2	B	0.15	0/807	0.41	0/1081
3	C	0.19	0/658	0.44	0/880
3	D	0.19	0/645	0.44	0/862
4	E	0.15	0/806	0.39	0/1091
4	F	0.15	0/789	0.39	0/1067
5	G	0.16	0/756	0.40	0/1017
5	H	0.15	0/722	0.38	0/972
6	I	0.20	0/3949	0.47	0/6087
7	J	0.20	0/4007	0.42	0/6188
8	M	0.19	0/5495	0.50	2/7442 (0.0%)
9	R	0.15	0/3429	0.39	2/4650 (0.0%)
10	S	0.21	1/1722 (0.1%)	0.41	0/2320
11	T	0.18	0/3433	0.47	0/4646
11	V	0.17	0/3375	0.45	0/4565
11	X	0.19	0/3439	0.49	0/4652
12	U	0.16	0/3333	0.45	0/4492
12	W	0.17	0/3361	0.45	0/4530
12	Y	0.18	0/3447	0.49	0/4649
All	All	0.18	1/44980 (0.0%)	0.45	4/62272 (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
8	M	0	2
11	T	0	4
11	V	0	2
11	X	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	U	0	1
12	W	0	3
12	Y	0	3
All	All	0	20

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	S	116	VAL	C-N	5.82	1.40	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	R	136	PHE	CA-C-N	6.38	124.26	120.24
9	R	136	PHE	C-N-CA	6.38	124.26	120.24
8	M	998	LEU	CA-C-N	5.38	135.68	126.32
8	M	998	LEU	C-N-CA	5.38	135.68	126.32

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	M	1067	CYS	Peptide
8	M	1344	ASN	Peptide
11	T	152	ALA	Peptide
11	T	160	GLY	Peptide
11	T	161	LYS	Peptide
11	T	162	THR	Peptide
12	U	222	VAL	Peptide
11	V	161	LYS	Peptide
11	V	162	THR	Peptide
12	W	205	SER	Mainchain
12	W	221	PHE	Peptide
12	W	222	VAL	Peptide
11	X	151	ASP	Peptide
11	X	152	ALA	Peptide
11	X	160	GLY	Peptide
11	X	161	LYS	Peptide
11	X	162	THR	Peptide
12	Y	205	SER	Mainchain
12	Y	206	PHE	Peptide

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Mol	Chain	Res	Type	Group
12	Y	222	VAL	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	Z	655	0	147	0	0
2	A	796	0	841	11	0
2	B	796	0	841	10	0
3	C	651	0	690	9	0
3	D	638	0	677	8	0
4	E	795	0	834	9	0
4	F	779	0	819	6	0
5	G	746	0	771	12	0
5	H	712	0	736	11	0
6	I	3525	0	1941	11	0
7	J	3568	0	1940	21	0
8	M	5398	0	5352	86	0
9	R	3335	0	3256	37	0
10	S	1695	0	1746	27	0
11	T	3391	0	3513	48	0
11	V	3336	0	3475	38	0
11	X	3397	0	3533	55	0
12	U	3299	0	3387	52	0
12	W	3325	0	3413	56	0
12	Y	3410	0	3466	59	0
13	M	27	0	12	3	0
13	R	27	0	12	0	0
13	T	27	0	12	0	0
13	U	27	0	12	0	0
13	V	27	0	12	0	0
13	W	27	0	12	0	0
13	X	27	0	12	2	0
13	Y	27	0	12	0	0
14	M	4	0	0	0	0
14	R	4	0	0	0	0
15	M	1	0	0	0	0
15	R	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	U	2	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	2	0	0	0	0
16	S	2	0	0	0	0
All	All	44481	0	41474	484	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (484) 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)
12:W:269:VAL:O	12:W:273:ILE:HB	1.65	0.97
12:U:269:VAL:O	12:U:273:ILE:HB	1.65	0.95
12:Y:269:VAL:O	12:Y:273:ILE:HB	1.65	0.93
3:C:62:LEU:O	3:C:66:ILE:HB	1.70	0.92
3:D:62:LEU:O	3:D:66:ILE:HB	1.70	0.92
10:S:176:GLN:O	10:S:180:LYS:HB2	1.70	0.90
9:R:116:ASP:O	9:R:120:PHE:HB2	1.73	0.87
9:R:77:ASP:O	9:R:81:PHE:HB2	1.74	0.86
8:M:1058:HIS:O	8:M:1062:ILE:HB	1.82	0.80
11:X:413:ARG:O	11:X:417:GLN:HB2	1.82	0.80
11:V:413:ARG:O	11:V:417:GLN:HB2	1.82	0.80
11:T:413:ARG:O	11:T:417:GLN:HB2	1.82	0.80
8:M:1089:PHE:O	8:M:1093:SER:HB3	1.85	0.77
12:W:175:MET:O	12:W:179:LEU:HB2	1.86	0.76
12:U:175:MET:O	12:U:179:LEU:HB2	1.86	0.74
9:R:118:VAL:O	9:R:122:GLU:HB2	1.88	0.74
12:Y:175:MET:O	12:Y:179:LEU:HB2	1.86	0.74
8:M:1133:ARG:HD2	12:Y:220:ARG:HB3	1.73	0.69
8:M:1057:TYR:O	8:M:1061:GLU:HB2	1.92	0.69
12:W:17:LEU:O	11:X:331:ASN:ND2	2.27	0.68
12:W:397:ARG:HG2	11:X:366:ARG:HA	1.79	0.64
11:T:286:GLN:O	11:T:290:LYS:HB2	1.98	0.64
5:G:110:ALA:O	5:G:114:VAL:HB	1.98	0.63
11:V:286:GLN:O	11:V:290:LYS:HB2	1.97	0.63
11:X:286:GLN:O	11:X:290:LYS:HB2	1.98	0.63
8:M:875:VAL:HG13	8:M:877:ASP:H	1.63	0.63
5:H:110:ALA:O	5:H:114:VAL:HB	1.98	0.62
11:T:413:ARG:HD3	12:U:350:ARG:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:119:GLU:O	11:V:123:GLU:HB2	1.99	0.62
12:W:327:ARG:HH22	11:X:353:VAL:HG13	1.65	0.62
5:H:108:GLU:HG2	10:S:44:ARG:HH11	1.64	0.62
11:T:119:GLU:O	11:T:123:GLU:HB2	1.99	0.62
11:V:127:ARG:NH2	12:W:267:SER:OG	2.32	0.62
12:W:18:SER:HA	11:X:331:ASN:HD22	1.65	0.61
11:X:119:GLU:O	11:X:123:GLU:HB2	1.99	0.61
11:X:462:TYR:HD1	12:Y:327:ARG:HA	1.65	0.61
12:W:126:GLY:HA2	12:W:240:SER:HA	1.83	0.61
11:X:331:ASN:OD1	11:X:331:ASN:N	2.34	0.60
12:U:126:GLY:HA2	12:U:240:SER:HA	1.83	0.60
12:Y:126:GLY:HA2	12:Y:240:SER:HA	1.83	0.60
8:M:806:VAL:O	8:M:810:GLN:HB3	2.02	0.60
11:X:149:PRO:HB3	11:X:162:THR:HG21	1.84	0.60
9:R:98:HIS:HD2	9:R:127:SER:HB2	1.67	0.60
11:V:109:GLU:HG2	12:W:114:THR:HG21	1.84	0.59
11:T:331:ASN:N	11:T:331:ASN:OD1	2.34	0.59
6:I:-79:DG:N2	7:J:79:DC:C2	2.70	0.59
11:T:313:VAL:HG21	11:T:338:LEU:HB3	1.85	0.59
11:V:331:ASN:OD1	11:V:331:ASN:N	2.34	0.59
9:R:228:LYS:HD2	9:R:239:MET:HA	1.84	0.59
11:V:313:VAL:HG21	11:V:338:LEU:HB3	1.85	0.59
11:X:453:THR:HG22	12:Y:341:HIS:HB2	1.85	0.59
8:M:1023:ARG:HG2	8:M:1027:LYS:HE2	1.85	0.59
11:T:54:ALA:O	11:T:58:CYS:HB2	2.03	0.58
11:V:149:PRO:HB3	11:V:162:THR:HG21	1.85	0.58
11:T:23:ARG:HH12	12:U:290:PRO:HB3	1.68	0.58
11:X:54:ALA:O	11:X:58:CYS:HB2	2.03	0.58
2:A:56:LYS:HG2	10:S:53:LEU:HD21	1.84	0.58
11:V:54:ALA:O	11:V:58:CYS:HB2	2.03	0.58
11:X:313:VAL:HG21	11:X:338:LEU:HB3	1.85	0.58
10:S:100:ARG:HH12	10:S:132:GLU:HA	1.69	0.58
12:U:127:ILE:HG12	12:U:288:ILE:HG22	1.86	0.58
12:W:127:ILE:HG12	12:W:288:ILE:HG22	1.86	0.57
9:R:5:PRO:HB3	9:R:98:HIS:HB2	1.86	0.57
11:T:395:VAL:HG22	11:T:434:ILE:HD12	1.87	0.57
11:T:445:LEU:HB3	12:U:53:ALA:HB2	1.87	0.56
12:Y:127:ILE:HG12	12:Y:288:ILE:HG22	1.86	0.56
8:M:778:GLY:HA3	8:M:782:GLN:HB2	1.88	0.56
11:X:395:VAL:HG22	11:X:434:ILE:HD12	1.87	0.56
3:D:77:LYS:HZ3	5:G:95:ARG:HH22	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:256:CYS:SG	10:S:257:VAL:N	2.76	0.56
11:X:42:LYS:O	11:X:55:ARG:NH2	2.39	0.56
8:M:995:HIS:ND1	8:M:1245:CYS:SG	2.79	0.55
9:R:228:LYS:O	9:R:232:SER:HB3	2.05	0.55
11:T:42:LYS:O	11:T:55:ARG:NH2	2.39	0.55
11:V:395:VAL:HG22	11:V:434:ILE:HD12	1.87	0.55
9:R:58:ARG:HB3	10:S:166:VAL:HG13	1.88	0.55
12:Y:128:LYS:HG2	12:Y:238:THR:HG22	1.88	0.55
12:W:128:LYS:HG2	12:W:238:THR:HG22	1.88	0.55
8:M:794:ASP:OD1	8:M:794:ASP:N	2.40	0.55
9:R:323:SER:O	10:S:101:ARG:NH1	2.40	0.55
12:U:128:LYS:HG2	12:U:238:THR:HG22	1.88	0.55
8:M:822:VAL:HG12	8:M:849:LEU:HB3	1.88	0.54
11:T:461:ASN:N	11:T:461:ASN:OD1	2.41	0.54
11:V:42:LYS:O	11:V:55:ARG:NH2	2.39	0.54
12:W:19:LEU:HD23	11:X:71:SER:HB2	1.88	0.54
5:G:107:GLY:O	5:G:111:LYS:HB2	2.08	0.54
11:V:380:ILE:HG13	11:V:412:LEU:HD13	1.88	0.54
11:V:41:ALA:HB3	11:V:52:ILE:HG23	1.90	0.54
12:W:115:GLU:OE2	12:W:270:ARG:NH2	2.41	0.54
11:T:380:ILE:HG13	11:T:412:LEU:HD13	1.88	0.54
11:V:461:ASN:N	11:V:461:ASN:OD1	2.40	0.54
8:M:1062:ILE:HD11	12:Y:220:ARG:HH21	1.73	0.54
12:U:38:ARG:O	12:U:51:ARG:NH2	2.40	0.54
5:H:107:GLY:O	5:H:111:LYS:HB2	2.08	0.54
8:M:695:ASN:O	13:M:1601:ADP:N6	2.41	0.54
11:X:312:GLU:OE2	11:X:341:ASN:ND2	2.41	0.54
11:X:380:ILE:HG13	11:X:412:LEU:HD13	1.88	0.54
2:B:51:ILE:O	2:B:55:GLN:HB2	2.08	0.53
8:M:1264:ARG:HB2	8:M:1333:ALA:HA	1.90	0.53
12:U:115:GLU:OE2	12:U:270:ARG:NH2	2.41	0.53
10:S:258:ASN:HD22	10:S:280:ARG:HA	1.73	0.53
12:Y:157:LYS:HG2	12:Y:170:GLU:HG2	1.90	0.53
2:A:51:ILE:O	2:A:55:GLN:HB2	2.08	0.53
11:T:41:ALA:HB3	11:T:52:ILE:HG23	1.90	0.53
12:W:157:LYS:HG2	12:W:170:GLU:HG2	1.90	0.53
11:X:289:ASN:HA	11:X:292:VAL:HB	1.90	0.53
8:M:1264:ARG:NH1	8:M:1314:ILE:O	2.42	0.53
11:T:289:ASN:HA	11:T:292:VAL:HB	1.90	0.53
11:X:461:ASN:OD1	11:X:461:ASN:N	2.40	0.53
4:E:55:VAL:HG21	5:G:101:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:198:THR:HB	9:R:216:LEU:HB2	1.91	0.53
11:X:413:ARG:NH1	13:X:501:ADP:O3A	2.41	0.53
9:R:197:CYS:SG	9:R:199:TRP:NE1	2.81	0.53
11:X:41:ALA:HB3	11:X:52:ILE:HG23	1.90	0.53
8:M:821:MET:HG2	8:M:845:THR:HG21	1.91	0.53
10:S:264:CYS:SG	10:S:265:SER:N	2.82	0.53
11:V:289:ASN:HA	11:V:292:VAL:HB	1.90	0.53
12:W:401:ASN:HD22	11:X:368:LEU:HD21	1.74	0.53
12:U:157:LYS:HG2	12:U:170:GLU:HG2	1.90	0.53
11:X:117:LYS:HD2	11:X:320:ILE:HD11	1.91	0.53
12:Y:38:ARG:O	12:Y:51:ARG:NH2	2.40	0.53
8:M:1200:ASN:O	8:M:1210:ARG:NH1	2.42	0.52
7:J:-19:DG:H5”	8:M:1272:THR:HG23	1.91	0.52
9:R:58:ARG:NH1	10:S:112:ASP:OD1	2.43	0.52
11:V:312:GLU:OE2	11:V:341:ASN:ND2	2.41	0.52
8:M:957:GLN:HE21	8:M:996:PRO:HD3	1.74	0.52
8:M:1210:ARG:O	8:M:1214:MET:HB2	2.09	0.52
9:R:258:VAL:O	9:R:368:ARG:NH1	2.42	0.52
11:T:312:GLU:OE2	11:T:341:ASN:ND2	2.41	0.52
12:U:311:ARG:O	12:U:311:ARG:NH2	2.42	0.52
12:Y:115:GLU:OE2	12:Y:270:ARG:NH2	2.41	0.52
3:D:77:LYS:HG2	5:G:95:ARG:HH12	1.75	0.52
8:M:1156:SER:HB3	11:X:206:THR:HB	1.91	0.52
10:S:275:THR:O	10:S:278:ARG:NH1	2.42	0.52
12:W:38:ARG:O	12:W:51:ARG:NH2	2.40	0.52
2:B:116:ARG:NH2	2:B:123:GLU:OE2	2.43	0.52
11:T:117:LYS:HD2	11:T:320:ILE:HD11	1.91	0.52
8:M:957:GLN:O	8:M:961:TYR:HB2	2.09	0.51
3:C:40:ARG:HH21	4:E:108:VAL:HG13	1.76	0.51
11:X:114:GLU:OE2	12:Y:250:ARG:NH1	2.43	0.51
9:R:117:GLN:O	9:R:121:GLU:HB2	2.10	0.51
12:Y:61:VAL:HG22	12:Y:320:ILE:HG21	1.92	0.51
12:Y:204:ARG:H	12:Y:221:PHE:HA	1.75	0.51
12:W:139:GLU:N	12:W:161:LYS:O	2.44	0.51
2:A:116:ARG:NH2	2:A:123:GLU:OE2	2.43	0.51
8:M:1202:ASP:N	8:M:1202:ASP:OD1	2.43	0.51
2:B:68:GLN:HE21	2:B:72:ARG:HE	1.58	0.51
8:M:1336:VAL:HB	8:M:1366:ILE:HG23	1.92	0.51
11:T:278:THR:OG1	11:T:279:GLU:N	2.44	0.51
11:V:71:SER:O	11:V:73:ARG:NH1	2.44	0.51
11:V:117:LYS:HD2	11:V:320:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:1222:ASN:ND2	8:M:1228:GLN:OE1	2.44	0.51
9:R:339:SER:OG	10:S:233:ARG:NH2	2.43	0.51
6:I:-59:DT:H1'	8:M:815:ARG:HH21	1.76	0.51
8:M:778:GLY:HA3	8:M:782:GLN:HE21	1.74	0.51
11:T:71:SER:O	11:T:73:ARG:NH1	2.44	0.51
11:T:286:GLN:HG2	12:Y:17:LEU:HB3	1.93	0.51
12:U:27:THR:HA	12:U:90:GLN:HG2	1.93	0.51
2:A:68:GLN:HE21	2:A:72:ARG:HE	1.58	0.51
8:M:685:ASP:OD2	8:M:701:LYS:NZ	2.42	0.51
8:M:1139:ASN:HB3	8:M:1143:LEU:HD13	1.93	0.51
12:U:61:VAL:HG22	12:U:320:ILE:HG21	1.92	0.51
12:U:122:ARG:HH12	12:U:274:ASN:HD21	1.59	0.51
12:W:61:VAL:HG22	12:W:320:ILE:HG21	1.92	0.51
2:B:100:LEU:HD23	3:C:37:LEU:HD13	1.93	0.50
8:M:1209:THR:O	8:M:1213:VAL:HB	2.10	0.50
8:M:1382:LYS:NZ	8:M:1393:VAL:O	2.44	0.50
12:W:122:ARG:HH12	12:W:274:ASN:HD21	1.59	0.50
4:F:30:ARG:HE	7:J:-45:DG:H5'	1.77	0.50
4:F:79:ILE:HD12	5:H:57:ILE:HG12	1.93	0.50
12:W:191:SER:HB3	12:W:202:LEU:HD11	1.94	0.50
11:X:119:GLU:O	11:X:123:GLU:CB	2.59	0.50
12:Y:122:ARG:HH12	12:Y:274:ASN:HD21	1.59	0.50
8:M:1357:ARG:NH1	13:M:1601:ADP:O5'	2.45	0.50
9:R:396:GLY:O	9:R:400:MET:HB2	2.11	0.50
10:S:10:LYS:HE3	11:V:178:THR:HG21	1.93	0.50
11:X:71:SER:O	11:X:73:ARG:NH1	2.44	0.50
2:A:100:LEU:HD23	3:D:37:LEU:HD13	1.94	0.50
12:U:436:SER:HB3	11:V:369:ILE:HD12	1.93	0.50
11:V:119:GLU:O	11:V:123:GLU:CB	2.59	0.50
12:W:311:ARG:O	12:W:311:ARG:NH2	2.42	0.50
12:U:156:GLY:HA3	12:U:176:ILE:HD11	1.94	0.50
12:Y:27:THR:HA	12:Y:90:GLN:HG2	1.93	0.50
8:M:1045:LEU:O	11:T:256:ASN:ND2	2.45	0.50
8:M:1085:LEU:HD11	8:M:1108:ASN:HB3	1.94	0.50
8:M:1212:LYS:HD2	11:T:265:VAL:HG21	1.94	0.50
9:R:414:VAL:HG22	9:R:431:ARG:HH11	1.76	0.50
12:U:191:SER:HB3	12:U:202:LEU:HD11	1.93	0.50
11:T:119:GLU:O	11:T:123:GLU:CB	2.59	0.50
11:V:278:THR:OG1	11:V:279:GLU:N	2.44	0.50
2:B:90:GLY:O	2:B:94:GLU:HB2	2.12	0.49
8:M:750:ILE:HD11	8:M:800:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:156:GLY:HA3	12:W:176:ILE:HD11	1.94	0.49
12:Y:156:GLY:HA3	12:Y:176:ILE:HD11	1.94	0.49
8:M:1025:LEU:HD11	12:U:239:VAL:HG11	1.93	0.49
12:W:29:LEU:H	12:W:91:SER:HB3	1.77	0.49
5:G:101:VAL:HG13	5:G:105:LEU:HD12	1.95	0.49
5:H:101:VAL:HG13	5:H:105:LEU:HD12	1.95	0.49
7:J:-25:DC:H2"	7:J:-24:DT:H5"	1.93	0.49
8:M:956:ARG:HD2	8:M:1002:ARG:HH21	1.78	0.49
12:W:27:THR:HA	12:W:90:GLN:HG2	1.93	0.49
8:M:772:LYS:H	8:M:797:HIS:HD2	1.59	0.49
8:M:1162:LEU:O	11:X:256:ASN:ND2	2.45	0.49
11:X:278:THR:OG1	11:X:279:GLU:N	2.44	0.49
8:M:1226:GLN:O	8:M:1230:LYS:HB2	2.12	0.49
12:Y:191:SER:HB3	12:Y:202:LEU:HD11	1.94	0.49
12:Y:185:LEU:H	12:Y:188:ASP:HB2	1.78	0.49
12:W:185:LEU:H	12:W:188:ASP:HB2	1.78	0.49
12:U:29:LEU:H	12:U:91:SER:HB3	1.77	0.49
12:W:149:ILE:HG13	12:W:150:THR:HG23	1.94	0.49
2:A:90:GLY:O	2:A:94:GLU:HB2	2.12	0.49
7:J:-46:DT:H2'	7:J:-45:DG:C8	2.48	0.49
9:R:124:GLU:OE2	9:R:416:ARG:NH2	2.46	0.49
11:V:65:ILE:HD13	11:V:96:LEU:HD11	1.94	0.49
11:X:65:ILE:HD13	11:X:96:LEU:HD11	1.94	0.48
11:T:65:ILE:HD13	11:T:96:LEU:HD11	1.94	0.48
12:Y:29:LEU:H	12:Y:91:SER:HB3	1.77	0.48
8:M:1214:MET:O	8:M:1218:PHE:HB2	2.13	0.48
4:F:86:LEU:O	4:F:90:ASN:HB2	2.13	0.48
11:T:428:THR:HG21	12:U:35:LEU:HD22	1.94	0.48
8:M:1061:GLU:HB3	12:Y:202:LEU:HD23	1.94	0.48
9:R:196:ASN:OD1	9:R:221:ARG:NH1	2.47	0.48
3:C:30:THR:HG21	7:J:-13:DA:H5"	1.96	0.48
12:Y:139:GLU:N	12:Y:161:LYS:O	2.44	0.48
12:Y:311:ARG:O	12:Y:311:ARG:NH2	2.42	0.48
12:U:185:LEU:H	12:U:188:ASP:HB2	1.78	0.48
4:E:86:LEU:O	4:E:90:ASN:HB2	2.13	0.48
9:R:435:GLN:NE2	10:S:221:ASP:OD2	2.47	0.48
12:Y:223:GLN:HG2	12:Y:225:PRO:HD3	1.96	0.48
5:H:100:ALA:HA	5:H:103:LEU:HD23	1.96	0.47
8:M:1209:THR:HG23	11:T:191:ARG:HH12	1.78	0.47
12:U:139:GLU:N	12:U:161:LYS:O	2.44	0.47
12:W:429:LEU:HB3	11:X:57:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:434:TYR:OH	10:S:221:ASP:OD1	2.32	0.47
12:W:204:ARG:H	12:W:221:PHE:HA	1.79	0.47
12:Y:20:ILE:HG21	12:Y:375:GLU:HG2	1.96	0.47
8:M:759:ASN:O	8:M:763:GLU:HB2	2.14	0.47
12:U:20:ILE:HG21	12:U:375:GLU:HG2	1.96	0.47
12:Y:310:ASN:O	12:Y:350:ARG:NH1	2.47	0.47
7:J:-19:DG:H2'	7:J:-18:DG:C8	2.50	0.47
7:J:11:DC:H2'	7:J:12:DG:C8	2.49	0.47
8:M:1086:GLN:O	8:M:1090:GLY:HA3	2.14	0.47
12:U:162:THR:OG1	12:U:163:THR:N	2.47	0.47
12:Y:185:LEU:HG	12:Y:208:ARG:HB2	1.96	0.47
5:G:100:ALA:HA	5:G:103:LEU:HD23	1.96	0.47
6:I:-58:DG:O4'	8:M:815:ARG:NH2	2.48	0.47
8:M:991:LYS:HG2	8:M:997:ASN:HB2	1.97	0.47
8:M:1045:LEU:HD21	11:T:291:VAL:HG21	1.97	0.47
12:U:310:ASN:O	12:U:350:ARG:NH1	2.47	0.47
12:W:310:ASN:O	12:W:350:ARG:NH1	2.47	0.47
8:M:1165:PRO:HB3	11:X:259:PRO:HD3	1.97	0.47
8:M:1340:ASP:OD1	8:M:1340:ASP:N	2.46	0.47
2:A:62:ILE:O	2:A:93:GLN:NE2	2.49	0.47
12:Y:402:LEU:HA	12:Y:405:VAL:HG22	1.97	0.47
2:A:96:VAL:HG13	3:D:58:LEU:HD21	1.96	0.46
11:T:80:GLY:HA2	12:Y:448:ILE:HD11	1.97	0.46
11:X:453:THR:HB	12:Y:340:PRO:HB2	1.97	0.46
12:Y:262:THR:OG1	12:Y:263:GLY:N	2.48	0.46
8:M:1065:LEU:HD22	12:Y:202:LEU:HB2	1.97	0.46
9:R:70:GLU:H	9:R:70:GLU:HG2	1.51	0.46
12:U:262:THR:OG1	12:U:263:GLY:N	2.48	0.46
12:W:145:ILE:HA	12:W:156:GLY:HA2	1.97	0.46
11:X:151:ASP:OD1	11:X:151:ASP:N	2.48	0.46
6:I:-59:DT:O2	8:M:815:ARG:NH2	2.49	0.46
12:W:20:ILE:HG21	12:W:375:GLU:HG2	1.96	0.46
12:W:162:THR:OG1	12:W:163:THR:N	2.47	0.46
12:W:262:THR:OG1	12:W:263:GLY:N	2.48	0.46
9:R:27:ARG:HE	9:R:394:LEU:HD21	1.80	0.46
12:W:402:LEU:HA	12:W:405:VAL:HG22	1.97	0.46
12:Y:145:ILE:HA	12:Y:156:GLY:HA2	1.97	0.46
12:Y:162:THR:OG1	12:Y:163:THR:N	2.47	0.46
7:J:25:DT:H2"	7:J:26:DA:C8	2.51	0.46
11:T:83:THR:O	11:T:375:TYR:OH	2.34	0.46
12:W:329:VAL:HG22	12:W:341:HIS:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:65:GLN:HE21	9:R:107:THR:HA	1.80	0.46
2:B:96:VAL:HG13	3:C:58:LEU:HD21	1.96	0.46
12:W:17:LEU:HD11	11:X:332:ILE:HD13	1.97	0.46
12:Y:329:VAL:HG22	12:Y:341:HIS:H	1.81	0.46
9:R:339:SER:O	9:R:346:ARG:NH2	2.49	0.45
8:M:1225:HIS:O	8:M:1229:THR:OG1	2.33	0.45
11:T:33:LEU:O	11:T:55:ARG:NH1	2.50	0.45
11:X:33:LEU:O	11:X:55:ARG:NH1	2.50	0.45
2:B:62:ILE:O	2:B:93:GLN:NE2	2.49	0.45
5:H:76:ILE:HG12	5:H:104:ILE:HD11	1.99	0.45
5:H:107:GLY:O	5:H:111:LYS:CB	2.65	0.45
4:E:42:GLN:OE1	4:F:39:ASN:ND2	2.49	0.45
11:T:158:GLY:HA2	12:Y:145:ILE:HB	1.99	0.45
12:W:14:LEU:HD12	12:W:15:LYS:HB2	1.98	0.45
4:F:89:ARG:NH1	4:F:98:LEU:O	2.49	0.45
5:G:76:ILE:HG12	5:G:104:ILE:HD11	1.99	0.45
12:U:145:ILE:HA	12:U:156:GLY:HA2	1.97	0.45
11:V:33:LEU:O	11:V:55:ARG:NH1	2.50	0.45
12:U:402:LEU:HA	12:U:405:VAL:HG22	1.97	0.45
10:S:257:VAL:HG21	12:U:166:GLU:HG2	1.99	0.45
12:U:28:GLY:H	12:U:90:GLN:HB3	1.82	0.45
12:U:189:VAL:HG11	12:U:223:GLN:HG2	1.99	0.45
12:U:243:GLU:HA	12:U:257:LEU:HD11	1.99	0.45
8:M:990:ARG:NH1	8:M:1376:GLU:OE2	2.50	0.45
8:M:1264:ARG:NH2	8:M:1312:SER:O	2.48	0.45
9:R:121:GLU:HB3	10:S:198:LEU:HD11	1.99	0.45
12:U:329:VAL:HG22	12:U:341:HIS:H	1.81	0.45
12:W:243:GLU:HA	12:W:257:LEU:HD11	1.99	0.45
11:X:72:GLY:N	11:X:333:ALA:O	2.45	0.45
12:Y:28:GLY:H	12:Y:90:GLN:HB3	1.82	0.45
4:E:89:ARG:NH1	4:E:98:LEU:O	2.49	0.44
12:Y:243:GLU:HA	12:Y:257:LEU:HD11	1.99	0.44
3:C:93:GLN:OE1	3:C:95:ARG:NH2	2.51	0.44
8:M:942:PRO:HB2	8:M:1363:ASP:HA	1.99	0.44
8:M:1300:ASP:O	8:M:1304:LEU:HB2	2.17	0.44
12:U:26:ILE:HG22	12:U:44:MET:HG2	1.99	0.44
12:W:26:ILE:HG22	12:W:44:MET:HG2	1.99	0.44
12:W:28:GLY:H	12:W:90:GLN:HB3	1.82	0.44
12:W:158:LEU:HD23	12:W:171:LEU:HD21	2.00	0.44
4:F:30:ARG:O	4:F:34:LEU:HB2	2.17	0.44
8:M:967:ARG:O	8:M:970:THR:OG1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:127:ARG:HH22	12:Y:271:ASP:HB2	1.81	0.44
8:M:1150:VAL:HG12	8:M:1152:TYR:H	1.83	0.44
11:V:71:SER:OG	11:V:331:ASN:O	2.36	0.44
12:W:402:LEU:HD22	12:W:426:ALA:HB1	1.99	0.44
5:G:107:GLY:O	5:G:111:LYS:CB	2.65	0.44
9:R:58:ARG:HD2	10:S:166:VAL:HG22	1.98	0.44
12:U:332:THR:OG1	12:U:335:THR:OG1	2.36	0.44
9:R:69:TRP:O	9:R:73:SER:CB	2.66	0.44
11:T:72:GLY:N	11:T:333:ALA:O	2.45	0.44
11:V:188:SER:HA	11:V:191:ARG:HD2	2.00	0.44
11:X:71:SER:OG	11:X:331:ASN:O	2.36	0.44
12:Y:26:ILE:HG22	12:Y:44:MET:HG2	1.99	0.44
12:Y:332:THR:OG1	12:Y:335:THR:OG1	2.36	0.44
4:E:30:ARG:O	4:E:34:LEU:HB2	2.17	0.44
7:J:15:DT:H6	7:J:15:DT:H2'	1.69	0.44
8:M:778:GLY:O	8:M:783:ARG:N	2.43	0.44
9:R:69:TRP:O	9:R:73:SER:HB2	2.17	0.44
12:W:201:LYS:HB2	12:W:201:LYS:HE2	1.72	0.44
11:X:188:SER:HA	11:X:191:ARG:HD2	2.00	0.44
6:I:22:DC:H2"	6:I:23:DA:H5"	2.00	0.44
7:J:-74:DC:H2"	7:J:-73:DA:C8	2.53	0.44
12:U:158:LEU:HD23	12:U:171:LEU:HD21	2.00	0.44
2:A:65:LEU:HB2	7:J:17:DA:H5"	2.00	0.43
5:G:34:LYS:HE2	5:G:34:LYS:HB2	1.88	0.43
10:S:54:ALA:O	10:S:58:ALA:HB2	2.18	0.43
10:S:261:ASN:HD22	10:S:272:HIS:HE1	1.66	0.43
7:J:23:DG:H2"	7:J:24:DC:H5"	2.01	0.43
11:T:71:SER:OG	11:T:331:ASN:O	2.36	0.43
12:U:137:GLU:HG2	12:U:191:SER:HB2	2.00	0.43
12:Y:402:LEU:HD22	12:Y:426:ALA:HB1	2.00	0.43
3:D:93:GLN:OE1	3:D:95:ARG:NH2	2.51	0.43
11:T:188:SER:HA	11:T:191:ARG:HD2	2.00	0.43
11:T:286:GLN:HA	12:Y:17:LEU:HD22	1.99	0.43
8:M:1321:SER:HB3	8:M:1347:MET:HE1	1.99	0.43
8:M:1200:ASN:OD1	8:M:1200:ASN:N	2.51	0.43
12:U:402:LEU:HD22	12:U:426:ALA:HB1	1.99	0.43
12:U:407:GLN:HE21	12:U:407:GLN:HB3	1.58	0.43
12:W:32:ASP:OD1	12:W:32:ASP:N	2.51	0.43
12:W:332:THR:OG1	12:W:335:THR:OG1	2.36	0.43
11:X:151:ASP:HA	11:X:161:LYS:HD3	2.00	0.43
12:Y:114:THR:O	12:Y:118:THR:OG1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:61:LEU:HD13	3:D:36:ARG:HB3	2.01	0.43
11:V:72:GLY:N	11:V:333:ALA:O	2.45	0.43
2:B:95:SER:O	2:B:99:TYR:HB3	2.19	0.43
6:I:-68:DG:N2	7:J:68:DC:C2	2.84	0.43
7:J:4:DG:H2"	7:J:5:DT:C5	2.53	0.43
5:G:54:ASP:OD1	5:G:54:ASP:N	2.50	0.43
10:S:268:CYS:O	10:S:272:HIS:HB2	2.18	0.43
11:T:362:ASP:OD1	11:T:362:ASP:N	2.45	0.43
11:V:54:ALA:O	11:V:58:CYS:CB	2.67	0.43
12:Y:158:LEU:HD23	12:Y:171:LEU:HD21	2.00	0.42
11:T:381:ARG:O	11:T:385:GLU:HB2	2.19	0.42
12:U:32:ASP:OD1	12:U:32:ASP:N	2.51	0.42
11:V:25:ALA:HB1	12:W:68:GLY:HA3	2.01	0.42
11:V:381:ARG:O	11:V:385:GLU:HB2	2.19	0.42
12:W:114:THR:O	12:W:118:THR:OG1	2.36	0.42
4:E:29:GLY:HA3	6:I:-44:DA:H3'	2.01	0.42
8:M:992:VAL:HG23	8:M:998:LEU:HD13	2.02	0.42
8:M:1144:LEU:HD22	12:Y:254:PHE:HZ	1.84	0.42
9:R:425:ASP:OD1	9:R:425:ASP:N	2.53	0.42
8:M:1030:LYS:HD2	8:M:1030:LYS:HA	1.80	0.42
8:M:1386:LYS:HE3	8:M:1386:LYS:HB3	1.88	0.42
12:Y:323:MET:HE1	12:Y:347:LEU:HD11	2.02	0.42
12:Y:455:GLN:OE1	12:Y:457:SER:OG	2.37	0.42
8:M:1004:ILE:H	8:M:1004:ILE:HG12	1.66	0.42
8:M:1276:ASP:OD1	8:M:1276:ASP:N	2.44	0.42
11:X:381:ARG:O	11:X:385:GLU:HB2	2.19	0.42
8:M:860:LEU:H	8:M:860:LEU:HG	1.69	0.42
9:R:227:LEU:HD13	9:R:313:ILE:HG13	2.01	0.42
11:X:54:ALA:O	11:X:58:CYS:CB	2.67	0.42
12:Y:103:GLY:N	12:Y:296:ASP:O	2.53	0.42
2:A:95:SER:O	2:A:99:TYR:HB3	2.19	0.42
8:M:1350:GLN:HE21	8:M:1354:ARG:HH12	1.68	0.42
8:M:1357:ARG:NH2	13:M:1601:ADP:O1B	2.41	0.42
12:W:103:GLY:N	12:W:296:ASP:O	2.53	0.42
11:X:76:LEU:HD21	11:X:369:ILE:HG12	2.02	0.42
11:X:225:GLU:HG3	11:X:227:GLU:H	1.85	0.42
2:B:61:LEU:HD13	3:C:36:ARG:HB3	2.02	0.42
5:G:109:LEU:O	5:G:113:ALA:CB	2.68	0.42
6:I:21:DC:OP2	8:M:831:ASN:ND2	2.52	0.42
8:M:1200:ASN:ND2	8:M:1202:ASP:O	2.53	0.42
11:T:106:VAL:HB	11:T:109:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:3:DC:H2"	7:J:4:DG:C8	2.55	0.42
8:M:1142:ASP:HA	8:M:1145:THR:HG22	2.02	0.42
11:T:225:GLU:HG3	11:T:227:GLU:H	1.85	0.42
12:U:102:ALA:HB3	12:U:105:GLU:HB2	2.02	0.42
12:U:103:GLY:N	12:U:296:ASP:O	2.53	0.42
12:U:134:GLU:OE2	12:U:232:ARG:NH2	2.43	0.42
11:V:106:VAL:HB	11:V:109:GLU:HG3	2.01	0.42
11:V:225:GLU:HG3	11:V:227:GLU:H	1.85	0.42
7:J:36:DA:H1'	7:J:37:DC:H5'	2.01	0.42
8:M:723:MET:H	8:M:723:MET:HG2	1.65	0.42
8:M:953:LEU:HD12	8:M:953:LEU:HA	1.95	0.42
11:T:54:ALA:O	11:T:58:CYS:CB	2.67	0.42
11:T:76:LEU:HD21	11:T:369:ILE:HG12	2.02	0.42
11:V:325:ASN:ND2	11:V:362:ASP:OD2	2.53	0.42
12:Y:32:ASP:OD1	12:Y:32:ASP:N	2.51	0.42
12:Y:102:ALA:HB3	12:Y:105:GLU:HB2	2.02	0.42
9:R:191:ILE:HG12	9:R:200:ILE:HG23	2.02	0.41
11:X:277:LYS:HE2	11:X:277:LYS:HB2	1.85	0.41
11:X:325:ASN:ND2	11:X:362:ASP:OD2	2.53	0.41
12:Y:407:GLN:HE21	12:Y:407:GLN:HB3	1.58	0.41
11:T:326:LYS:HE3	11:T:326:LYS:HB3	1.92	0.41
12:U:455:GLN:OE1	12:U:457:SER:OG	2.37	0.41
11:V:212:VAL:HG12	11:V:230:VAL:HG11	2.02	0.41
12:W:361:GLU:HG3	12:W:392:VAL:HG21	2.02	0.41
5:H:109:LEU:O	5:H:113:ALA:CB	2.68	0.41
9:R:13:TYR:HA	9:R:59:ARG:HH22	1.85	0.41
11:T:351:GLU:OE1	12:Y:331:LYS:NZ	2.50	0.41
12:U:361:GLU:HG3	12:U:392:VAL:HG21	2.02	0.41
12:W:323:MET:HE1	12:W:347:LEU:HD11	2.01	0.41
7:J:-76:DT:H2"	7:J:-75:DG:C8	2.55	0.41
12:U:323:MET:HE1	12:U:347:LEU:HD11	2.02	0.41
12:W:102:ALA:HB3	12:W:105:GLU:HB2	2.02	0.41
12:Y:159:THR:HA	12:Y:168:ILE:HA	2.03	0.41
6:I:72:DG:H1'	6:I:73:DT:H5'	2.02	0.41
9:R:8:ILE:HG12	9:R:17:PHE:HB2	2.03	0.41
9:R:233:PHE:HB3	10:S:276:ARG:HH11	1.85	0.41
11:T:51:GLN:HG3	11:T:54:ALA:HB3	2.03	0.41
3:D:85:ASP:O	3:D:89:ALA:HB2	2.20	0.41
8:M:1069:LYS:HE2	8:M:1069:LYS:HB2	1.86	0.41
11:T:325:ASN:ND2	11:T:362:ASP:OD2	2.53	0.41
12:U:159:THR:HA	12:U:168:ILE:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:76:LEU:HD21	11:V:369:ILE:HG12	2.02	0.41
11:V:277:LYS:HB2	11:V:277:LYS:HE2	1.85	0.41
12:W:159:THR:HA	12:W:168:ILE:HA	2.03	0.41
7:J:-24:DT:H2"	7:J:-23:DT:H5'	2.02	0.41
8:M:987:MET:O	8:M:991:LYS:HB2	2.20	0.41
12:U:146:ASP:O	12:U:155:GLN:N	2.51	0.41
12:W:19:LEU:H	11:X:331:ASN:HB3	1.85	0.41
11:X:51:GLN:HG3	11:X:54:ALA:HB3	2.03	0.41
11:X:106:VAL:HB	11:X:109:GLU:HG3	2.01	0.41
3:C:85:ASP:O	3:C:89:ALA:HB2	2.20	0.41
8:M:1241:LEU:HD11	8:M:1277:VAL:HG13	2.03	0.41
11:T:117:LYS:HE3	11:T:117:LYS:HB2	1.92	0.41
12:U:21:ALA:HB3	12:U:24:SER:HB2	2.03	0.41
3:C:77:LYS:HG2	5:H:95:ARG:HH12	1.85	0.41
10:S:128:ARG:O	10:S:132:GLU:HB2	2.21	0.41
12:U:114:THR:O	12:U:118:THR:OG1	2.36	0.41
11:V:51:GLN:HG3	11:V:54:ALA:HB3	2.03	0.41
12:W:146:ASP:O	12:W:155:GLN:N	2.51	0.41
12:Y:146:ASP:O	12:Y:155:GLN:N	2.51	0.41
2:B:101:VAL:HG11	4:E:108:VAL:HG11	2.03	0.41
6:I:-70:DG:H2"	6:I:-69:DA:C8	2.57	0.41
9:R:229:GLU:OE1	10:S:101:ARG:NH2	2.55	0.41
9:R:237:ASN:OD1	9:R:237:ASN:N	2.49	0.41
11:T:212:VAL:HG12	11:T:230:VAL:HG11	2.02	0.41
11:T:456:LEU:HD23	12:U:329:VAL:HG23	2.03	0.41
12:W:455:GLN:OE1	12:W:457:SER:OG	2.37	0.41
11:X:48:PHE:HA	13:X:501:ADP:HN62	1.85	0.41
12:Y:361:GLU:HG3	12:Y:392:VAL:HG21	2.02	0.41
4:E:78:ARG:HH11	7:J:58:DC:H5'	1.85	0.40
8:M:722:GLU:HB2	8:M:933:LEU:HA	2.04	0.40
8:M:836:ARG:HA	8:M:839:ALA:HB3	2.03	0.40
8:M:1068:VAL:HG13	8:M:1126:ASN:HD21	1.86	0.40
11:X:326:LYS:HE3	11:X:326:LYS:HB3	1.92	0.40
5:H:54:ASP:OD1	5:H:54:ASP:N	2.50	0.40
11:V:405:THR:O	11:V:409:GLU:HB2	2.21	0.40
11:X:212:VAL:HG12	11:X:230:VAL:HG11	2.02	0.40
6:I:-86:DA:H2"	6:I:-85:DT:C6	2.56	0.40
8:M:1055:THR:HA	8:M:1141:ILE:H	1.86	0.40
7:J:88:DC:H2"	7:J:89:DA:C8	2.57	0.40
10:S:54:ALA:O	10:S:58:ALA:CB	2.69	0.40
10:S:258:ASN:OD1	10:S:258:ASN:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:21:ALA:HB3	12:W:24:SER:HB2	2.03	0.40
11:X:462:TYR:HB2	12:Y:327:ARG:HD3	2.02	0.40
8:M:1045:LEU:HD23	8:M:1045:LEU:HA	1.84	0.40
8:M:1331:THR:HG22	8:M:1357:ARG:HB2	2.03	0.40
10:S:246:ILE:HG13	10:S:268:CYS:HB3	2.04	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	A	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
2	B	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
3	C	80/103 (78%)	78 (98%)	2 (2%)	0	100	100
3	D	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
4	E	101/132 (76%)	101 (100%)	0	0	100	100
4	F	99/132 (75%)	99 (100%)	0	0	100	100
5	G	94/131 (72%)	90 (96%)	4 (4%)	0	100	100
5	H	89/131 (68%)	87 (98%)	2 (2%)	0	100	100
8	M	684/1514 (45%)	627 (92%)	56 (8%)	1 (0%)	48	79
9	R	407/438 (93%)	401 (98%)	6 (2%)	0	100	100
10	S	200/280 (71%)	199 (100%)	1 (0%)	0	100	100
11	T	441/463 (95%)	417 (95%)	23 (5%)	1 (0%)	43	72
11	V	430/463 (93%)	411 (96%)	19 (4%)	0	100	100
11	X	440/463 (95%)	420 (96%)	20 (4%)	0	100	100
12	U	426/471 (90%)	414 (97%)	12 (3%)	0	100	100
12	W	429/471 (91%)	415 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	Y	445/471 (94%)	427 (96%)	18 (4%)	0	100	100
All	All	4633/6038 (77%)	4448 (96%)	183 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	M	1345	PRO
11	T	161	LYS

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	A	84/113 (74%)	83 (99%)	1 (1%)	63	73
2	B	84/113 (74%)	83 (99%)	1 (1%)	63	73
3	C	68/81 (84%)	64 (94%)	4 (6%)	18	45
3	D	67/81 (83%)	63 (94%)	4 (6%)	17	45
4	E	82/99 (83%)	80 (98%)	2 (2%)	43	63
4	F	80/99 (81%)	78 (98%)	2 (2%)	42	63
5	G	83/109 (76%)	80 (96%)	3 (4%)	31	56
5	H	78/109 (72%)	76 (97%)	2 (3%)	40	62
8	M	574/1376 (42%)	510 (89%)	64 (11%)	6	27
9	R	372/396 (94%)	355 (95%)	17 (5%)	24	51
10	S	199/261 (76%)	189 (95%)	10 (5%)	22	49
11	T	371/391 (95%)	335 (90%)	36 (10%)	8	31
11	V	368/391 (94%)	332 (90%)	36 (10%)	7	31
11	X	374/391 (96%)	335 (90%)	39 (10%)	7	29
12	U	367/403 (91%)	325 (89%)	42 (11%)	5	26
12	W	369/403 (92%)	326 (88%)	43 (12%)	5	25
12	Y	372/403 (92%)	328 (88%)	44 (12%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3992/5219 (76%)	3642 (91%)	350 (9%)	11 33

All (350) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	96	VAL
2	B	96	VAL
3	C	58	LEU
3	C	66	ILE
3	C	92	ARG
3	C	97	LEU
3	D	58	LEU
3	D	66	ILE
3	D	92	ARG
3	D	97	LEU
4	E	18	ARG
4	E	34	LEU
4	F	18	ARG
4	F	34	LEU
5	G	103	LEU
5	G	114	VAL
5	G	128	THR
5	H	103	LEU
5	H	114	VAL
8	M	686	VAL
8	M	692	LEU
8	M	696	LEU
8	M	756	VAL
8	M	757	LEU
8	M	764	PHE
8	M	794	ASP
8	M	806	VAL
8	M	814	LYS
8	M	845	THR
8	M	854	THR
8	M	860	LEU
8	M	867	LEU
8	M	876	ILE
8	M	934	LYS
8	M	937	VAL
8	M	989	LEU
8	M	999	PHE

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Mol	Chain	Res	Type
8	M	1001	VAL
8	M	1004	ILE
8	M	1018	TYR
8	M	1028	LEU
8	M	1038	VAL
8	M	1040	LEU
8	M	1046	VAL
8	M	1052	LYS
8	M	1054	LEU
8	M	1055	THR
8	M	1062	ILE
8	M	1066	THR
8	M	1068	VAL
8	M	1075	VAL
8	M	1082	ASN
8	M	1085	LEU
8	M	1135	ILE
8	M	1138	LYS
8	M	1143	LEU
8	M	1151	LYS
8	M	1158	ILE
8	M	1162	LEU
8	M	1163	ILE
8	M	1166	LEU
8	M	1188	VAL
8	M	1195	LEU
8	M	1199	LEU
8	M	1205	VAL
8	M	1209	THR
8	M	1213	VAL
8	M	1229	THR
8	M	1233	ILE
8	M	1238	LYS
8	M	1251	LEU
8	M	1254	LEU
8	M	1274	VAL
8	M	1278	LEU
8	M	1280	GLN
8	M	1282	LEU
8	M	1298	ILE
8	M	1326	LEU
8	M	1328	ILE

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Mol	Chain	Res	Type
8	M	1352	GLN
8	M	1358	ILE
8	M	1386	LYS
8	M	1392	VAL
9	R	3	THR
9	R	15	ILE
9	R	42	LEU
9	R	63	LEU
9	R	66	LEU
9	R	70	GLU
9	R	120	PHE
9	R	128	LEU
9	R	133	VAL
9	R	149	THR
9	R	189	LEU
9	R	204	LEU
9	R	266	THR
9	R	331	VAL
9	R	345	VAL
9	R	406	THR
9	R	425	ASP
10	S	8	ILE
10	S	46	VAL
10	S	107	THR
10	S	126	VAL
10	S	182	THR
10	S	192	THR
10	S	217	LEU
10	S	242	THR
10	S	254	SER
10	S	266	VAL
11	T	42	LYS
11	T	49	VAL
11	T	105	LEU
11	T	115	VAL
11	T	121	LEU
11	T	133	ILE
11	T	148	THR
11	T	159	TYR
11	T	182	ASP
11	T	202	ILE
11	T	226	THR

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Mol	Chain	Res	Type
11	T	241	LYS
11	T	243	ILE
11	T	244	VAL
11	T	247	VAL
11	T	258	ARG
11	T	273	LEU
11	T	274	LYS
11	T	277	LYS
11	T	278	THR
11	T	284	LEU
11	T	292	VAL
11	T	303	LEU
11	T	312	GLU
11	T	322	THR
11	T	331	ASN
11	T	336	VAL
11	T	337	VAL
11	T	364	ILE
11	T	369	ILE
11	T	380	ILE
11	T	384	ILE
11	T	417	GLN
11	T	435	VAL
11	T	456	LEU
11	T	461	ASN
12	U	15	LYS
12	U	19	LEU
12	U	26	ILE
12	U	29	LEU
12	U	32	ASP
12	U	69	ARG
12	U	106	ILE
12	U	111	LEU
12	U	118	THR
12	U	135	LEU
12	U	149	ILE
12	U	150	THR
12	U	153	HIS
12	U	158	LEU
12	U	171	LEU
12	U	182	GLU
12	U	183	LYS

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Mol	Chain	Res	Type
12	U	191	SER
12	U	198	LYS
12	U	202	LEU
12	U	222	VAL
12	U	234	THR
12	U	236	VAL
12	U	252	GLN
12	U	257	LEU
12	U	266	ARG
12	U	268	GLU
12	U	273	ILE
12	U	296	ASP
12	U	298	VAL
12	U	320	ILE
12	U	339	SER
12	U	352	ILE
12	U	367	ILE
12	U	386	LEU
12	U	396	LEU
12	U	397	ARG
12	U	407	GLN
12	U	420	VAL
12	U	437	VAL
12	U	448	ILE
12	U	456	ILE
11	V	42	LYS
11	V	49	VAL
11	V	105	LEU
11	V	115	VAL
11	V	121	LEU
11	V	133	ILE
11	V	148	THR
11	V	162	THR
11	V	182	ASP
11	V	202	ILE
11	V	226	THR
11	V	241	LYS
11	V	243	ILE
11	V	244	VAL
11	V	247	VAL
11	V	258	ARG
11	V	273	LEU

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Mol	Chain	Res	Type
11	V	274	LYS
11	V	277	LYS
11	V	278	THR
11	V	284	LEU
11	V	292	VAL
11	V	303	LEU
11	V	312	GLU
11	V	322	THR
11	V	331	ASN
11	V	336	VAL
11	V	337	VAL
11	V	364	ILE
11	V	369	ILE
11	V	380	ILE
11	V	384	ILE
11	V	417	GLN
11	V	435	VAL
11	V	456	LEU
11	V	461	ASN
12	W	14	LEU
12	W	15	LYS
12	W	19	LEU
12	W	26	ILE
12	W	29	LEU
12	W	32	ASP
12	W	69	ARG
12	W	106	ILE
12	W	111	LEU
12	W	118	THR
12	W	135	LEU
12	W	147	ARG
12	W	158	LEU
12	W	171	LEU
12	W	182	GLU
12	W	183	LYS
12	W	191	SER
12	W	198	LYS
12	W	201	LYS
12	W	202	LEU
12	W	206	PHE
12	W	222	VAL
12	W	234	THR

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Mol	Chain	Res	Type
12	W	236	VAL
12	W	252	GLN
12	W	257	LEU
12	W	266	ARG
12	W	268	GLU
12	W	273	ILE
12	W	296	ASP
12	W	298	VAL
12	W	320	ILE
12	W	339	SER
12	W	352	ILE
12	W	367	ILE
12	W	386	LEU
12	W	396	LEU
12	W	397	ARG
12	W	407	GLN
12	W	420	VAL
12	W	437	VAL
12	W	448	ILE
12	W	456	ILE
11	X	42	LYS
11	X	49	VAL
11	X	105	LEU
11	X	115	VAL
11	X	121	LEU
11	X	133	ILE
11	X	148	THR
11	X	153	GLU
11	X	161	LYS
11	X	162	THR
11	X	163	ILE
11	X	182	ASP
11	X	202	ILE
11	X	226	THR
11	X	241	LYS
11	X	243	ILE
11	X	244	VAL
11	X	247	VAL
11	X	258	ARG
11	X	273	LEU
11	X	274	LYS
11	X	277	LYS

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Mol	Chain	Res	Type
11	X	278	THR
11	X	284	LEU
11	X	292	VAL
11	X	303	LEU
11	X	312	GLU
11	X	322	THR
11	X	331	ASN
11	X	336	VAL
11	X	337	VAL
11	X	364	ILE
11	X	369	ILE
11	X	380	ILE
11	X	384	ILE
11	X	417	GLN
11	X	435	VAL
11	X	456	LEU
11	X	461	ASN
12	Y	14	LEU
12	Y	15	LYS
12	Y	19	LEU
12	Y	26	ILE
12	Y	29	LEU
12	Y	32	ASP
12	Y	69	ARG
12	Y	106	ILE
12	Y	111	LEU
12	Y	118	THR
12	Y	135	LEU
12	Y	158	LEU
12	Y	171	LEU
12	Y	182	GLU
12	Y	183	LYS
12	Y	191	SER
12	Y	198	LYS
12	Y	202	LEU
12	Y	219	THR
12	Y	220	ARG
12	Y	221	PHE
12	Y	222	VAL
12	Y	223	GLN
12	Y	234	THR
12	Y	236	VAL

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Mol	Chain	Res	Type
12	Y	252	GLN
12	Y	257	LEU
12	Y	266	ARG
12	Y	268	GLU
12	Y	273	ILE
12	Y	296	ASP
12	Y	298	VAL
12	Y	320	ILE
12	Y	339	SER
12	Y	352	ILE
12	Y	367	ILE
12	Y	386	LEU
12	Y	396	LEU
12	Y	397	ARG
12	Y	407	GLN
12	Y	420	VAL
12	Y	437	VAL
12	Y	448	ILE
12	Y	456	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
4	E	16	GLN
4	E	42	GLN
4	F	39	ASN
4	F	42	GLN
4	F	74	ASN
5	G	52	HIS
5	H	52	HIS
8	M	716	ASN
8	M	782	GLN
8	M	797	HIS
8	M	808	GLN
8	M	857	GLN
8	M	922	HIS
8	M	988	GLN
8	M	1126	ASN
8	M	1139	ASN
8	M	1226	GLN
8	M	1249	GLN
8	M	1283	ASN

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Mol	Chain	Res	Type
8	M	1356	HIS
8	M	1360	GLN
9	R	45	HIS
9	R	98	HIS
9	R	235	HIS
9	R	251	GLN
9	R	289	ASN
10	S	272	HIS
11	T	124	ASN
11	T	238	HIS
11	T	263	GLN
11	T	271	GLN
11	T	357	HIS
12	U	23	HIS
12	U	47	GLN
12	U	63	ASN
12	U	173	ASN
12	U	252	GLN
12	U	272	GLN
12	U	299	HIS
12	U	341	HIS
12	U	407	GLN
12	U	408	GLN
12	U	416	ASN
11	V	124	ASN
11	V	263	GLN
11	V	271	GLN
11	V	357	HIS
11	V	394	GLN
12	W	47	GLN
12	W	63	ASN
12	W	272	GLN
12	W	401	ASN
12	W	407	GLN
12	W	408	GLN
12	W	416	ASN
11	X	124	ASN
11	X	238	HIS
11	X	256	ASN
11	X	263	GLN
11	X	271	GLN
11	X	289	ASN

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Mol	Chain	Res	Type
11	X	357	HIS
11	X	394	GLN
12	Y	23	HIS
12	Y	47	GLN
12	Y	63	ASN
12	Y	252	GLN
12	Y	272	GLN
12	Y	341	HIS
12	Y	407	GLN
12	Y	416	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
13	ADP	M	1601	14	27,29,29	1.36	4 (14%)	42,45,45	1.91	10 (23%)
14	BEF	M	1602	13	0,3,3	-	-	-		
13	ADP	X	501	15	27,29,29	1.37	4 (14%)	42,45,45	1.98	11 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	ADP	T	501	15	27,29,29	1.36	4 (14%)	42,45,45	1.97	11 (26%)
13	ADP	V	501	15	27,29,29	1.36	4 (14%)	42,45,45	1.97	11 (26%)
13	ADP	W	501	15	27,29,29	1.38	4 (14%)	42,45,45	2.02	9 (21%)
13	ADP	Y	502	15	27,29,29	1.35	4 (14%)	42,45,45	1.93	11 (26%)
13	ADP	U	502	15	27,29,29	1.37	4 (14%)	42,45,45	2.11	9 (21%)
14	BEF	R	502	13	0,3,3	-	-	-		
13	ADP	R	501	15,14	27,29,29	1.37	4 (14%)	42,45,45	1.92	10 (23%)

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
13	ADP	M	1601	14	-	6/16/32/32	0/3/3/3
13	ADP	X	501	15	-	2/16/32/32	0/3/3/3
13	ADP	T	501	15	-	3/16/32/32	0/3/3/3
13	ADP	V	501	15	-	3/16/32/32	0/3/3/3
13	ADP	W	501	15	-	0/16/32/32	0/3/3/3
13	ADP	Y	502	15	-	1/16/32/32	0/3/3/3
13	ADP	U	502	15	-	2/16/32/32	0/3/3/3
13	ADP	R	501	15,14	-	4/16/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	W	501	ADP	C5-C4	4.70	1.47	1.39
13	U	502	ADP	C5-C4	4.66	1.47	1.39
13	R	501	ADP	C5-C4	4.57	1.47	1.39
13	X	501	ADP	C5-C4	4.57	1.47	1.39
13	M	1601	ADP	C5-C4	4.55	1.47	1.39
13	Y	502	ADP	C5-C4	4.54	1.47	1.39
13	V	501	ADP	C5-C4	4.50	1.47	1.39
13	T	501	ADP	C5-C4	4.48	1.47	1.39
13	V	501	ADP	C5-C6	2.77	1.48	1.41
13	W	501	ADP	C5-C6	2.76	1.48	1.41
13	U	502	ADP	C5-C6	2.72	1.48	1.41
13	X	501	ADP	C5-C6	2.72	1.48	1.41
13	R	501	ADP	C5-C6	2.72	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	501	ADP	C5-C6	2.71	1.48	1.41
13	M	1601	ADP	C5-C6	2.69	1.48	1.41
13	Y	502	ADP	C5-C6	2.64	1.48	1.41
13	X	501	ADP	C8-N7	2.48	1.36	1.31
13	R	501	ADP	C8-N7	2.44	1.36	1.31
13	Y	502	ADP	C8-N7	2.43	1.36	1.31
13	V	501	ADP	C8-N7	2.43	1.36	1.31
13	M	1601	ADP	C8-N7	2.43	1.36	1.31
13	T	501	ADP	C8-N7	2.41	1.36	1.31
13	W	501	ADP	C8-N7	2.35	1.36	1.31
13	U	502	ADP	C5-N7	-2.32	1.34	1.39
13	W	501	ADP	C5-N7	-2.24	1.34	1.39
13	U	502	ADP	C8-N7	2.23	1.35	1.31
13	T	501	ADP	C5-N7	-2.19	1.34	1.39
13	M	1601	ADP	C5-N7	-2.16	1.34	1.39
13	X	501	ADP	C5-N7	-2.14	1.35	1.39
13	R	501	ADP	C5-N7	-2.12	1.35	1.39
13	V	501	ADP	C5-N7	-2.10	1.35	1.39
13	Y	502	ADP	C5-N7	-2.10	1.35	1.39

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	U	502	ADP	C5-C4-N3	-7.06	117.54	126.75
13	W	501	ADP	C5-C4-N3	-6.77	117.92	126.75
13	X	501	ADP	C5-C4-N3	-6.20	118.66	126.75
13	T	501	ADP	C5-C4-N3	-6.17	118.69	126.75
13	M	1601	ADP	C5-C4-N3	-6.14	118.73	126.75
13	V	501	ADP	C5-C4-N3	-6.13	118.75	126.75
13	R	501	ADP	C5-C4-N3	-6.12	118.77	126.75
13	Y	502	ADP	C5-C4-N3	-5.59	119.46	126.75
13	U	502	ADP	N3-C4-N9	5.58	136.28	127.08
13	W	501	ADP	N3-C4-N9	5.36	135.91	127.08
13	X	501	ADP	N3-C4-N9	4.85	135.07	127.08
13	M	1601	ADP	N3-C4-N9	4.83	135.05	127.08
13	R	501	ADP	N3-C4-N9	4.77	134.95	127.08
13	V	501	ADP	N3-C4-N9	4.77	134.94	127.08
13	T	501	ADP	N3-C4-N9	4.75	134.92	127.08
13	Y	502	ADP	N3-C4-N9	4.41	134.35	127.08
13	U	502	ADP	C2-N3-C4	4.15	121.56	111.75
13	W	501	ADP	C2-N3-C4	4.06	121.34	111.75
13	M	1601	ADP	C2-N3-C4	3.89	120.94	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	V	501	ADP	C2-N3-C4	3.88	120.92	111.75
13	X	501	ADP	C2-N3-C4	3.88	120.92	111.75
13	R	501	ADP	C2-N3-C4	3.84	120.82	111.75
13	T	501	ADP	C2-N3-C4	3.82	120.77	111.75
13	U	502	ADP	PA-O3A-PB	-3.78	119.84	132.83
13	Y	502	ADP	C2-N3-C4	3.77	120.65	111.75
13	Y	502	ADP	PA-O3A-PB	-3.73	120.02	132.83
13	W	501	ADP	PA-O3A-PB	-3.64	120.33	132.83
13	T	501	ADP	C4-C5-N7	-3.48	106.37	110.62
13	X	501	ADP	PA-O3A-PB	-3.37	121.25	132.83
13	V	501	ADP	PA-O3A-PB	-3.34	121.35	132.83
13	Y	502	ADP	N3-C2-N1	-3.34	123.38	128.60
13	V	501	ADP	C4-C5-N7	-3.32	106.58	110.62
13	T	501	ADP	PA-O3A-PB	-3.31	121.48	132.83
13	U	502	ADP	C4-C5-N7	-3.29	106.61	110.62
13	R	501	ADP	C4-C5-N7	-3.27	106.63	110.62
13	X	501	ADP	C4-C5-N7	-3.26	106.64	110.62
13	M	1601	ADP	C4-C5-N7	-3.21	106.71	110.62
13	M	1601	ADP	N3-C2-N1	-3.20	123.60	128.60
13	X	501	ADP	N3-C2-N1	-3.18	123.64	128.60
13	V	501	ADP	N3-C2-N1	-3.17	123.65	128.60
13	R	501	ADP	N3-C2-N1	-3.16	123.66	128.60
13	W	501	ADP	C4-C5-N7	-3.13	106.80	110.62
13	U	502	ADP	N3-C2-N1	-3.10	123.75	128.60
13	W	501	ADP	N3-C2-N1	-3.09	123.77	128.60
13	Y	502	ADP	C4-C5-N7	-3.08	106.87	110.62
13	T	501	ADP	N3-C2-N1	-3.04	123.85	128.60
13	Y	502	ADP	C2'-C1'-N9	-3.03	105.63	113.30
13	T	501	ADP	C5-N7-C8	2.96	107.72	103.51
13	U	502	ADP	C5-N7-C8	2.92	107.66	103.51
13	V	501	ADP	C5-N7-C8	2.79	107.47	103.51
13	X	501	ADP	C5-N7-C8	2.74	107.41	103.51
13	R	501	ADP	C5-N7-C8	2.73	107.39	103.51
13	M	1601	ADP	C5-N7-C8	2.73	107.39	103.51
13	Y	502	ADP	C4-N9-C8	2.68	108.64	105.73
13	T	501	ADP	C4-N9-C8	2.67	108.62	105.73
13	R	501	ADP	C4-N9-C8	2.62	108.57	105.73
13	W	501	ADP	C5-N7-C8	2.61	107.22	103.51
13	V	501	ADP	C4-N9-C8	2.60	108.55	105.73
13	X	501	ADP	C4-N9-C8	2.59	108.54	105.73
13	M	1601	ADP	C4-N9-C8	2.57	108.51	105.73
13	Y	502	ADP	C5-N7-C8	2.54	107.12	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	1601	ADP	C3'-C2'-C1'	2.43	106.04	101.43
13	R	501	ADP	C3'-C2'-C1'	2.41	106.01	101.43
13	Y	502	ADP	C6-C5-N7	2.39	136.47	132.02
13	U	502	ADP	C3'-C2'-C1'	2.37	105.93	101.43
13	X	501	ADP	C3'-C2'-C1'	2.37	105.93	101.43
13	W	501	ADP	C3'-C2'-C1'	2.30	105.80	101.43
13	T	501	ADP	C6-C5-N7	2.30	136.31	132.02
13	T	501	ADP	C3'-C2'-C1'	2.27	105.73	101.43
13	V	501	ADP	C6-C5-N7	2.27	136.25	132.02
13	R	501	ADP	C6-C5-N7	2.21	136.15	132.02
13	M	1601	ADP	C6-C5-N7	2.21	136.14	132.02
13	V	501	ADP	C3'-C2'-C1'	2.20	105.61	101.43
13	T	501	ADP	N9-C8-N7	-2.20	110.90	113.91
13	X	501	ADP	C6-C5-N7	2.18	136.08	132.02
13	U	502	ADP	C4-N9-C8	2.15	108.06	105.73
13	W	501	ADP	C4-N9-C8	2.13	108.04	105.73
13	V	501	ADP	N9-C8-N7	-2.06	111.09	113.91
13	R	501	ADP	N9-C8-N7	-2.04	111.13	113.91
13	X	501	ADP	N9-C8-N7	-2.03	111.14	113.91
13	M	1601	ADP	N9-C8-N7	-2.00	111.17	113.91
13	Y	502	ADP	N9-C8-N7	-2.00	111.18	113.91

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	M	1601	ADP	PA-O3A-PB-O2B
13	M	1601	ADP	C5'-O5'-PA-O1A
13	M	1601	ADP	C5'-O5'-PA-O2A
13	R	501	ADP	C5'-O5'-PA-O1A
13	R	501	ADP	C5'-O5'-PA-O2A
13	R	501	ADP	C5'-O5'-PA-O3A
13	T	501	ADP	C5'-O5'-PA-O1A
13	T	501	ADP	C5'-O5'-PA-O2A
13	V	501	ADP	C5'-O5'-PA-O1A
13	V	501	ADP	C5'-O5'-PA-O2A
13	X	501	ADP	C5'-O5'-PA-O3A
13	Y	502	ADP	C5'-O5'-PA-O1A
13	U	502	ADP	O4'-C4'-C5'-O5'
13	U	502	ADP	C3'-C4'-C5'-O5'
13	T	501	ADP	C5'-O5'-PA-O3A
13	X	501	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
13	M	1601	ADP	PA-O3A-PB-O1B
13	R	501	ADP	C3'-C4'-C5'-O5'
13	M	1601	ADP	C5'-O5'-PA-O3A
13	V	501	ADP	C5'-O5'-PA-O3A
13	M	1601	ADP	O4'-C4'-C5'-O5'

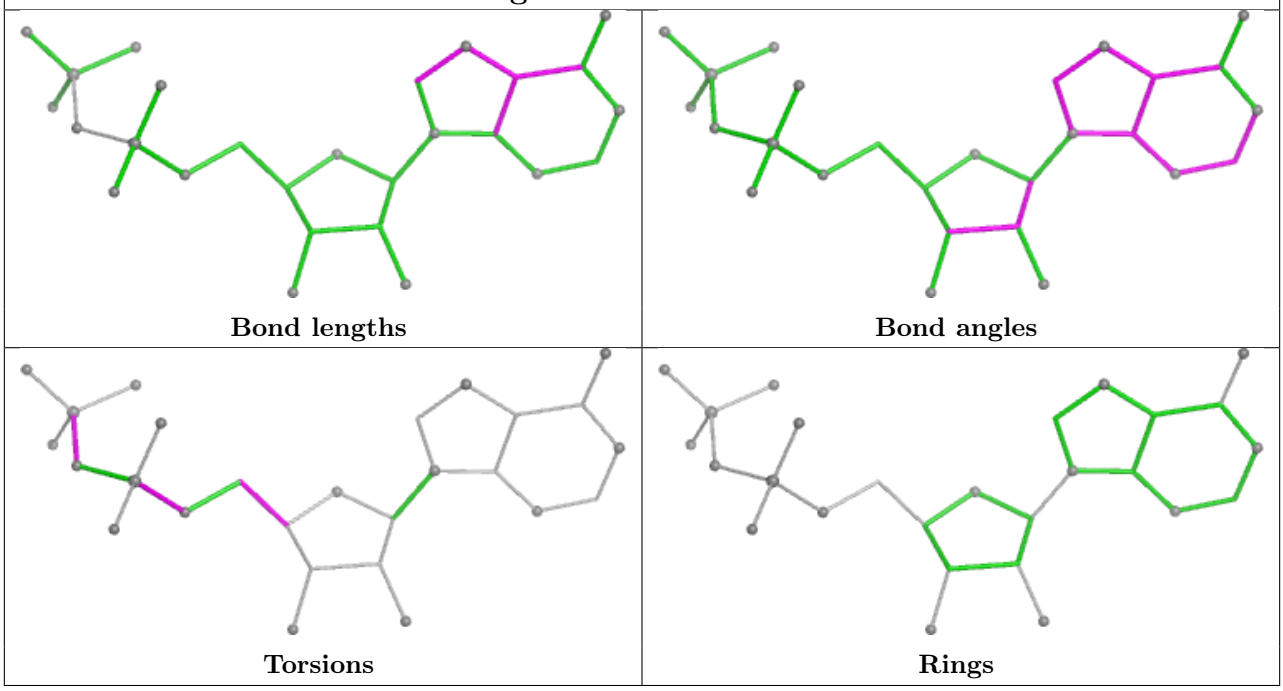
There are no ring outliers.

2 monomers are involved in 5 short contacts:

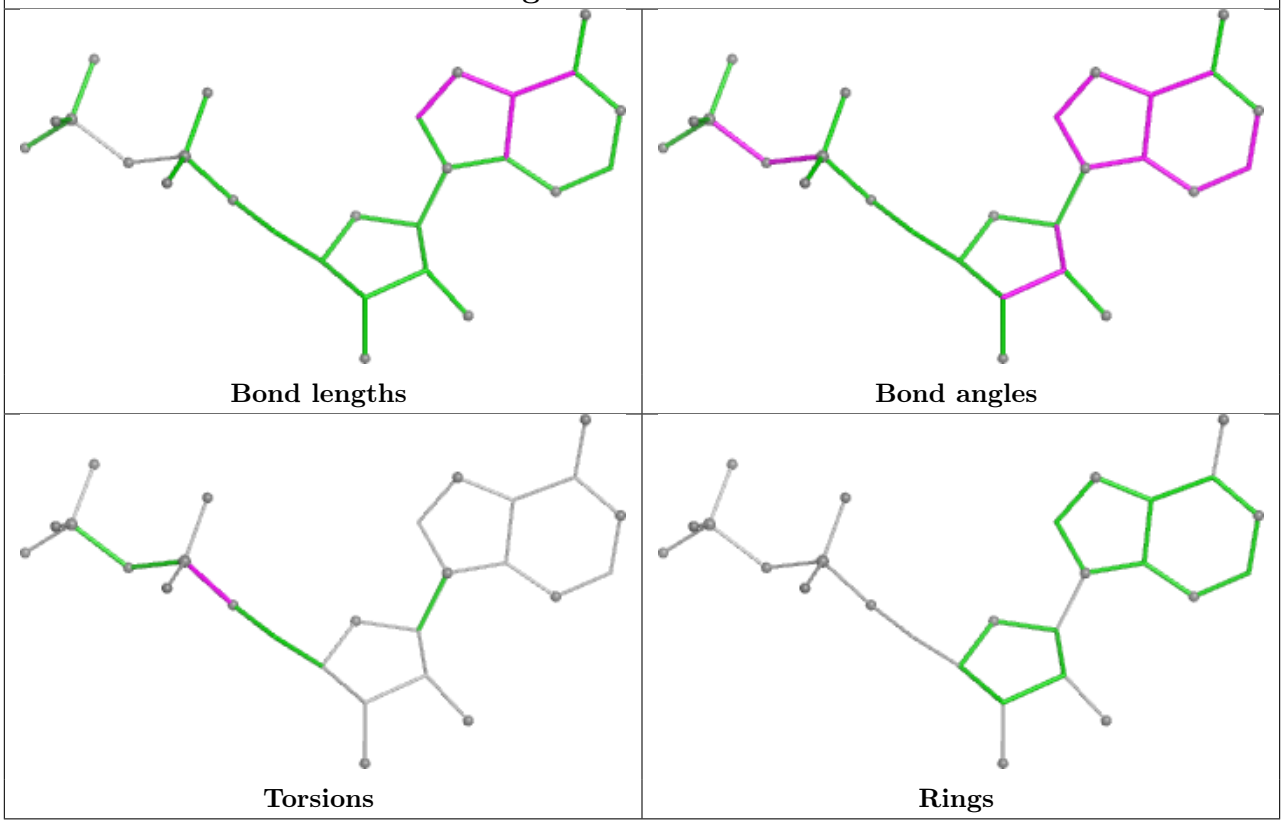
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1601	ADP	3	0
13	X	501	ADP	2	0

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 then 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.

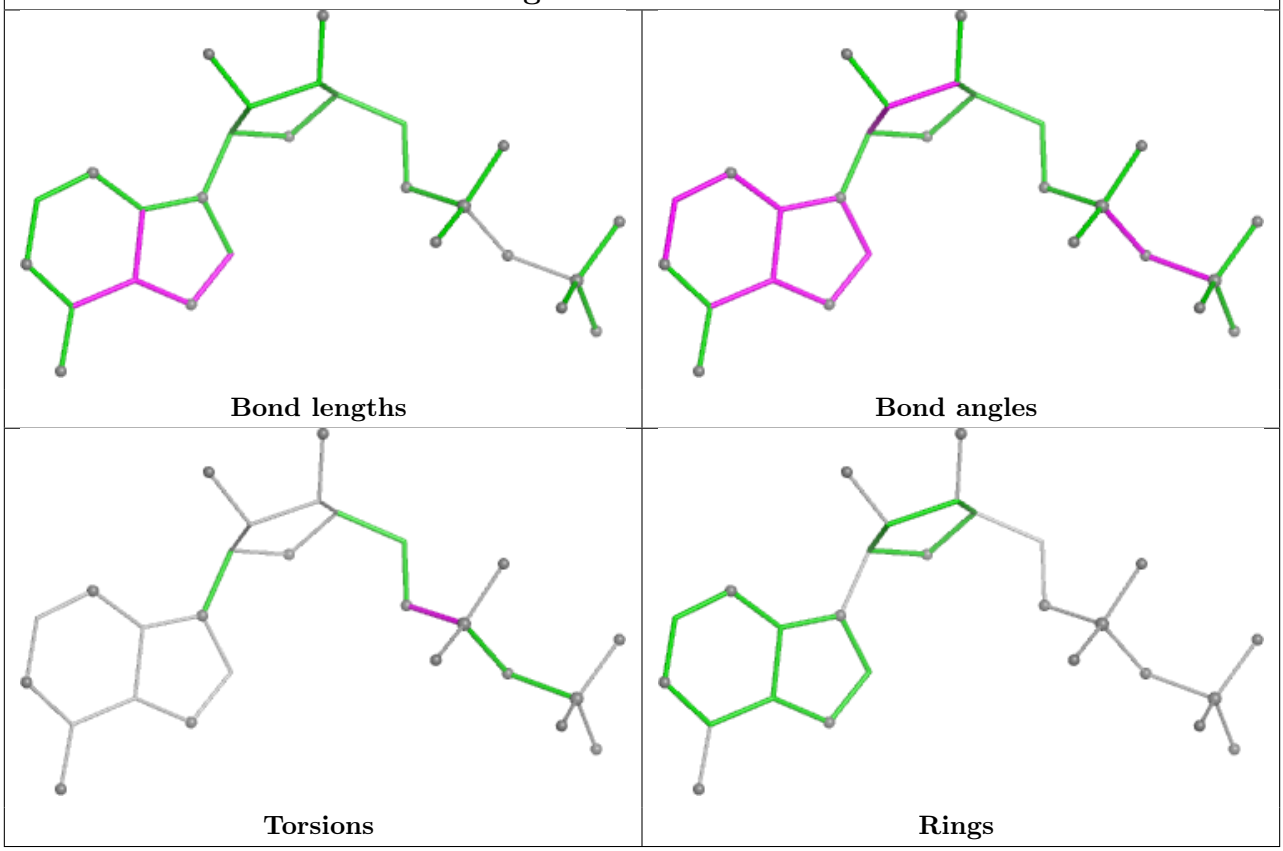
Ligand ADP M 1601



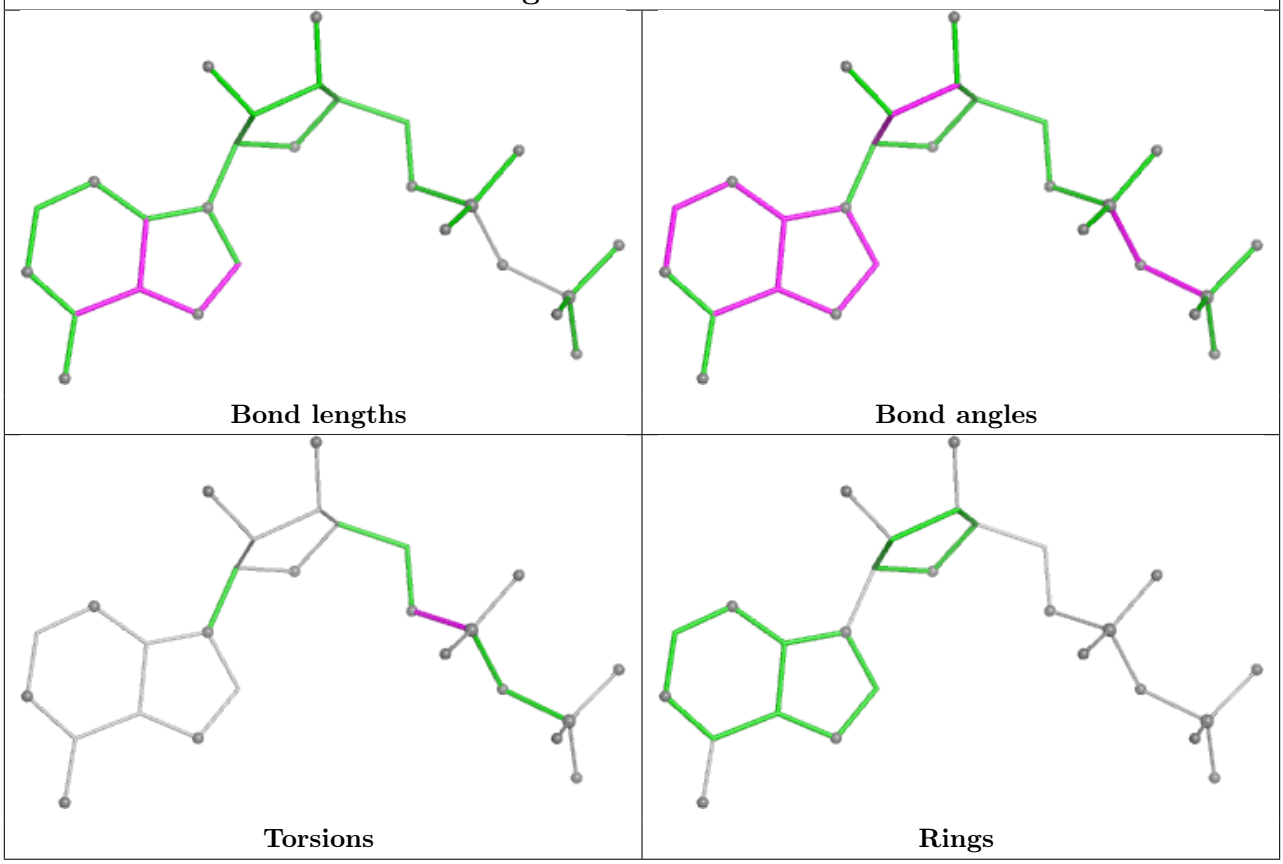
Ligand ADP X 501



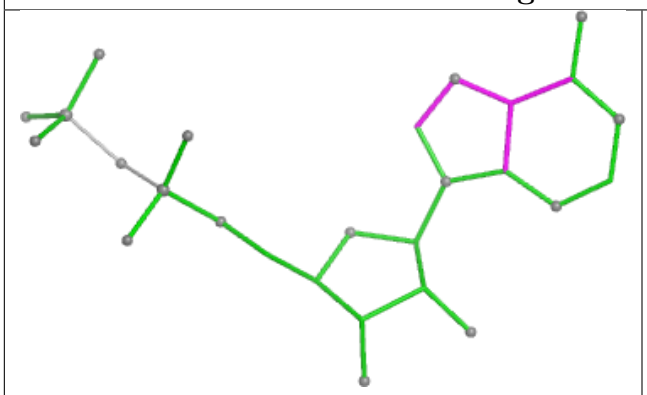
Ligand ADP T 501



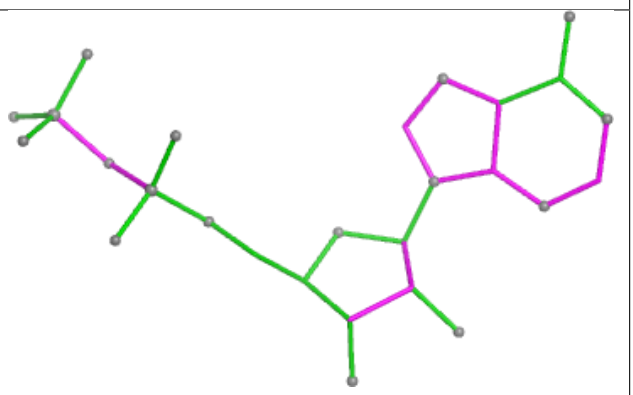
Ligand ADP V 501



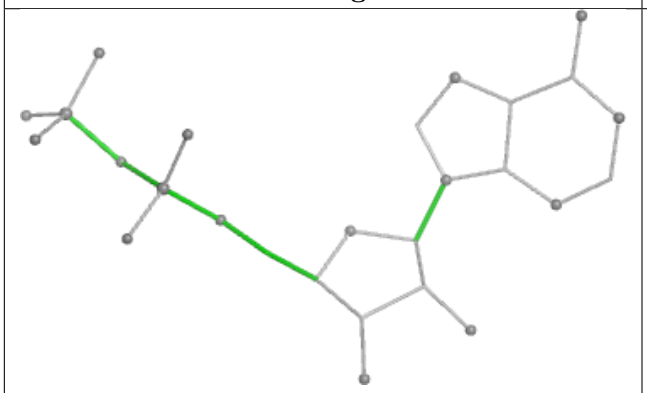
Ligand ADP W 501



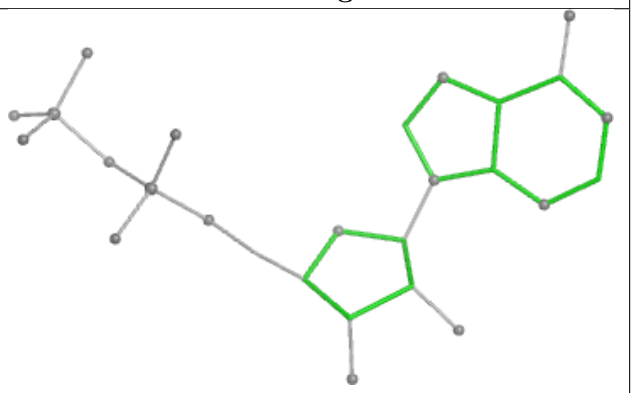
Bond lengths



Bond angles

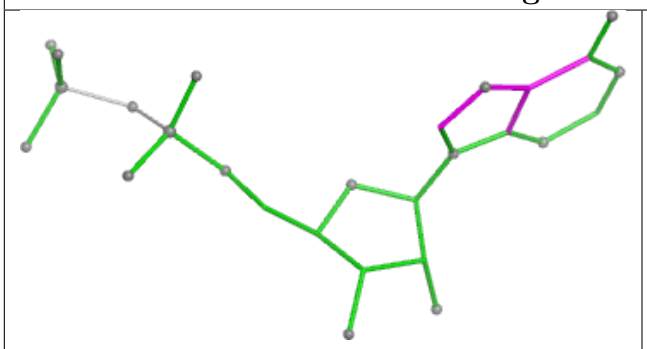


Torsions

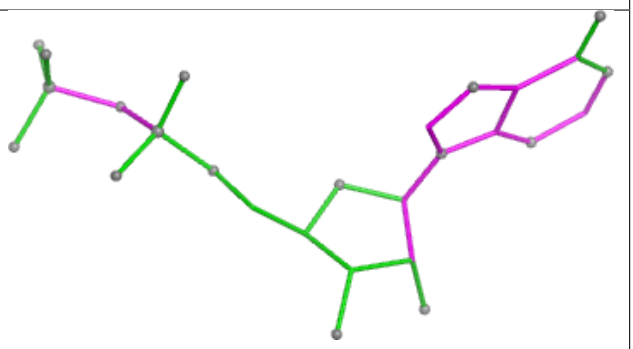


Rings

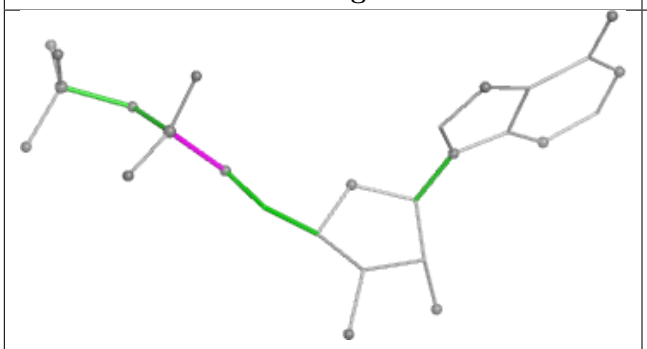
Ligand ADP Y 502



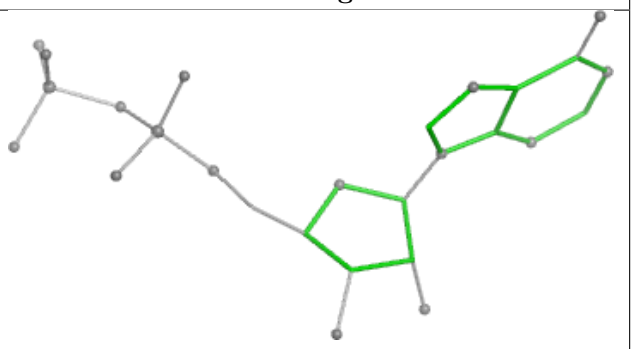
Bond lengths



Bond angles

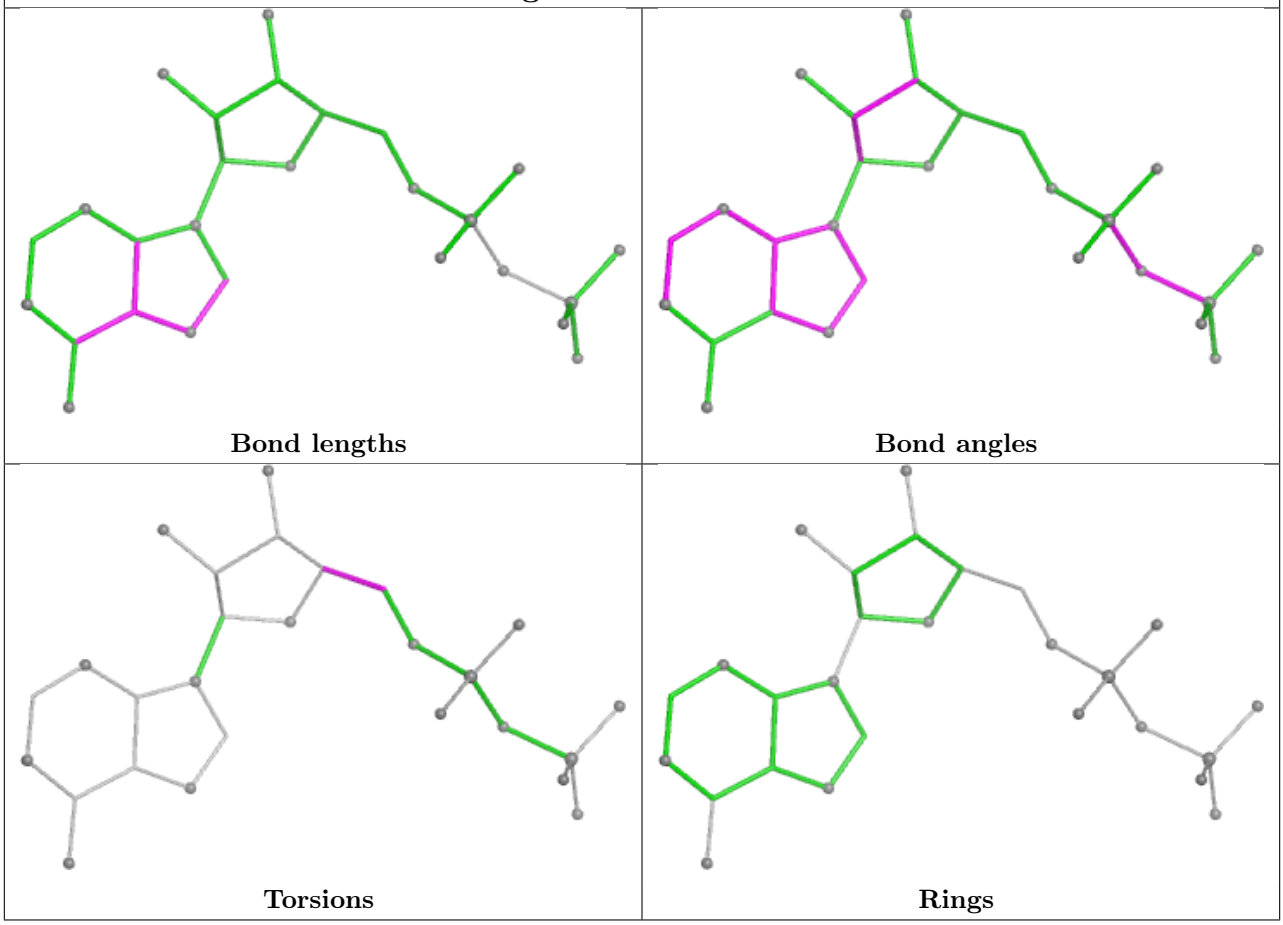


Torsions

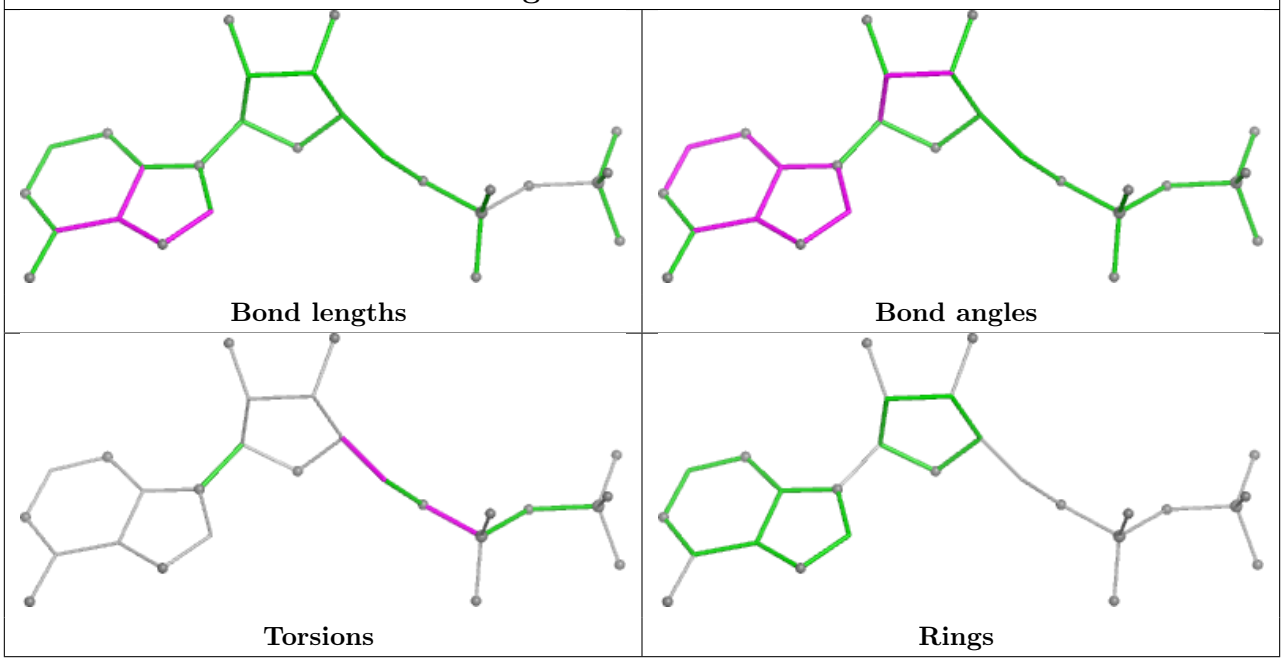


Rings

Ligand ADP U 502



Ligand ADP R 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

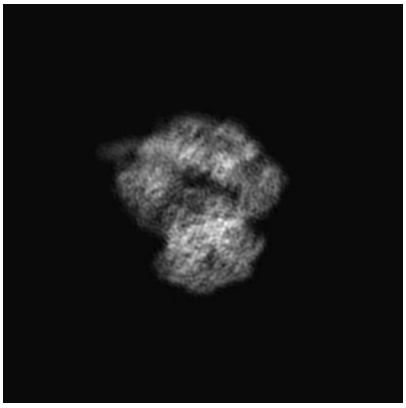
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4396. These allow visual inspection of the internal detail of the map and identification of artifacts.

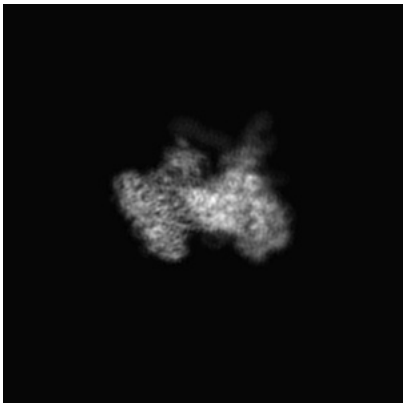
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

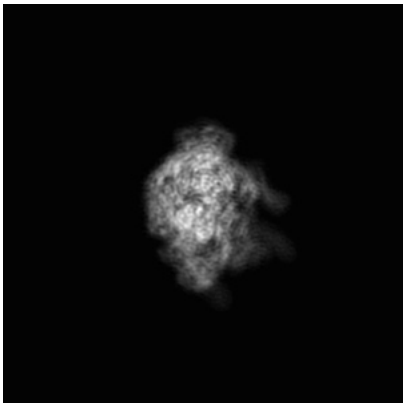
6.1.1 Primary map



X



Y

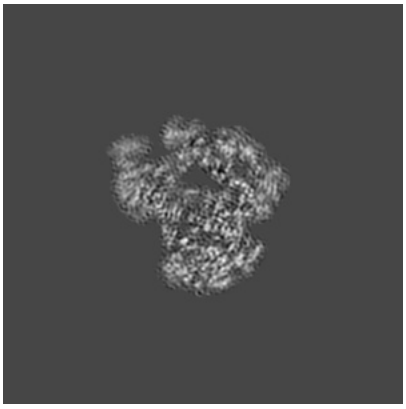


Z

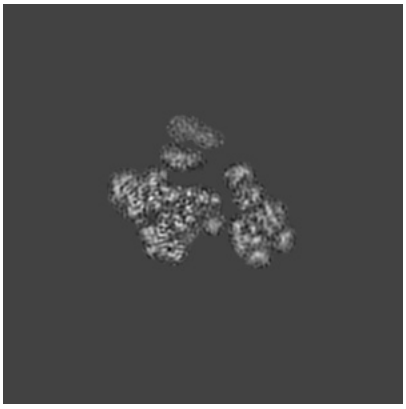
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

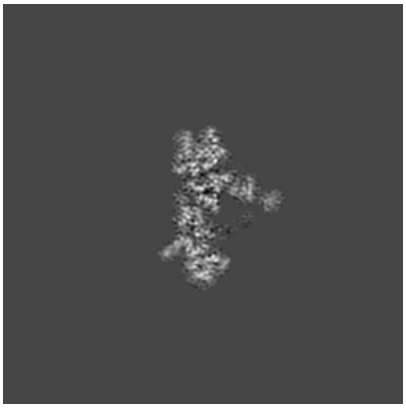
6.2.1 Primary map



X Index: 192



Y Index: 192

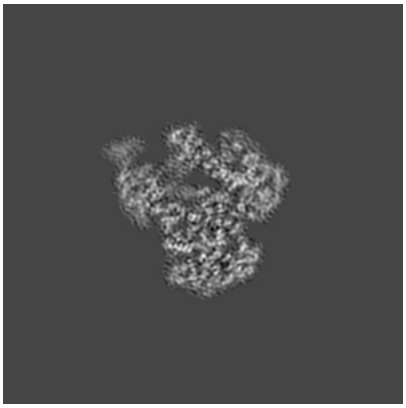


Z Index: 192

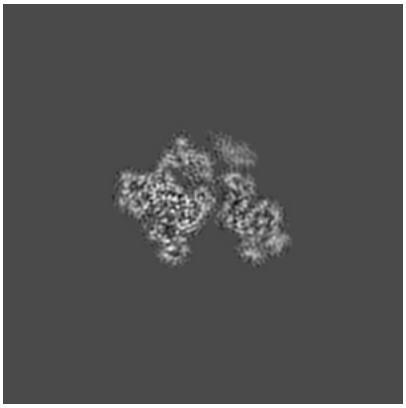
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 197



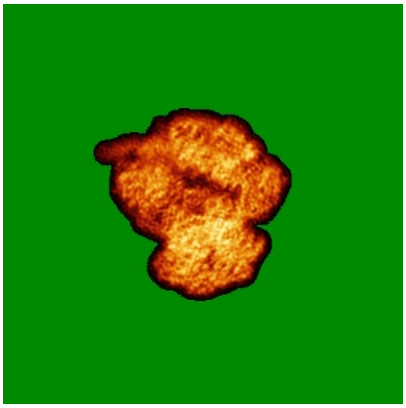
Y Index: 207

Z Index: 154

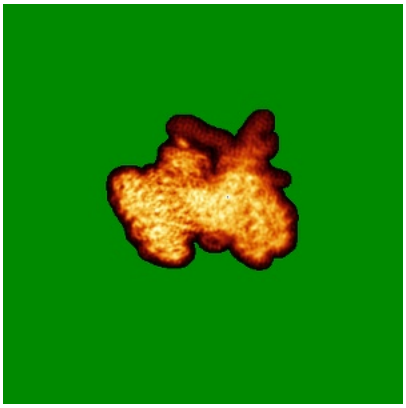
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

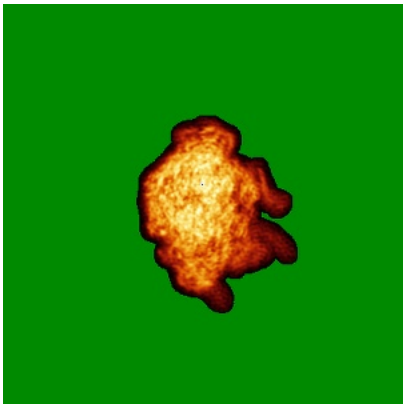
6.4.1 Primary map



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

The images above show the 3D surface view of the map at the recommended contour level 0.0359. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

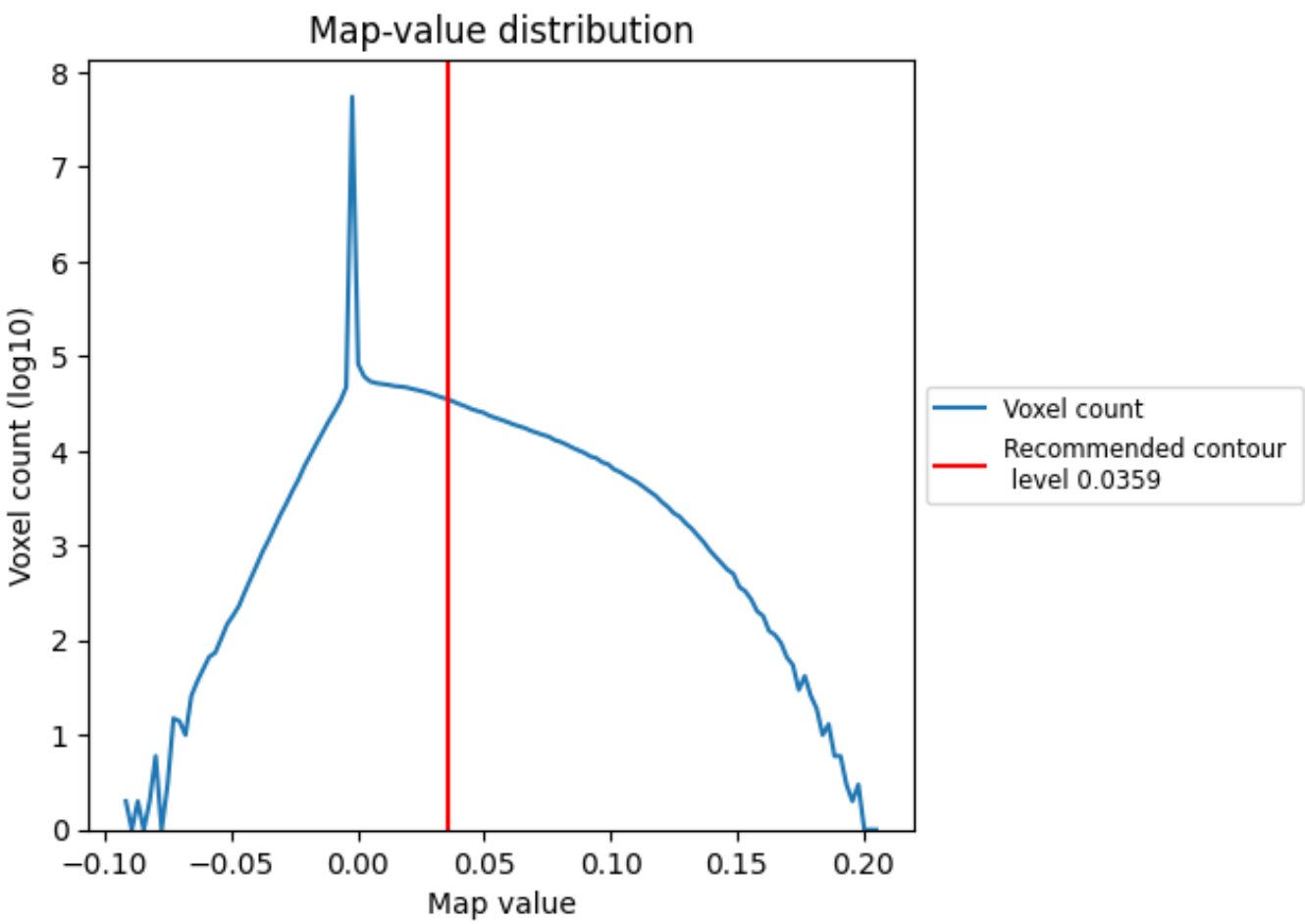
6.6 Mask visualisation (i)

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

7 Map analysis (i)

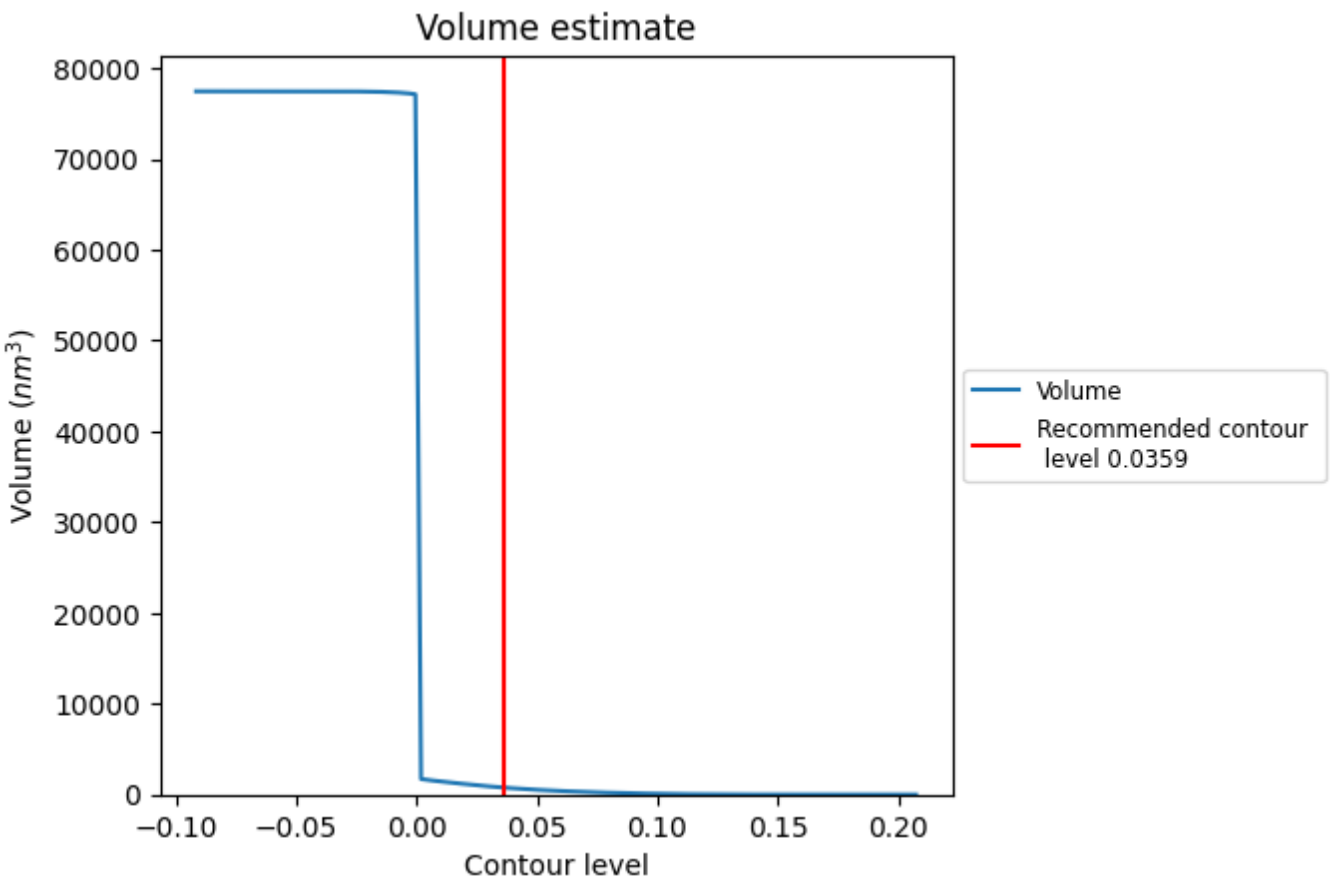
This section contains the results of statistical analysis of the map.

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.

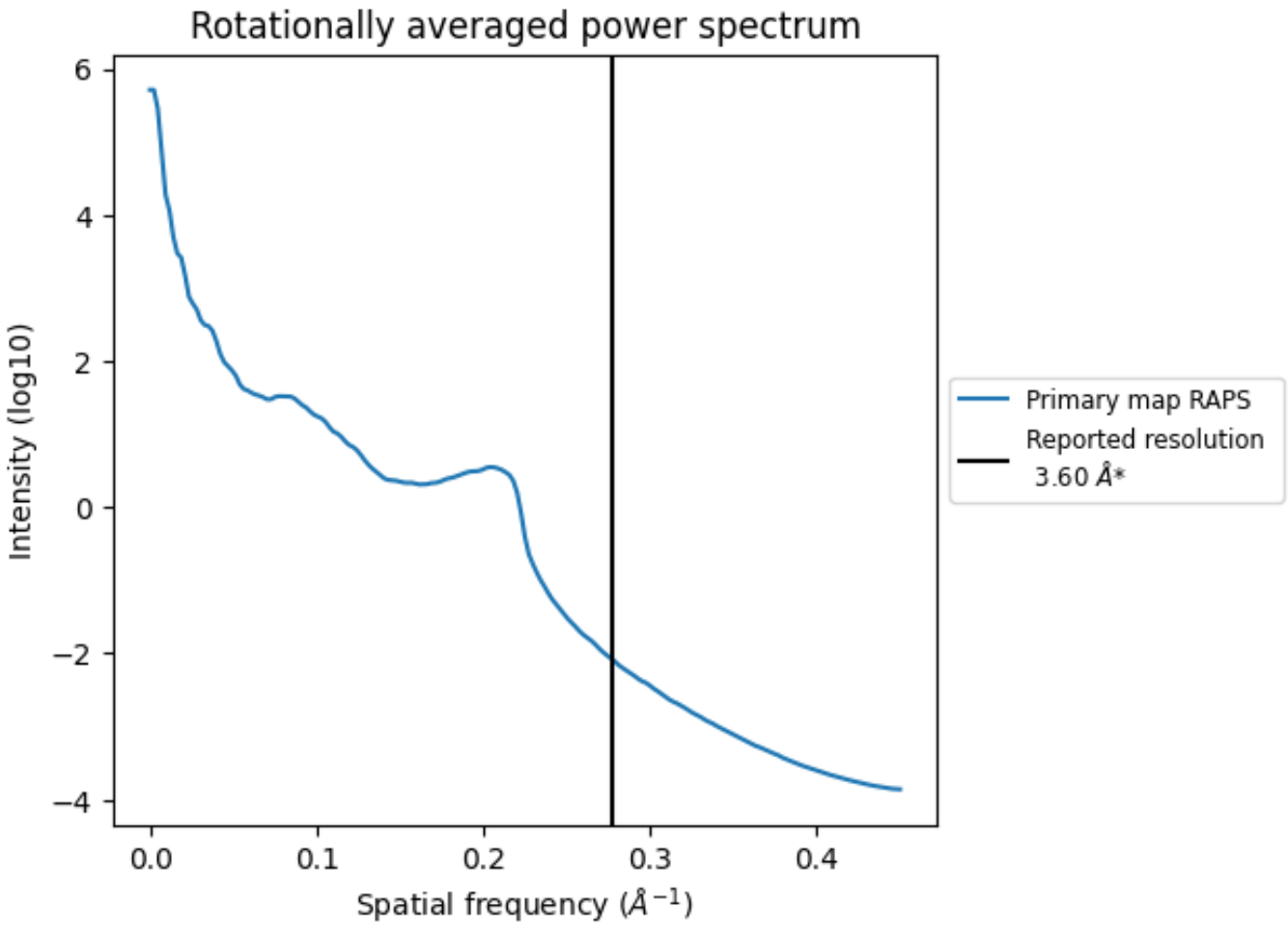
7.2 Volume estimate (i)



The volume at the recommended contour level is 773 nm^3; this corresponds to an approximate mass of 699 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 0.278 Å^{-1}

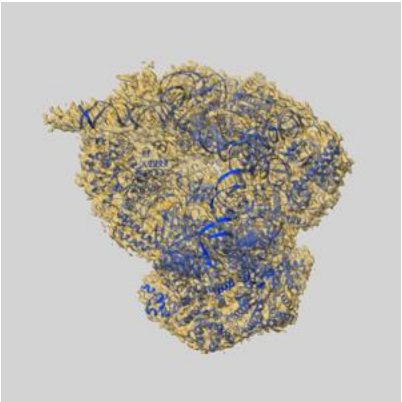
8 Fourier-Shell correlation (i)

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

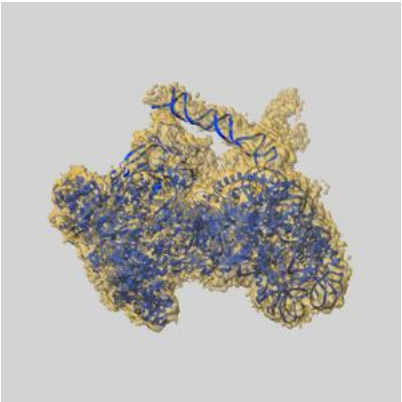
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4396 and PDB model 6GEN. Per-residue inclusion information can be found in section 3 on page 9.

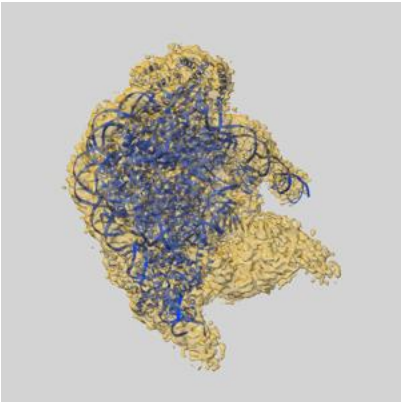
9.1 Map-model overlay (i)



X



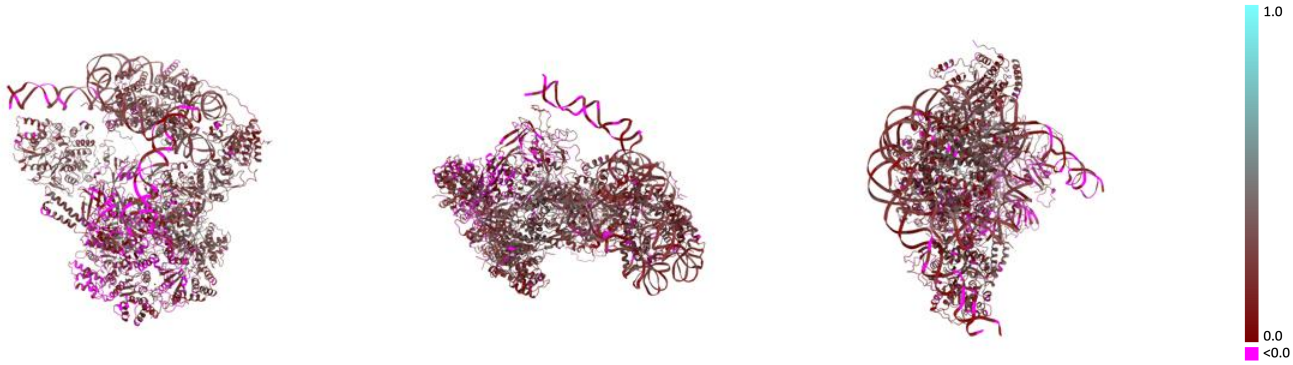
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0359 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.

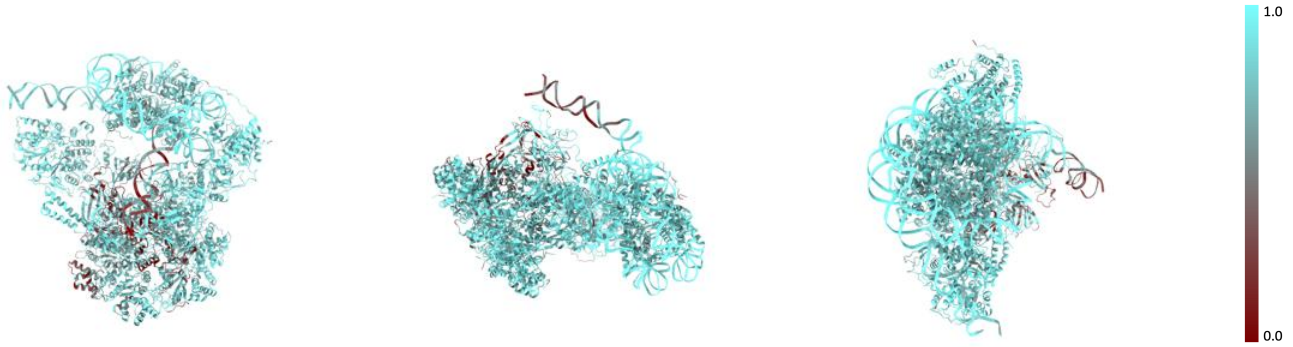
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

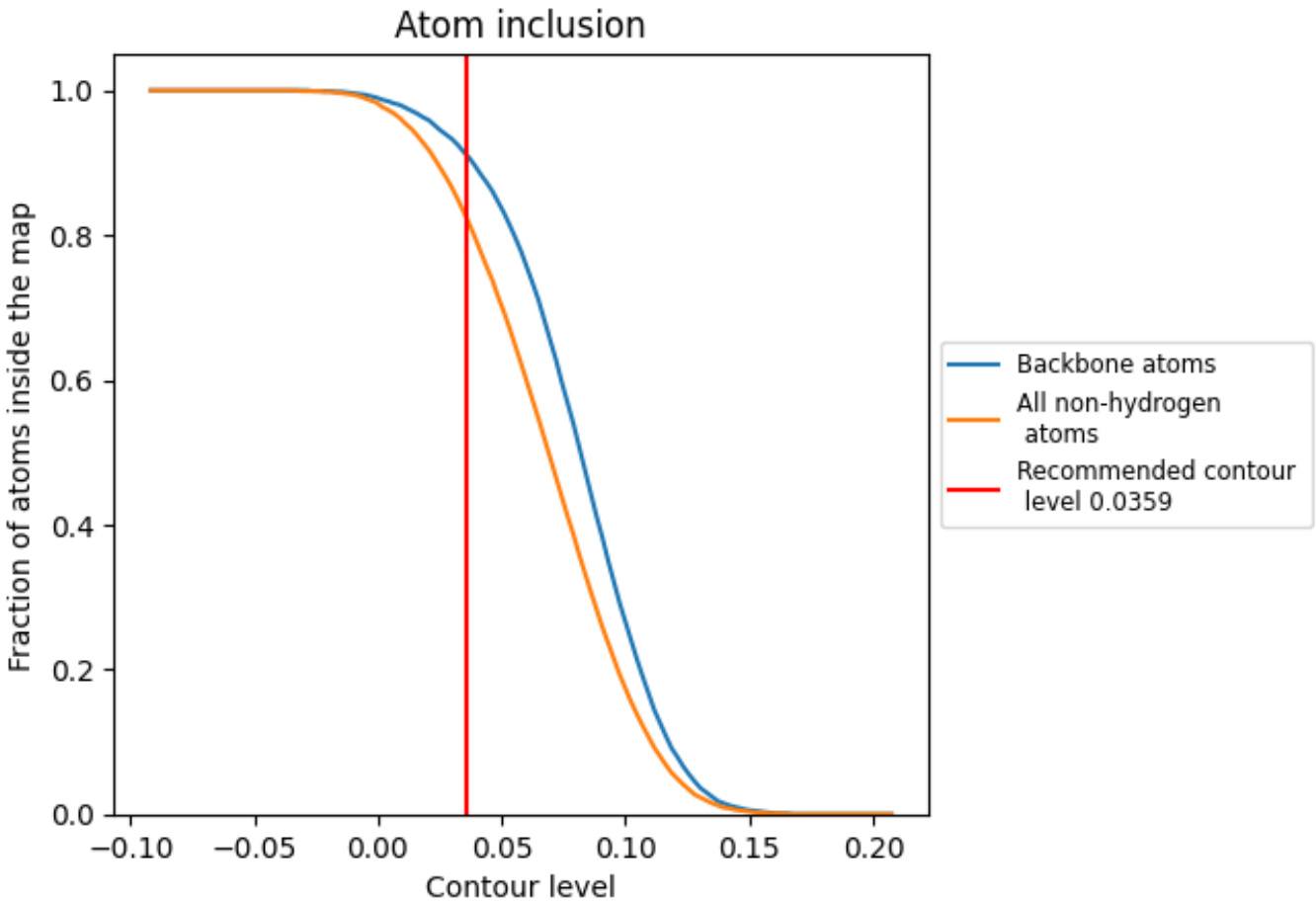
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0359).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0359) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8230	0.1950
A	0.8400	0.2140
B	0.8510	0.2570
C	0.8370	0.2540
D	0.8220	0.2200
E	0.8630	0.2360
F	0.8400	0.2110
G	0.8470	0.2050
H	0.8410	0.2100
I	0.8930	0.1780
J	0.8690	0.1740
M	0.8820	0.2540
R	0.8890	0.2410
S	0.8510	0.2350
T	0.7380	0.1230
U	0.8180	0.2130
V	0.8580	0.2770
W	0.8710	0.2680
X	0.6410	0.0630
Y	0.6730	0.0610
Z	0.8850	0.1990