Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 05:22 pm GMT

PDB ID	:	5O09
EMDB ID	:	EMD-3726
Title	:	BtubABC mini microtubule
Authors	:	Deng, X.; Bharat, T.A.M.; Lowe, J.
Deposited on	:	2017-05-16
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 (1)) were used in the production of this report:

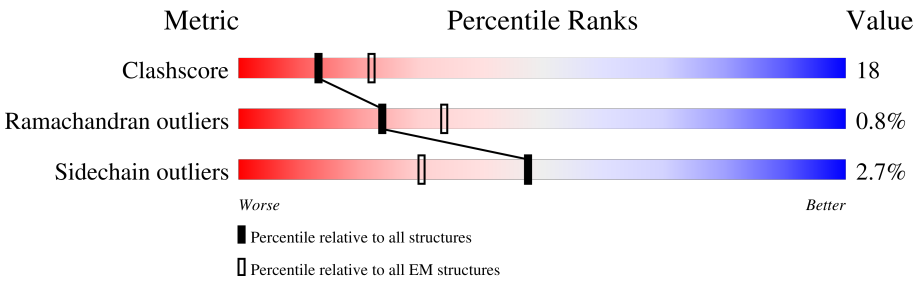
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1A	433	• 73% 26% •
1	2A	433	5% 72% 27% •
1	3A	433	10% 74% 25% •
1	4A	433	10% 73% 25% •
1	5A	433	13% 70% 28% •
1	6A	433	17% 68% 31% •
1	7A	433	22% 69% 29% •
1	8A	433	29% 70% 29% •

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Mol	Chain	Length	Quality of chain
2	1B	426	66% 29%
2	2B	426	5% 65% 30%
2	3B	426	6% 66% 29%
2	4B	426	8% 67% 27%
2	5B	426	13% 69% 25%
2	6B	426	16% 71% 24%
2	7B	426	16% 71% 24%
2	8B	426	32% 71% 24%
3	1C	238	89% 86% 11%
3	2C	238	92% 87% 11%
3	3C	238	97% 86% 11%
3	4C	238	100% 87% 10%
3	5C	238	95% 86% 11%
3	6C	238	93% 87% 11%
3	7C	238	100% 86% 11%
3	8C	238	100% 86% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 67424 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 Tubulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1A	433	3307	2105	556	629	17	0	0
1	2A	433	3307	2105	556	629	17	0	0
1	3A	433	3307	2105	556	629	17	0	0
1	4A	433	3307	2105	556	629	17	0	0
1	5A	433	3307	2105	556	629	17	0	0
1	6A	433	3307	2105	556	629	17	0	0
1	7A	433	3307	2105	556	629	17	0	0
1	8A	433	3307	2105	556	629	17	0	0

- Molecule 2 is a protein called Tubulin BtubB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1B	410	3167	2007	554	594	12	0	0
2	2B	410	3167	2007	554	594	12	0	0
2	3B	410	3167	2007	554	594	12	0	0
2	4B	410	3167	2007	554	594	12	0	0
2	5B	410	3167	2007	554	594	12	0	0
2	6B	410	3167	2007	554	594	12	0	0
2	7B	410	3167	2007	554	594	12	0	0

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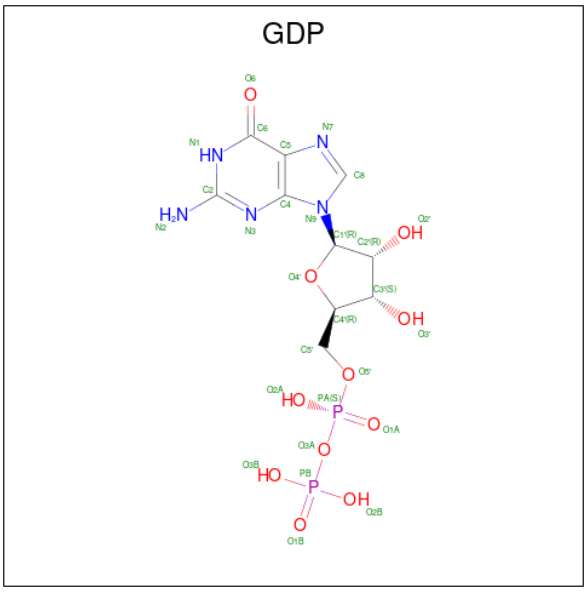
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	8B	410	3167	2007	554	594	12	0	0

- Molecule 3 is a protein called Bacterial kinesin light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1C	238	1898	1185	348	357	8	0	0
3	2C	238	1898	1185	348	357	8	0	0
3	3C	238	1898	1185	348	357	8	0	0
3	4C	238	1898	1185	348	357	8	0	0
3	5C	238	1898	1185	348	357	8	0	0
3	6C	238	1898	1185	348	357	8	0	0
3	7C	238	1898	1185	348	357	8	0	0
3	8C	238	1898	1185	348	357	8	0	0

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



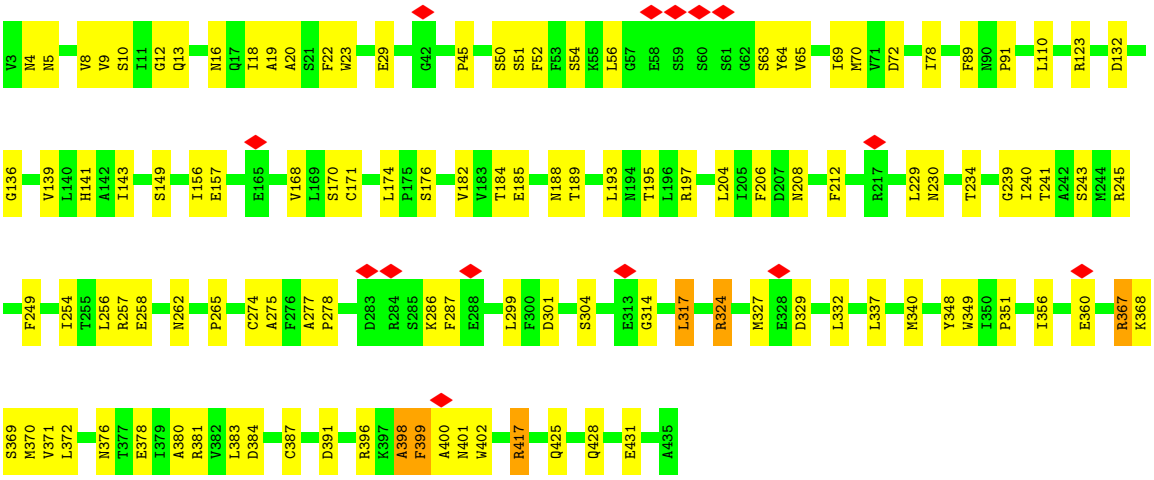
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	1A	1	28	10	5	11	2	0
4	1B	1	28	10	5	11	2	0
4	2A	1	28	10	5	11	2	0
4	2B	1	28	10	5	11	2	0
4	3A	1	28	10	5	11	2	0
4	3B	1	28	10	5	11	2	0
4	4A	1	28	10	5	11	2	0
4	4B	1	28	10	5	11	2	0
4	5A	1	28	10	5	11	2	0
4	5B	1	28	10	5	11	2	0
4	6A	1	28	10	5	11	2	0
4	6B	1	28	10	5	11	2	0
4	7A	1	28	10	5	11	2	0
4	7B	1	28	10	5	11	2	0
4	8A	1	28	10	5	11	2	0
4	8B	1	28	10	5	11	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.

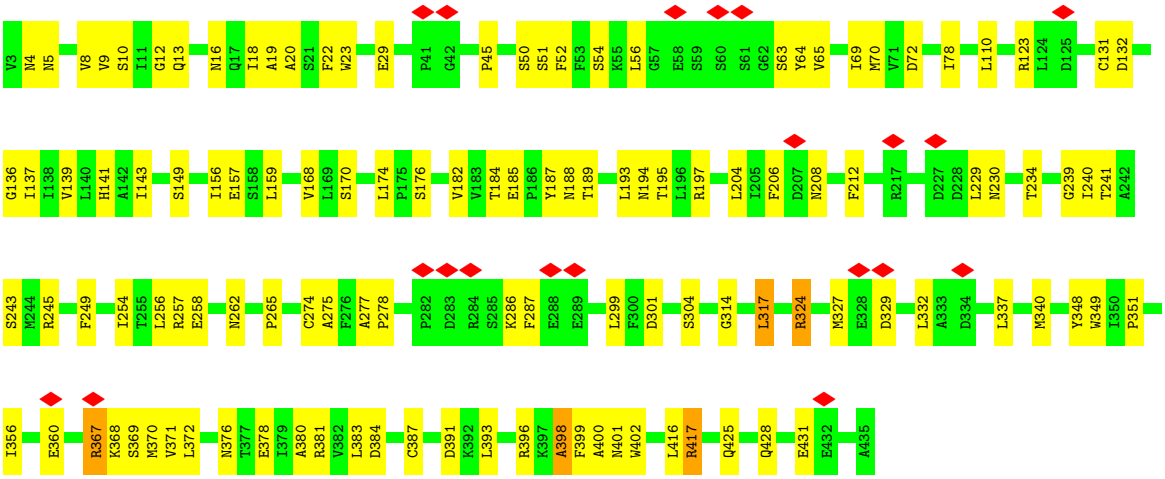
- Molecule 1: Tubulin

Chain 1A:



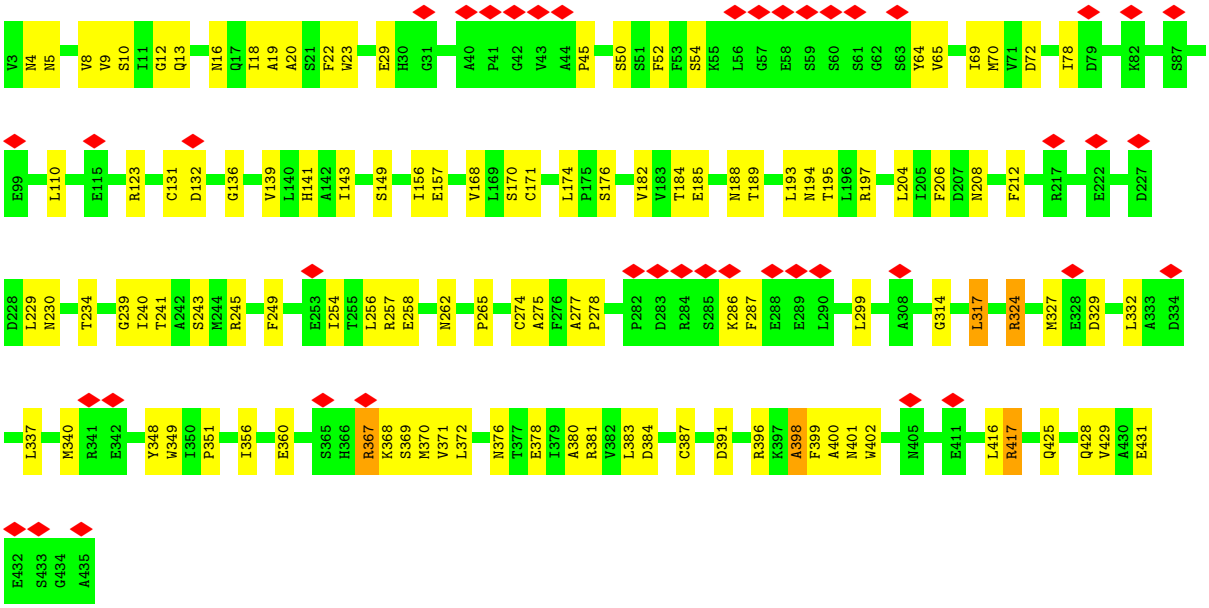
- Molecule 1: Tubulin

Chain 2A:



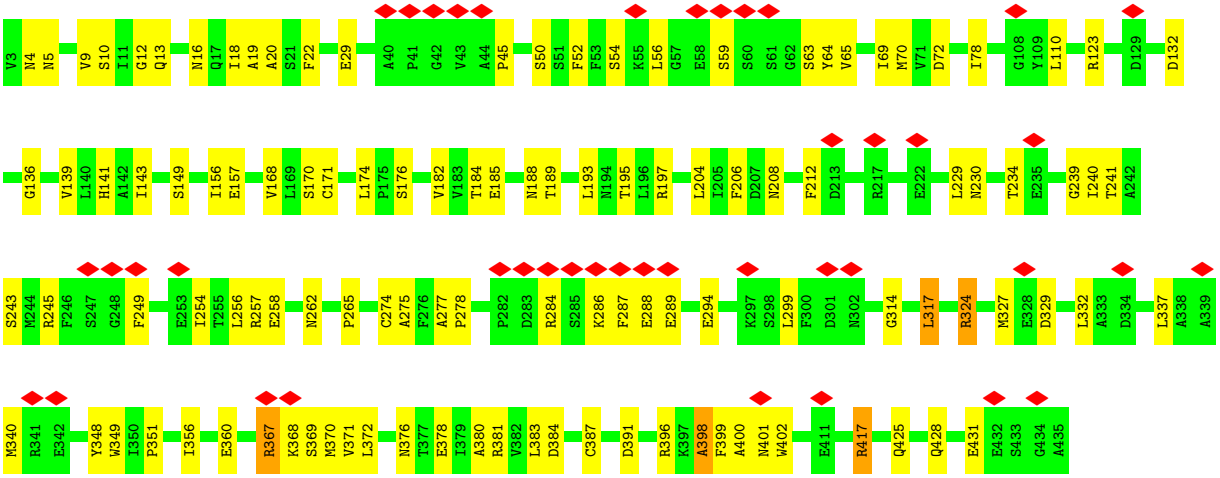
- Molecule 1: Tubulin

Chain 3A:



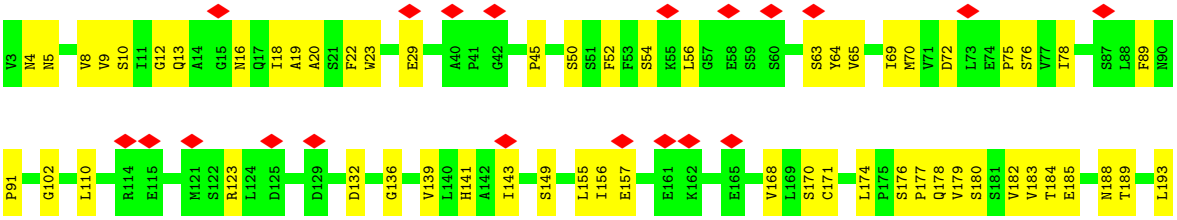
- Molecule 1: Tubulin

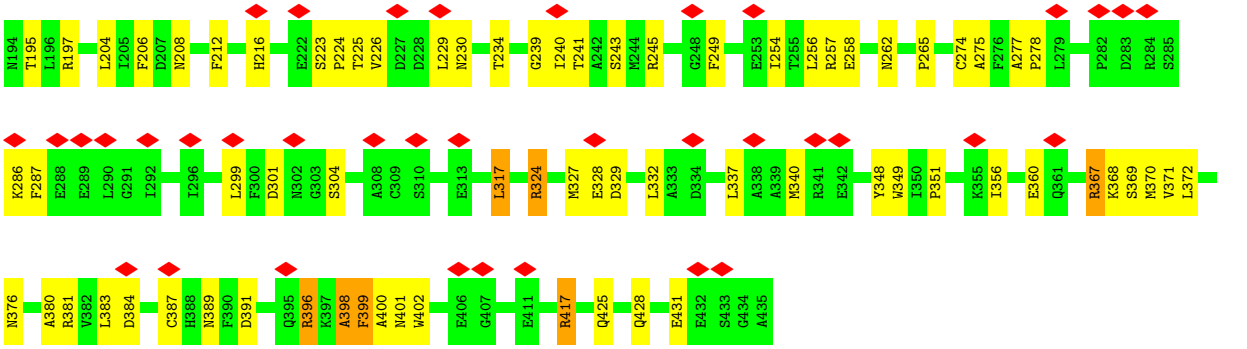
Chain 4A:



- Molecule 1: Tubulin

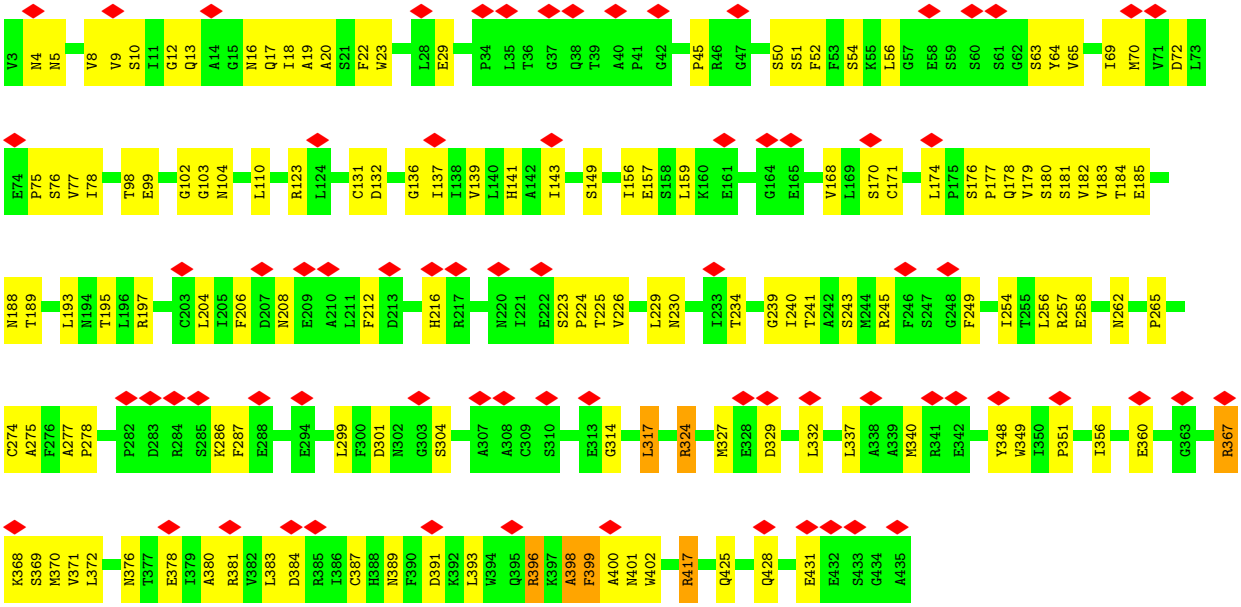
Chain 5A:





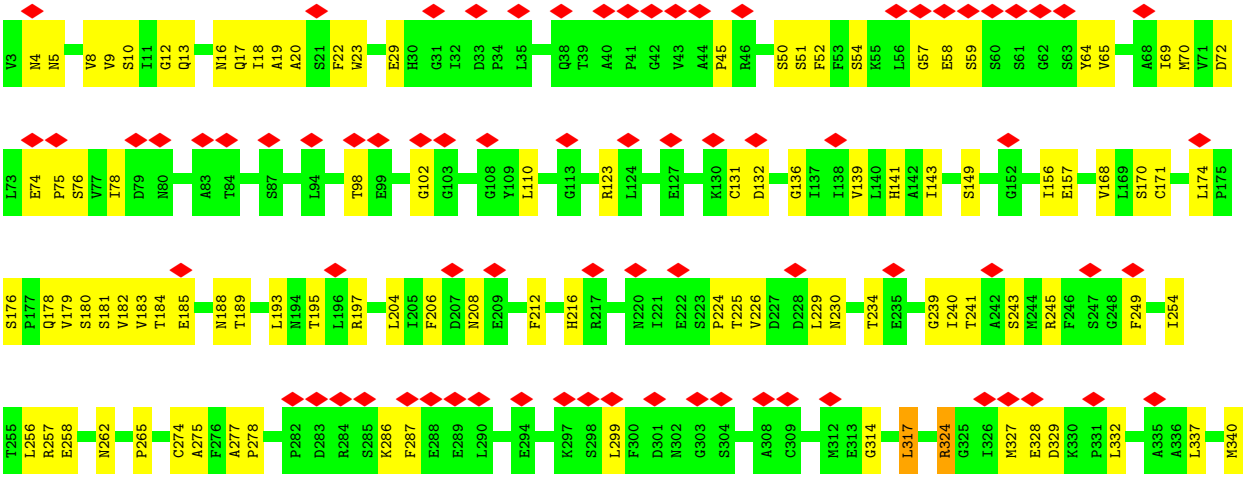
- Molecule 1: Tubulin

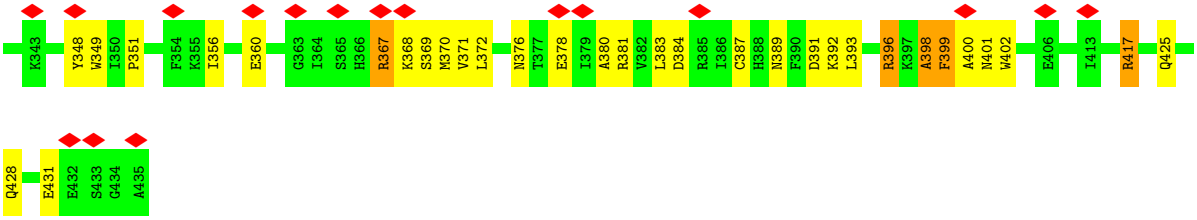
Chain 6A:



- Molecule 1: Tubulin

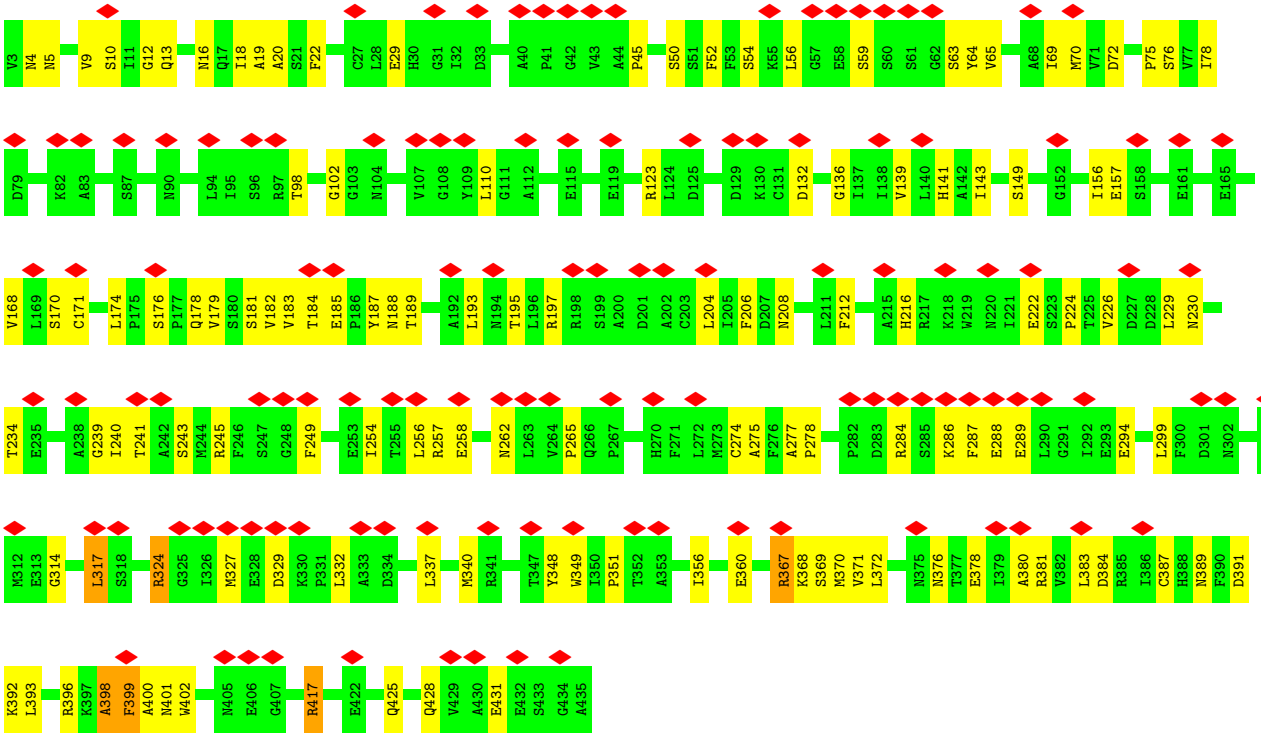
Chain 7A:





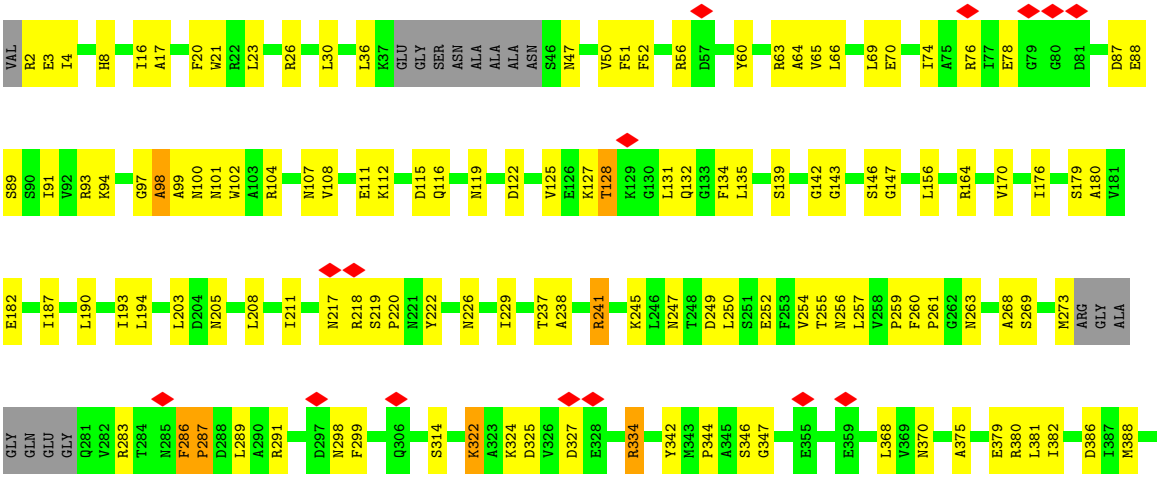
• Molecule 1: Tubulin

Chain 8A:



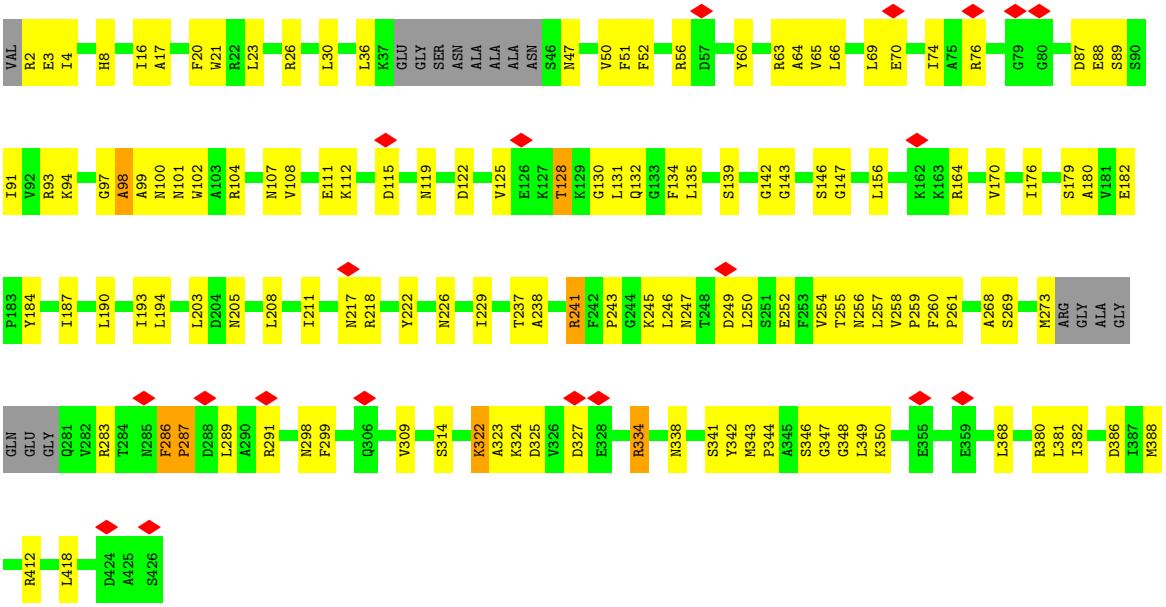
• Molecule 2: Tubulin BtubB

Chain 1B:



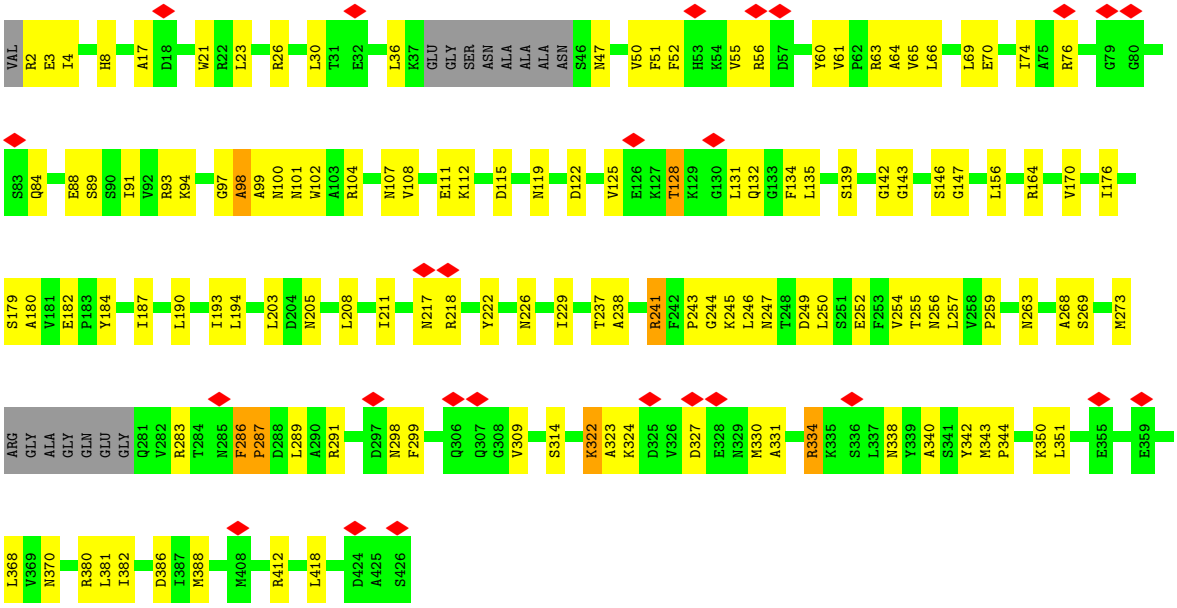
• Molecule 2: Tubulin BtubB

Chain 2B:



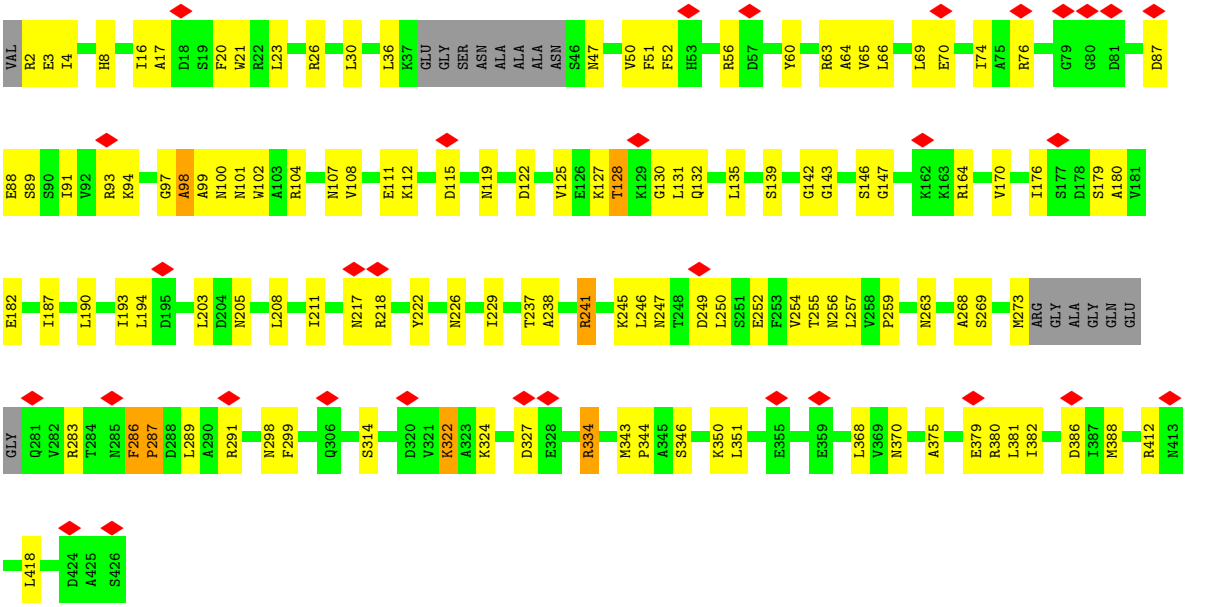
• Molecule 2: Tubulin BtubB

Chain 3B:



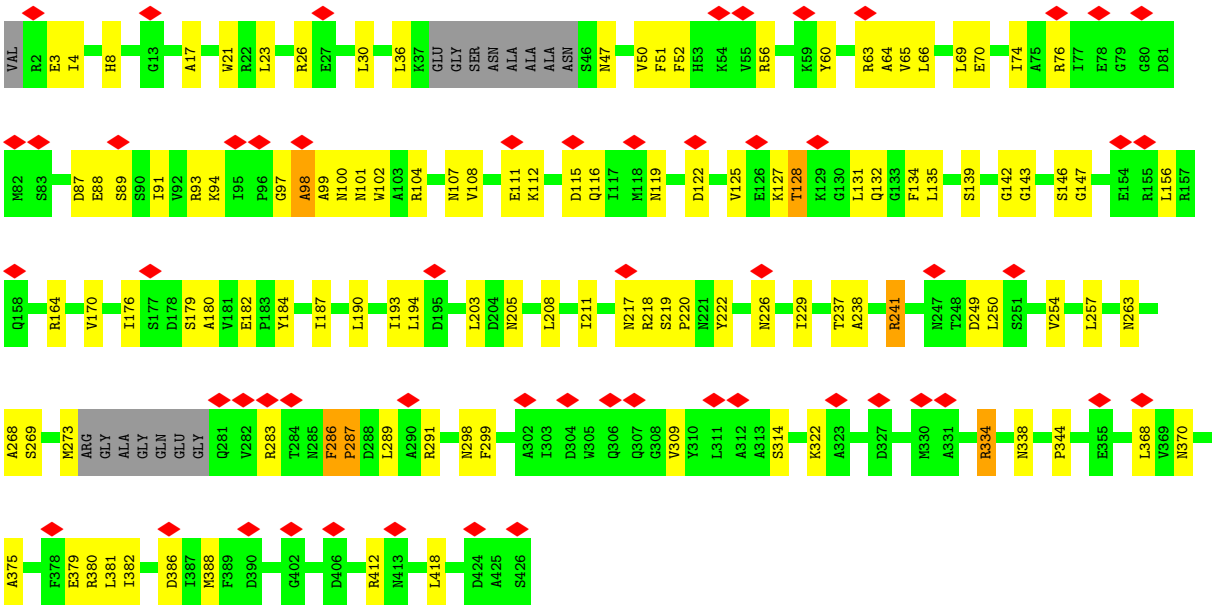
• Molecule 2: Tubulin BtubB

Chain 4B:



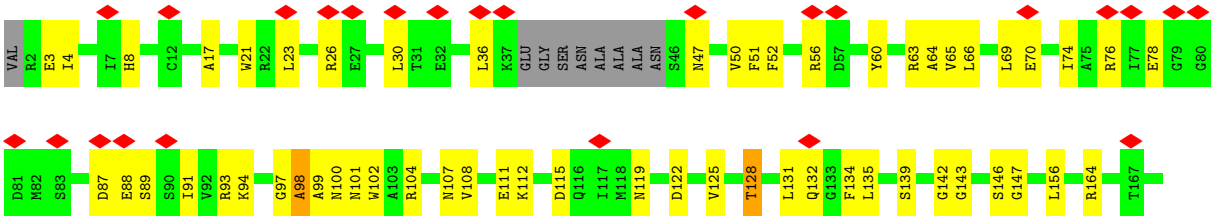
- Molecule 2: Tubulin BtubB

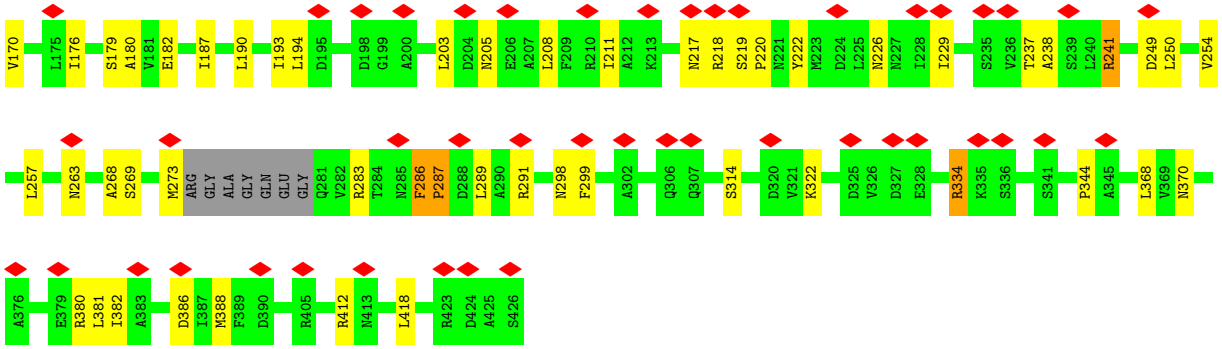
Chain 5B:



- Molecule 2: Tubulin BtubB

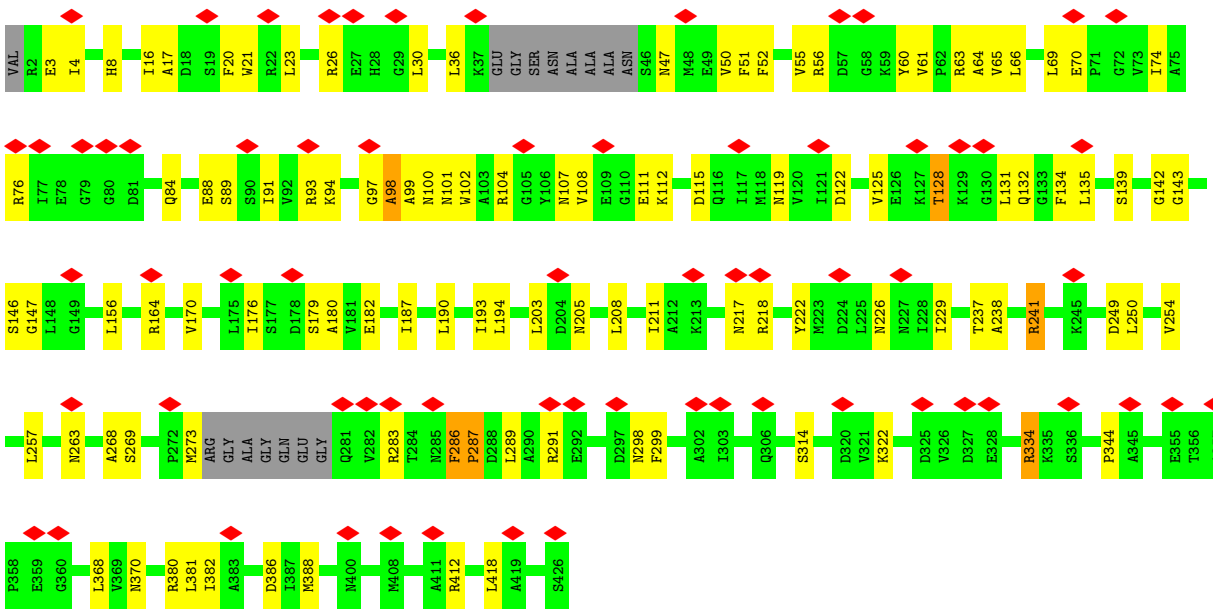
Chain 6B:





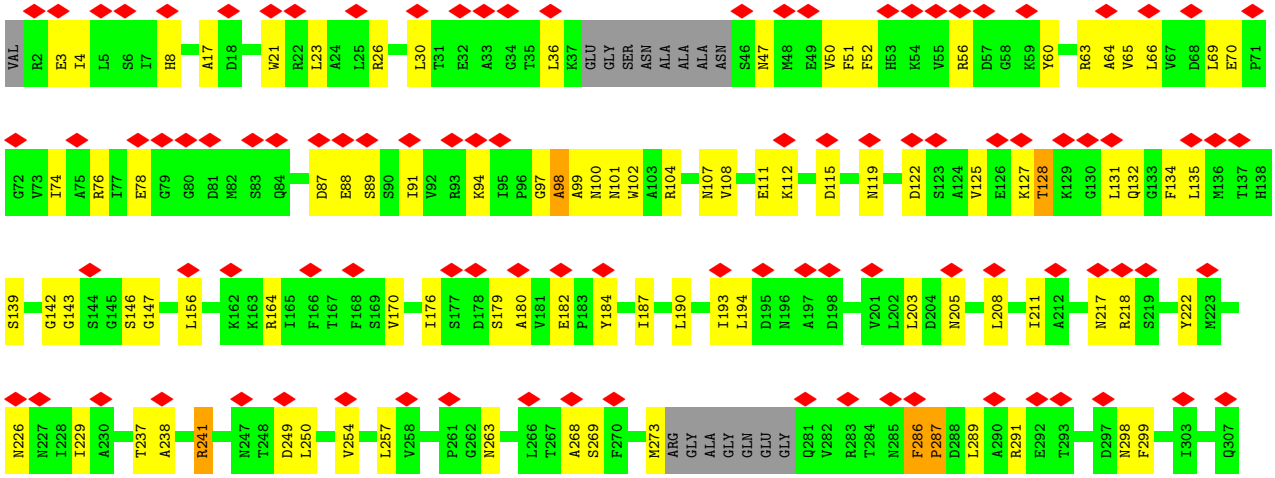
- Molecule 2: Tubulin BtubB

Chain 7B:



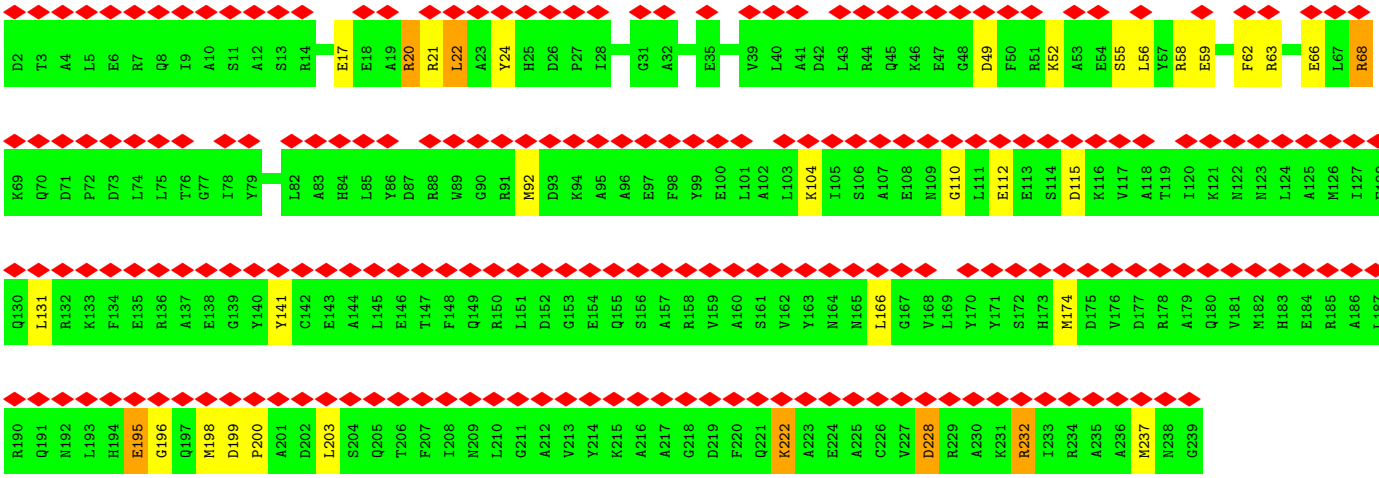
- Molecule 2: Tubulin BtubB

Chain 8B:



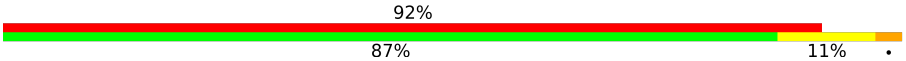
• Molecule 3: Bacterial kinesin light chain

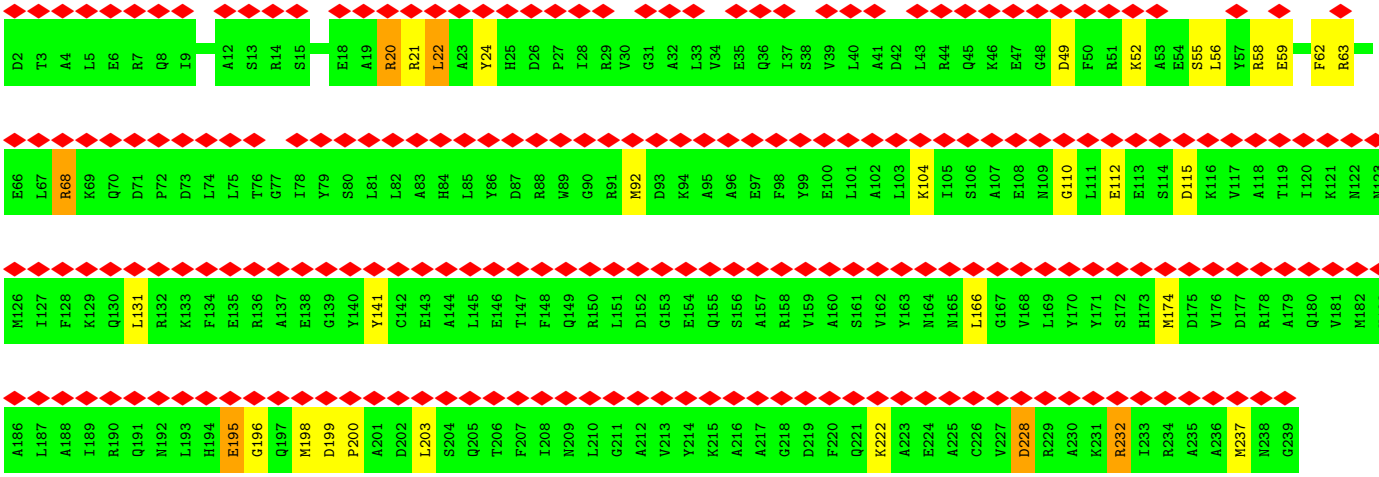
Chain 1C:



• Molecule 3: Bacterial kinesin light chain

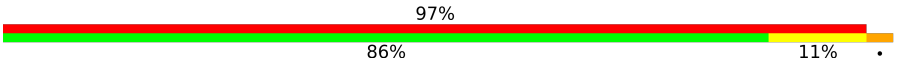
Chain 2C:





• Molecule 3: Bacterial kinesin light chain

Chain 3C:



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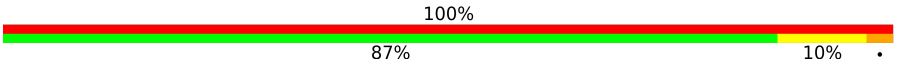
F62 R63 A64 Q65 E66 L67 R68 K69 Q70 D71 P72 D73 L74 L75 T76 G77 I78 Y79 S80 L81 L82 A83 H84 L85 Y86 D87 R88 W89 G90 R91 M92 D93 K94 A95 A96 E97 F98 Y99 E100 L101 A102 L103 K104 I105 S106 A107 E108 N109 G110 L111 E112 E113 S114 D115 K116 V117 A118 T119 I120 K121

N122 N123 L124 A125 M126 I127 F128 K129 Q130 L131 R132 K133 F134 E135 R136 A137 E138 G139 Y140 Y141 C142 E143 A144 L145 E146 T147 F148 Q149 R150 L151 D152 G153 E154 Q155 S156 A157 R158 V159 A160 S161 V162 Y163 N164 N165 L166 G167 V168 L169 Y170 Y171 S172 H173 M174 D175 V176 D177 R178 A179 Q180 V181

M182 H183 E184 R185 A186 L187 A188 I189 R190 Q191 N192 L193 H194 E195 G196 Q197 M198 D199 P200 A201 D202 L203 S204 Q205 T206 F207 I208 N209 L210 G211 A212 V213 Y214 K215 A216 A217 G218 D219 F220 Q221 K222 A223 E224 A225 C226 V227 D228 R229 A230 K231 R232 I233 R234 A235 A236 M237 N238 G239

- Molecule 3: Bacterial kinesin light chain

Chain 4C:



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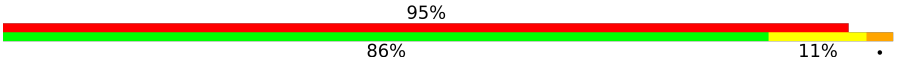
F62 R63 A64 Q65 E66 L67 R68 K69 Q70 D71 P72 D73 L74 L75 T76 G77 I78 Y79 S80 L81 L82 A83 H84 L85 Y86 D87 R88 W89 G90 R91 M92 D93 K94 A95 A96 E97 F98 Y99 E100 L101 A102 L103 K104 I105 S106 A107 E108 N109 G110 L111 E112 E113 S114 D115 K116 V117 A118 T119 I120 K121

N122 N123 L124 A125 M126 I127 F128 K129 Q130 L131 R132 K133 F134 E135 R136 A137 E138 G139 Y140 Y141 C142 E143 A144 L145 E146 T147 F148 Q149 R150 L151 D152 G153 E154 Q155 S156 A157 R158 V159 A160 S161 V162 Y163 N164 N165 L166 G167 V168 L169 Y170 Y171 S172 H173 M174 D175 V176 D177 R178 A179 Q180 V181

M182 H183 E184 R185 A186 L187 A188 I189 R190 Q191 N192 L193 H194 E195 G196 Q197 M198 D199 P200 A201 D202 L203 S204 Q205 T206 F207 I208 N209 L210 G211 A212 V213 Y214 K215 A216 A217 G218 D219 F220 Q221 K222 A223 E224 A225 C226 V227 D228 R229 A230 K231 R232 I233 R234 A235 A236 M237 N238 G239

- Molecule 3: Bacterial kinesin light chain

Chain 5C:



D2 T3 A4 L5 E6 R7 Q8 I9 A10 S11 A12 S13 R14 S15 V16 E17 E18 A19 R20 R21 L22 A23 Y24 H25 D26 P27 I28 R29 V30 G31 A32 L33 V34 E35 Q36 I37 S38 V39 L40 A41 D42 L43 R44 Q45 K46 E47 G48 D49 F50 R51 K52 A53 E54 S55 L56 Y57 R58 E59 A60 L61

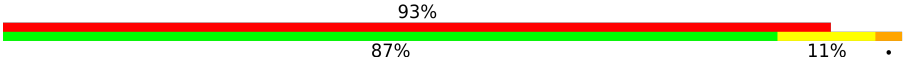
F62 R63 A64 Q65 E66 L67 R68 K69 Q70 D71 P72 D73 L74 L75 T76 G77 I78 Y79 S80 L81 L82 A83 H84 L85 Y86 D87 R88 W89 G90 R91 M92 D93 K94 A95 A96 E97 F98 Y99 E100 L101 A102 L103 K104 I105 S106 A107 E108 N109 G110 L111 E112 E113 S114 D115 K116 V117 A118 T119 I120 K121

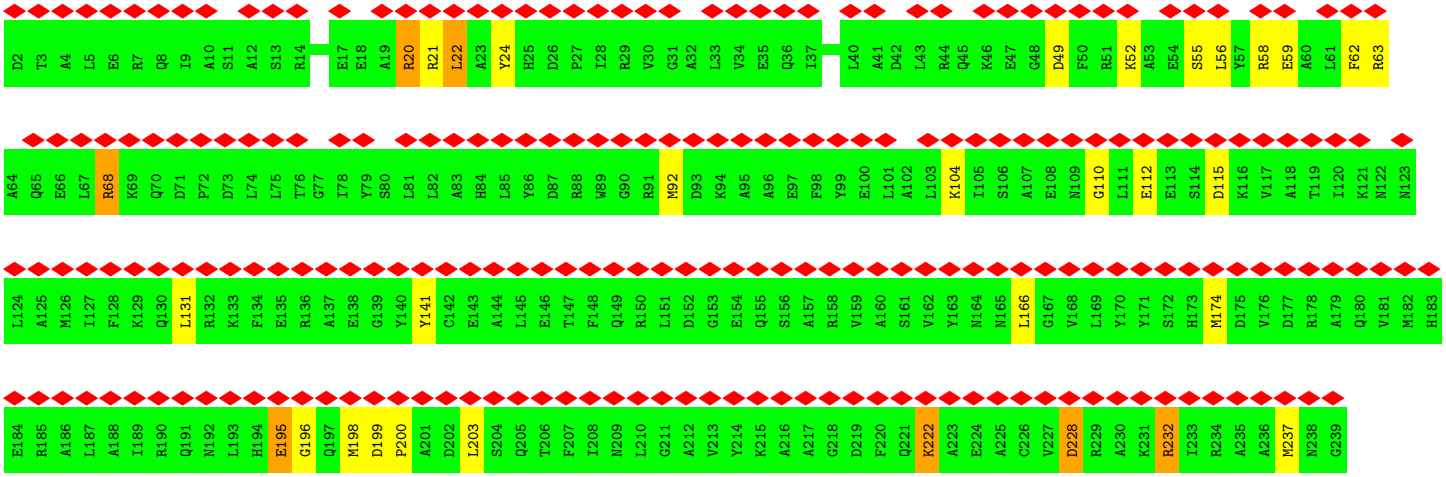
N122 N123 L124 A125 M126 I127 F128 K129 Q130 L131 R132 K133 F134 E135 R136 A137 E138 G139 Y140 Y141 C142 E143 A144 L145 E146 T147 F148 Q149 R150 L151 D152 G153 E154 Q155 S156 A157 R158 V159 A160 S161 V162 Y163 N164 N165 L166 G167 V168 L169 Y170 Y171 S172 H173 M174 D175 V176 D177 R178 A179 Q180 V181

M182 H183 E184 R185 A186 L187 A188 I189 R190 Q191 N192 L193 H194 E195 G196 Q197 M198 D199 P200 A201 D202 L203 S204 Q205 T206 F207 I208 N209 L210 G211 A212 V213 Y214 K215 A216 A217 G218 D219 F220 Q221 K222 A223 E224 A225 C226 V227 D228 R229 A230 K231 R232 I233 R234 A235 A236 M237 N238 G239

• Molecule 3: Bacterial kinesin light chain

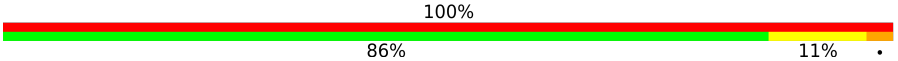
Chain 6C:

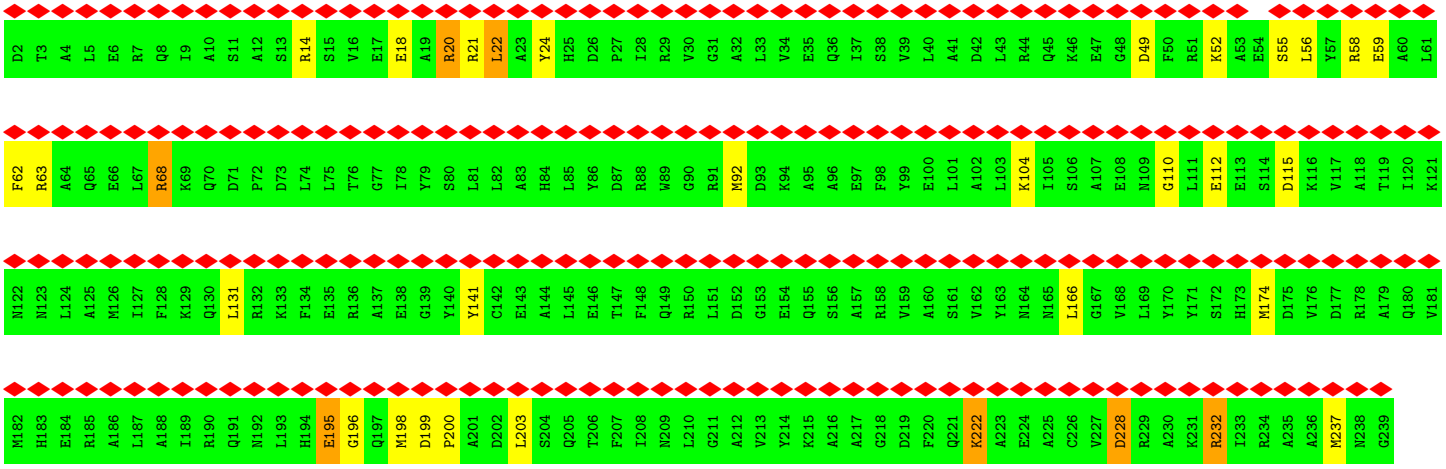




• Molecule 3: Bacterial kinesin light chain

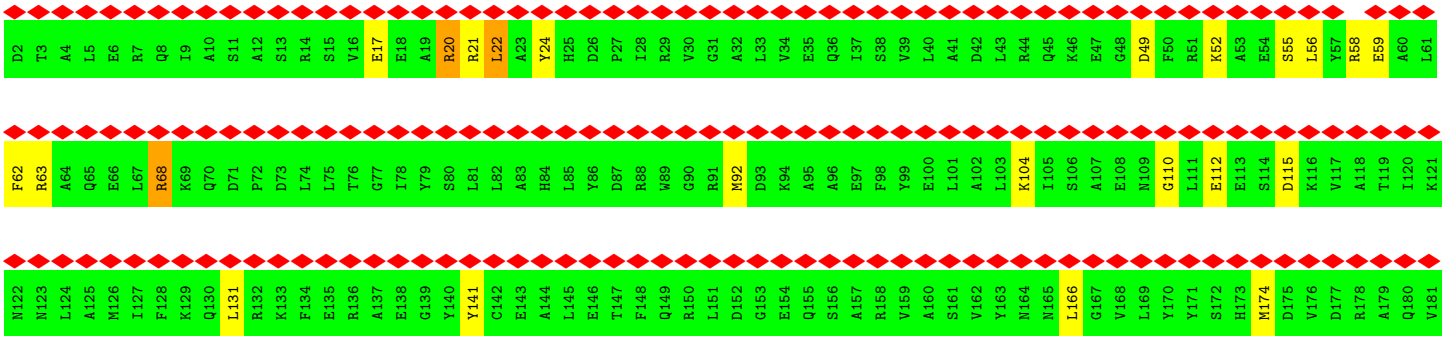
Chain 7C:

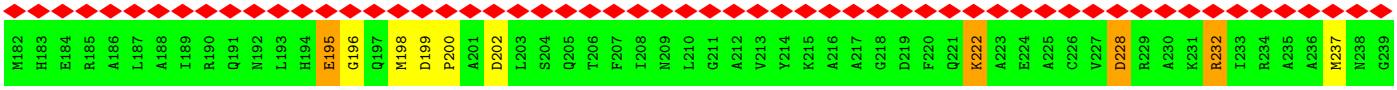




• Molecule 3: Bacterial kinesin light chain

Chain 8C:




M182
H183
E184
R185
A186
L187
A188
I189
R190
Q191
N192
L193
H194
E195
G196
Q197
M198
D199
P200
A201
D202
L203
S204
Q205
T206
F207
I208
N209
L210
G211
A212
V213
Y214
K215
A216
A217
G218
D219
F220
Q221
K222
A223
E224
A225
C226
V227
D228
R229
A230
K231
R232
I233
R234
A235
A236
M237
N238
G239

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-5.54°, rise=79.31 Å, axial sym=C1	Depositor
Number of segments used	257661	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.730	Depositor
Minimum map value	-0.430	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.0967	Depositor
Map size (Å)	375.2, 375.2, 375.2	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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: GDP

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	1A	0.70	0/3376	0.75	3/4588 (0.1%)
1	2A	0.70	0/3376	0.75	3/4588 (0.1%)
1	3A	0.70	0/3376	0.75	3/4588 (0.1%)
1	4A	0.70	0/3376	0.75	3/4588 (0.1%)
1	5A	0.70	0/3376	0.75	3/4588 (0.1%)
1	6A	0.70	0/3376	0.75	3/4588 (0.1%)
1	7A	0.70	0/3376	0.75	3/4588 (0.1%)
1	8A	0.70	0/3376	0.75	3/4588 (0.1%)
2	1B	0.72	0/3228	0.77	3/4369 (0.1%)
2	2B	0.72	0/3228	0.77	3/4369 (0.1%)
2	3B	0.72	0/3228	0.77	3/4369 (0.1%)
2	4B	0.72	0/3228	0.77	3/4369 (0.1%)
2	5B	0.72	0/3228	0.77	3/4369 (0.1%)
2	6B	0.72	0/3228	0.77	3/4369 (0.1%)
2	7B	0.72	0/3228	0.77	3/4369 (0.1%)
2	8B	0.72	0/3228	0.77	3/4369 (0.1%)
3	1C	0.76	0/1926	0.89	3/2589 (0.1%)
3	2C	0.76	0/1926	0.89	3/2589 (0.1%)
3	3C	0.76	0/1926	0.89	3/2589 (0.1%)
3	4C	0.76	0/1926	0.89	3/2589 (0.1%)
3	5C	0.76	0/1926	0.89	3/2589 (0.1%)
3	6C	0.76	0/1926	0.89	3/2589 (0.1%)
3	7C	0.76	0/1926	0.89	3/2589 (0.1%)
3	8C	0.76	0/1926	0.89	3/2589 (0.1%)
All	All	0.72	0/68240	0.79	72/92368 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1A	0	2
1	2A	0	2
1	3A	0	2
1	4A	0	2
1	5A	0	2
1	6A	0	2
1	7A	0	2
1	8A	0	2
2	1B	0	3
2	2B	0	3
2	3B	0	3
2	4B	0	3
2	5B	0	3
2	6B	0	3
2	7B	0	3
2	8B	0	3
3	1C	0	1
3	2C	0	1
3	3C	0	1
3	4C	0	1
3	5C	0	1
3	6C	0	1
3	7C	0	1
3	8C	0	1
All	All	0	48

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5A	396	ARG	NE-CZ-NH2	7.84	124.22	120.30
1	8A	396	ARG	NE-CZ-NH2	7.78	124.19	120.30
1	4A	396	ARG	NE-CZ-NH2	7.77	124.19	120.30
1	1A	396	ARG	NE-CZ-NH2	7.75	124.18	120.30
1	6A	396	ARG	NE-CZ-NH2	7.73	124.16	120.30
1	7A	396	ARG	NE-CZ-NH2	7.69	124.14	120.30
1	3A	396	ARG	NE-CZ-NH2	7.69	124.14	120.30
1	2A	396	ARG	NE-CZ-NH2	7.68	124.14	120.30
3	2C	20	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	6A	396	ARG	NE-CZ-NH1	-7.33	116.63	120.30
3	3C	20	ARG	NE-CZ-NH1	7.33	123.96	120.30
3	6C	20	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	8A	396	ARG	NE-CZ-NH1	-7.32	116.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	4A	396	ARG	NE-CZ-NH1	-7.30	116.65	120.30
3	7C	20	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	3A	396	ARG	NE-CZ-NH1	-7.29	116.66	120.30
3	1C	20	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	2A	396	ARG	NE-CZ-NH1	-7.26	116.67	120.30
3	5C	20	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	7A	396	ARG	NE-CZ-NH1	-7.23	116.69	120.30
1	5A	396	ARG	NE-CZ-NH1	-7.22	116.69	120.30
1	1A	396	ARG	NE-CZ-NH1	-7.22	116.69	120.30
3	4C	20	ARG	NE-CZ-NH1	7.13	123.86	120.30
3	8C	20	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	7A	257	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	3A	257	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	5A	257	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	1A	257	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	6A	257	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	2A	257	ARG	NE-CZ-NH2	6.09	123.35	120.30
2	4B	65	VAL	CG1-CB-CG2	-6.08	101.17	110.90
2	8B	65	VAL	CG1-CB-CG2	-6.08	101.18	110.90
2	6B	65	VAL	CG1-CB-CG2	-6.06	101.20	110.90
2	5B	65	VAL	CG1-CB-CG2	-6.06	101.21	110.90
2	2B	65	VAL	CG1-CB-CG2	-6.06	101.21	110.90
2	7B	65	VAL	CG1-CB-CG2	-6.05	101.22	110.90
2	1B	65	VAL	CG1-CB-CG2	-6.05	101.22	110.90
2	3B	65	VAL	CG1-CB-CG2	-6.05	101.23	110.90
1	4A	257	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	8A	257	ARG	NE-CZ-NH2	5.89	123.25	120.30
3	6C	20	ARG	NE-CZ-NH2	-5.76	117.42	120.30
3	7C	20	ARG	NE-CZ-NH2	-5.75	117.43	120.30
3	3C	20	ARG	NE-CZ-NH2	-5.72	117.44	120.30
3	5C	20	ARG	NE-CZ-NH2	-5.67	117.47	120.30
3	2C	20	ARG	NE-CZ-NH2	-5.67	117.47	120.30
3	4C	20	ARG	NE-CZ-NH2	-5.66	117.47	120.30
3	8C	20	ARG	NE-CZ-NH2	-5.63	117.49	120.30
3	1C	20	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	5B	380	ARG	NE-CZ-NH2	5.48	123.04	120.30
2	4B	380	ARG	NE-CZ-NH2	5.47	123.03	120.30
2	8B	380	ARG	NE-CZ-NH2	5.46	123.03	120.30
2	1B	380	ARG	NE-CZ-NH2	5.46	123.03	120.30
2	3B	380	ARG	NE-CZ-NH2	5.46	123.03	120.30
2	2B	380	ARG	NE-CZ-NH2	5.43	123.02	120.30
2	7B	380	ARG	NE-CZ-NH2	5.43	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6B	380	ARG	NE-CZ-NH2	5.41	123.00	120.30
3	4C	22	LEU	CA-CB-CG	5.28	127.43	115.30
3	8C	22	LEU	CA-CB-CG	5.27	127.42	115.30
3	2C	22	LEU	CA-CB-CG	5.27	127.42	115.30
3	6C	22	LEU	CA-CB-CG	5.27	127.41	115.30
3	1C	22	LEU	CA-CB-CG	5.26	127.39	115.30
3	3C	22	LEU	CA-CB-CG	5.25	127.38	115.30
3	5C	22	LEU	CA-CB-CG	5.25	127.38	115.30
3	7C	22	LEU	CA-CB-CG	5.24	127.36	115.30
2	7B	241	ARG	NE-CZ-NH2	5.17	122.89	120.30
2	8B	241	ARG	NE-CZ-NH2	5.16	122.88	120.30
2	5B	241	ARG	NE-CZ-NH2	5.16	122.88	120.30
2	4B	241	ARG	NE-CZ-NH2	5.15	122.87	120.30
2	6B	241	ARG	NE-CZ-NH2	5.14	122.87	120.30
2	1B	241	ARG	NE-CZ-NH2	5.13	122.86	120.30
2	3B	241	ARG	NE-CZ-NH2	5.11	122.86	120.30
2	2B	241	ARG	NE-CZ-NH2	5.09	122.85	120.30

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1A	348	TYR	Peptide
1	1A	398	ALA	Peptide
2	1B	128	THR	Peptide
2	1B	286	PHE	Peptide
2	1B	98	ALA	Peptide
3	1C	110	GLY	Peptide
1	2A	348	TYR	Peptide
1	2A	398	ALA	Peptide
2	2B	128	THR	Peptide
2	2B	286	PHE	Peptide
2	2B	98	ALA	Peptide
3	2C	110	GLY	Peptide
1	3A	348	TYR	Peptide
1	3A	398	ALA	Peptide
2	3B	128	THR	Peptide
2	3B	286	PHE	Peptide
2	3B	98	ALA	Peptide
3	3C	110	GLY	Peptide
1	4A	348	TYR	Peptide
1	4A	398	ALA	Peptide

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Mol	Chain	Res	Type	Group
2	4B	128	THR	Peptide
2	4B	286	PHE	Peptide
2	4B	98	ALA	Peptide
3	4C	110	GLY	Peptide
1	5A	348	TYR	Peptide
1	5A	398	ALA	Peptide
2	5B	128	THR	Peptide
2	5B	286	PHE	Peptide
2	5B	98	ALA	Peptide
3	5C	110	GLY	Peptide
1	6A	348	TYR	Peptide
1	6A	398	ALA	Peptide
2	6B	128	THR	Peptide
2	6B	286	PHE	Peptide
2	6B	98	ALA	Peptide
3	6C	110	GLY	Peptide
1	7A	348	TYR	Peptide
1	7A	398	ALA	Peptide
2	7B	128	THR	Peptide
2	7B	286	PHE	Peptide
2	7B	98	ALA	Peptide
3	7C	110	GLY	Peptide
1	8A	348	TYR	Peptide
1	8A	398	ALA	Peptide
2	8B	128	THR	Peptide
2	8B	286	PHE	Peptide
2	8B	98	ALA	Peptide
3	8C	110	GLY	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	1A	3307	0	3293	108	0
1	2A	3307	0	3293	105	0
1	3A	3307	0	3293	85	0
1	4A	3307	0	3291	149	0
1	5A	3307	0	3287	223	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6A	3307	0	3289	245	0
1	7A	3307	0	3286	281	0
1	8A	3307	0	3285	267	0
2	1B	3167	0	3138	261	0
2	2B	3167	0	3136	282	0
2	3B	3167	0	3138	372	0
2	4B	3167	0	3137	250	0
2	5B	3167	0	3143	145	0
2	6B	3167	0	3143	139	0
2	7B	3167	0	3140	179	0
2	8B	3167	0	3143	126	0
3	1C	1898	0	1875	89	0
3	2C	1898	0	1874	89	0
3	3C	1898	0	1873	102	0
3	4C	1898	0	1875	84	0
3	5C	1898	0	1875	91	0
3	6C	1898	0	1874	91	0
3	7C	1898	0	1873	101	0
3	8C	1898	0	1875	83	0
4	1A	28	0	12	2	0
4	1B	28	0	12	3	0
4	2A	28	0	12	2	0
4	2B	28	0	12	3	0
4	3A	28	0	12	2	0
4	3B	28	0	12	3	0
4	4A	28	0	12	2	0
4	4B	28	0	12	3	0
4	5A	28	0	12	2	0
4	5B	28	0	12	3	0
4	6A	28	0	12	5	0
4	6B	28	0	12	3	0
4	7A	28	0	12	7	0
4	7B	28	0	12	3	0
4	8A	28	0	12	6	0
4	8B	28	0	12	3	0
All	All	67424	0	66621	2456	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 18.

All (2456) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:256:ASN:HB3	1:7A:183:VAL:CG2	1.26	1.65
2:7B:61:VAL:CG2	1:8A:287:PHE:CE2	1.78	1.60
2:2B:252:GLU:HG2	1:6A:102:GLY:CA	1.26	1.59
2:3B:61:VAL:CG2	1:4A:287:PHE:CE2	1.78	1.56
2:3B:2:ARG:HH11	1:7A:75:PRO:CG	0.95	1.55
2:7B:56:ARG:HB2	1:8A:286:LYS:CE	1.30	1.54
2:3B:61:VAL:CG2	1:4A:287:PHE:CZ	1.88	1.53
2:4B:245:LYS:HG2	1:8A:226:VAL:CG2	1.32	1.53
3:3C:18:GLU:HG3	1:4A:288:GLU:CD	1.15	1.52
2:4B:245:LYS:CG	1:8A:226:VAL:HG21	1.07	1.52
2:3B:61:VAL:HG21	1:4A:287:PHE:CE2	0.98	1.51
2:7B:61:VAL:HG21	1:8A:287:PHE:CE2	0.98	1.51
3:7C:18:GLU:HG3	1:8A:288:GLU:CD	1.15	1.51
2:7B:61:VAL:CG2	1:8A:287:PHE:CZ	1.88	1.50
2:4B:324:LYS:NZ	1:8A:216:HIS:CB	1.70	1.50
2:2B:324:LYS:HB2	1:6A:224:PRO:C	1.28	1.49
2:7B:56:ARG:CG	1:8A:286:LYS:HE2	0.99	1.45
2:3B:56:ARG:CG	1:4A:286:LYS:HE2	0.99	1.45
2:4B:324:LYS:NZ	1:8A:216:HIS:CG	1.83	1.44
2:2B:2:ARG:NE	1:6A:75:PRO:CG	1.77	1.43
2:2B:324:LYS:CB	1:6A:224:PRO:O	1.65	1.42
2:3B:84:GLN:NE2	1:4A:284:ARG:CZ	1.81	1.42
2:8B:119:ASN:HD21	3:8C:55:SER:C	1.21	1.42
1:1A:287:PHE:CE1	1:4A:65:VAL:CG1	2.01	1.41
2:2B:342:TYR:O	1:6A:393:LEU:CD2	1.66	1.41
2:4B:324:LYS:CB	1:8A:224:PRO:HD2	1.49	1.40
1:5A:287:PHE:CE1	1:8A:65:VAL:CG1	2.01	1.40
2:3B:56:ARG:CG	1:4A:286:LYS:CE	1.92	1.40
2:3B:56:ARG:HB2	1:4A:286:LYS:CE	1.30	1.40
2:7B:84:GLN:NE2	1:8A:284:ARG:CZ	1.82	1.40
2:7B:56:ARG:CB	1:8A:286:LYS:HE2	1.41	1.40
2:4B:119:ASN:HD21	3:4C:55:SER:C	1.22	1.39
2:7B:56:ARG:CG	1:8A:286:LYS:CE	1.92	1.38
2:2B:2:ARG:HE	1:6A:75:PRO:CG	1.26	1.38
2:2B:259:PRO:O	1:6A:400:ALA:CB	1.69	1.37
2:3B:56:ARG:CB	1:4A:286:LYS:HE2	1.41	1.37
2:2B:119:ASN:HD21	3:2C:55:SER:C	1.27	1.37
2:3B:2:ARG:NH1	1:7A:75:PRO:HG2	1.07	1.37
2:6B:115:ASP:OD2	3:6C:58:ARG:CB	1.73	1.36
2:1B:245:LYS:HG2	1:5A:226:VAL:CG2	1.54	1.35
2:7B:56:ARG:CB	1:8A:286:LYS:CE	1.85	1.35
1:5A:56:LEU:HD12	1:6A:286:LYS:NZ	1.40	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6B:119:ASN:HD21	3:6C:55:SER:C	1.27	1.35
2:1B:256:ASN:HA	1:5A:183:VAL:CG2	1.55	1.35
1:1A:56:LEU:HD12	1:2A:286:LYS:NZ	1.40	1.34
2:1B:324:LYS:HZ1	1:5A:216:HIS:CB	1.37	1.34
2:2B:115:ASP:OD2	3:2C:58:ARG:CB	1.73	1.34
2:3B:119:ASN:HD21	3:3C:55:SER:C	1.29	1.34
2:7B:119:ASN:HD21	3:7C:55:SER:C	1.29	1.34
2:2B:246:LEU:N	1:6A:13:GLN:HE22	1.21	1.33
2:2B:246:LEU:N	1:6A:13:GLN:NE2	1.76	1.32
2:3B:112:LYS:O	3:3C:62:PHE:CD2	1.83	1.32
2:3B:252:GLU:HG2	1:7A:102:GLY:C	1.29	1.32
2:7B:112:LYS:O	3:7C:62:PHE:CD2	1.83	1.31
2:5B:94:LYS:CE	3:5C:66:GLU:OE2	1.78	1.31
2:5B:119:ASN:HD21	3:5C:55:SER:C	1.35	1.30
2:8B:115:ASP:OD2	3:8C:58:ARG:HB3	1.31	1.30
2:4B:327:ASP:OD2	1:8A:212:PHE:HD2	1.06	1.30
2:2B:259:PRO:O	1:6A:400:ALA:HB2	1.18	1.30
2:1B:94:LYS:CE	3:1C:66:GLU:OE2	1.78	1.29
3:3C:18:GLU:CA	1:4A:288:GLU:OE2	1.80	1.29
3:7C:18:GLU:HG3	1:8A:288:GLU:OE1	1.30	1.29
2:2B:347:GLY:CA	1:6A:180:SER:OG	1.80	1.29
2:6B:115:ASP:OD2	3:6C:58:ARG:HB3	1.11	1.28
3:7C:18:GLU:CA	1:8A:288:GLU:OE2	1.80	1.28
2:2B:252:GLU:CG	1:6A:102:GLY:CA	2.08	1.28
2:2B:2:ARG:CZ	1:6A:75:PRO:HG2	1.60	1.28
2:6B:88:GLU:HG2	3:6C:24:TYR:CD2	1.68	1.28
2:1B:119:ASN:HD21	3:1C:55:SER:C	1.35	1.27
1:5A:287:PHE:CE1	1:8A:65:VAL:HG11	1.63	1.27
2:1B:259:PRO:HA	1:5A:399:PHE:CD1	1.70	1.26
2:3B:115:ASP:OD2	3:3C:58:ARG:CB	1.83	1.26
2:5B:115:ASP:OD2	3:5C:58:ARG:HB3	1.30	1.26
2:2B:88:GLU:HG2	3:2C:24:TYR:CD2	1.68	1.26
2:2B:252:GLU:CG	1:6A:102:GLY:HA3	1.64	1.26
2:3B:56:ARG:CB	1:4A:286:LYS:CE	1.85	1.26
2:2B:347:GLY:HA2	1:6A:180:SER:CB	1.66	1.26
2:3B:256:ASN:CB	1:7A:183:VAL:CG2	2.12	1.25
2:2B:115:ASP:OD2	3:2C:58:ARG:HB3	1.11	1.25
2:3B:88:GLU:HG2	3:3C:24:TYR:CD2	1.71	1.25
2:7B:88:GLU:HG2	3:7C:24:TYR:CD2	1.71	1.25
2:4B:115:ASP:OD2	3:4C:58:ARG:HB3	1.31	1.24
2:7B:115:ASP:OD2	3:7C:58:ARG:CB	1.83	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:287:PHE:CE1	1:4A:65:VAL:HG11	1.63	1.24
2:1B:256:ASN:O	1:5A:183:VAL:HG21	1.32	1.24
2:2B:94:LYS:NZ	3:2C:63:ARG:HH21	1.35	1.24
2:1B:324:LYS:NZ	1:5A:216:HIS:HB2	1.48	1.23
3:3C:18:GLU:HG3	1:4A:288:GLU:OE1	1.30	1.23
3:3C:18:GLU:CG	1:4A:288:GLU:OE1	1.86	1.23
2:4B:2:ARG:NH1	1:8A:76:SER:OG	1.68	1.23
2:7B:56:ARG:CD	1:8A:286:LYS:HE2	1.69	1.23
3:7C:18:GLU:CG	1:8A:288:GLU:OE1	1.86	1.23
2:3B:246:LEU:CD1	1:7A:181:SER:OG	1.86	1.22
2:3B:344:PRO:HB2	1:7A:389:ASN:ND2	1.52	1.22
2:6B:122:ASP:OD2	3:6C:52:LYS:CE	1.87	1.22
3:7C:18:GLU:CG	1:8A:288:GLU:CD	2.08	1.22
2:2B:122:ASP:OD2	3:2C:52:LYS:CE	1.87	1.22
2:3B:56:ARG:CD	1:4A:286:LYS:HE2	1.69	1.22
2:4B:324:LYS:NZ	1:8A:216:HIS:HB2	1.35	1.22
2:3B:84:GLN:CD	1:4A:284:ARG:NH1	1.93	1.22
2:3B:327:ASP:OD2	1:7A:212:PHE:CD2	1.93	1.22
2:6B:94:LYS:NZ	3:6C:63:ARG:HH21	1.35	1.22
1:1A:287:PHE:HE1	1:4A:65:VAL:CG1	1.45	1.21
3:3C:18:GLU:CG	1:4A:288:GLU:CD	2.08	1.21
2:1B:115:ASP:OD2	3:1C:58:ARG:HB3	1.30	1.21
2:4B:327:ASP:OD2	1:8A:212:PHE:CD2	1.94	1.21
1:5A:287:PHE:HE1	1:8A:65:VAL:CG1	1.45	1.21
2:1B:324:LYS:NZ	1:5A:216:HIS:CB	1.99	1.21
2:7B:84:GLN:CD	1:8A:284:ARG:NH1	1.93	1.21
2:7B:122:ASP:OD2	3:7C:52:LYS:CE	1.89	1.21
2:1B:94:LYS:NZ	3:1C:66:GLU:OE2	1.73	1.20
2:3B:122:ASP:OD2	3:3C:52:LYS:CE	1.89	1.20
2:3B:344:PRO:HA	1:7A:392:LYS:CE	1.71	1.20
2:2B:2:ARG:NE	1:6A:75:PRO:HG3	1.41	1.20
2:3B:344:PRO:CB	1:7A:389:ASN:HD22	1.54	1.20
2:7B:115:ASP:OD2	3:7C:58:ARG:HB3	1.03	1.20
2:2B:322:LYS:HB2	1:6A:225:THR:CG2	1.71	1.20
2:3B:252:GLU:CG	1:7A:102:GLY:C	1.91	1.20
2:5B:94:LYS:NZ	3:5C:66:GLU:OE2	1.73	1.20
2:2B:246:LEU:H	1:6A:13:GLN:NE2	1.32	1.19
2:4B:245:LYS:CD	1:8A:226:VAL:CG2	2.19	1.19
2:4B:259:PRO:O	1:8A:399:PHE:C	1.79	1.19
2:3B:324:LYS:HA	1:7A:212:PHE:CZ	1.78	1.19
2:2B:347:GLY:HA2	1:6A:180:SER:OG	1.06	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4B:259:PRO:C	1:8A:399:PHE:O	1.81	1.18
2:3B:2:ARG:HG3	1:7A:98:THR:O	1.43	1.18
2:3B:115:ASP:OD2	3:3C:58:ARG:HB3	1.03	1.18
2:3B:252:GLU:CG	1:7A:102:GLY:O	1.90	1.18
2:3B:61:VAL:HG23	1:4A:287:PHE:CZ	1.62	1.18
1:1A:286:LYS:NZ	1:4A:63:SER:OG	1.76	1.18
2:4B:245:LYS:CG	1:8A:226:VAL:CG2	1.99	1.18
2:3B:2:ARG:CG	1:7A:98:THR:O	1.93	1.17
2:3B:245:LYS:HA	1:7A:13:GLN:NE2	1.57	1.17
2:4B:283:ARG:HH21	1:7A:58:GLU:N	1.32	1.17
2:8B:87:ASP:CG	3:8C:21:ARG:NH2	1.98	1.16
2:1B:2:ARG:CZ	1:5A:76:SER:OG	1.92	1.16
2:2B:342:TYR:O	1:6A:393:LEU:HD23	0.99	1.15
2:4B:115:ASP:CG	3:4C:58:ARG:HB3	1.64	1.15
2:4B:283:ARG:HH21	1:7A:57:GLY:C	1.49	1.15
1:5A:286:LYS:NZ	1:8A:63:SER:OG	1.76	1.15
2:8B:119:ASN:ND2	3:8C:55:SER:C	2.00	1.15
2:3B:89:SER:HB2	3:3C:21:ARG:NH1	1.61	1.15
2:7B:94:LYS:NZ	3:7C:63:ARG:HH21	1.44	1.15
2:8B:115:ASP:CG	3:8C:58:ARG:HB3	1.65	1.15
2:4B:119:ASN:ND2	3:4C:55:SER:C	2.00	1.15
2:2B:119:ASN:ND2	3:2C:55:SER:C	1.98	1.14
2:2B:249:ASP:OD2	1:6A:99:GLU:O	1.66	1.14
2:4B:87:ASP:CG	3:4C:21:ARG:NH2	1.98	1.14
2:6B:119:ASN:ND2	3:6C:55:SER:C	1.98	1.14
3:7C:18:GLU:HA	1:8A:288:GLU:OE2	1.33	1.14
2:1B:259:PRO:CA	1:5A:399:PHE:HD1	1.60	1.14
2:1B:324:LYS:CD	1:5A:224:PRO:HD3	1.36	1.14
2:3B:94:LYS:NZ	3:3C:63:ARG:HH21	1.44	1.14
3:3C:18:GLU:HA	1:4A:288:GLU:OE2	1.33	1.14
1:6A:65:VAL:CG1	1:7A:287:PHE:CE1	2.30	1.14
1:2A:65:VAL:CG1	1:3A:287:PHE:CE1	2.30	1.13
2:2B:252:GLU:HG2	1:6A:102:GLY:HA2	1.23	1.13
2:7B:61:VAL:HG23	1:8A:287:PHE:CZ	1.62	1.13
2:7B:89:SER:HB2	3:7C:21:ARG:NH1	1.61	1.13
2:3B:115:ASP:CG	3:3C:58:ARG:HB3	1.68	1.12
2:4B:324:LYS:CG	1:8A:224:PRO:HD2	1.77	1.12
2:3B:256:ASN:HB3	1:7A:183:VAL:HG22	1.17	1.12
2:4B:245:LYS:CD	1:8A:226:VAL:HG21	1.78	1.12
2:5B:283:ARG:HD2	2:8B:56:ARG:CZ	1.81	1.11
2:1B:256:ASN:HA	1:5A:183:VAL:HG22	1.19	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6A:63:SER:OG	1:7A:286:LYS:NZ	1.84	1.11
2:1B:324:LYS:NZ	1:5A:216:HIS:ND1	1.98	1.11
2:2B:252:GLU:CG	1:6A:102:GLY:HA2	1.76	1.11
2:3B:344:PRO:HB2	1:7A:389:ASN:HD22	0.96	1.11
2:4B:245:LYS:HE2	1:8A:226:VAL:HG23	1.24	1.11
2:7B:56:ARG:HG3	1:8A:286:LYS:CE	1.67	1.11
2:7B:115:ASP:CG	3:7C:58:ARG:HB3	1.68	1.10
2:3B:119:ASN:ND2	3:3C:55:SER:C	2.05	1.10
2:8B:112:LYS:O	3:8C:62:PHE:CG	2.05	1.10
2:1B:324:LYS:NZ	1:5A:216:HIS:CG	2.19	1.10
2:3B:252:GLU:HG2	1:7A:102:GLY:O	0.94	1.10
2:4B:112:LYS:O	3:4C:62:PHE:CG	2.05	1.10
2:4B:344:PRO:CB	1:8A:389:ASN:ND2	2.14	1.10
2:1B:283:ARG:HD2	2:4B:56:ARG:CZ	1.81	1.09
1:2A:63:SER:OG	1:3A:286:LYS:NZ	1.84	1.09
2:3B:2:ARG:CD	1:7A:98:THR:O	2.00	1.09
2:1B:2:ARG:HE	1:5A:75:PRO:HG2	0.97	1.09
2:1B:324:LYS:HZ3	1:5A:216:HIS:CG	1.69	1.09
2:2B:324:LYS:HD2	1:6A:223:SER:HA	1.24	1.09
2:4B:344:PRO:CA	1:8A:392:LYS:HE2	1.81	1.09
2:1B:346:SER:O	1:5A:179:VAL:HA	1.51	1.09
2:2B:94:LYS:NZ	3:2C:63:ARG:NH2	2.01	1.09
2:4B:344:PRO:HA	1:8A:392:LYS:CE	1.81	1.09
2:7B:119:ASN:ND2	3:7C:55:SER:C	2.05	1.09
2:4B:344:PRO:HB3	1:8A:389:ASN:HD22	1.09	1.09
1:1A:287:PHE:HE1	1:4A:65:VAL:HG13	1.17	1.09
2:4B:115:ASP:HB2	3:4C:62:PHE:CE2	1.87	1.08
2:4B:283:ARG:NH2	1:7A:58:GLU:N	2.00	1.08
2:2B:243:PRO:HB3	1:6A:76:SER:HB3	1.33	1.08
2:3B:256:ASN:HB3	1:7A:183:VAL:HG21	1.14	1.08
2:6B:115:ASP:OD2	3:6C:58:ARG:HD3	1.52	1.08
1:1A:65:VAL:HG11	1:2A:287:PHE:HE1	1.16	1.08
2:2B:115:ASP:OD2	3:2C:58:ARG:HD3	1.52	1.08
2:4B:119:ASN:ND2	3:4C:55:SER:O	1.87	1.08
2:4B:255:THR:HG22	1:8A:184:THR:HG21	1.11	1.08
2:6B:94:LYS:NZ	3:6C:63:ARG:NH2	2.01	1.08
2:8B:88:GLU:HG2	3:8C:24:TYR:HB3	1.33	1.08
2:3B:327:ASP:OD2	1:7A:212:PHE:CE2	2.05	1.08
2:7B:61:VAL:CG2	1:8A:287:PHE:HE2	1.37	1.08
1:1A:65:VAL:HG11	1:2A:287:PHE:CE1	1.89	1.08
2:6B:115:ASP:CG	3:6C:58:ARG:CB	2.22	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:88:GLU:CG	3:2C:24:TYR:CD2	2.37	1.07
2:2B:256:ASN:O	1:6A:183:VAL:HG21	1.52	1.07
2:3B:56:ARG:HG3	1:4A:286:LYS:HE2	1.09	1.07
2:2B:324:LYS:HB2	1:6A:224:PRO:O	0.90	1.07
2:4B:246:LEU:HD22	1:8A:181:SER:OG	1.53	1.07
2:6B:88:GLU:CG	3:6C:24:TYR:CD2	2.37	1.07
2:7B:61:VAL:HG21	1:8A:287:PHE:CZ	1.72	1.07
2:8B:115:ASP:HB2	3:8C:62:PHE:CE2	1.87	1.07
2:1B:256:ASN:C	1:5A:183:VAL:HG21	1.74	1.07
2:1B:256:ASN:CA	1:5A:183:VAL:CG2	2.30	1.07
2:2B:255:THR:HG21	1:6A:104:ASN:HB2	1.21	1.07
2:3B:112:LYS:O	3:3C:62:PHE:CG	2.08	1.07
1:5A:287:PHE:HE1	1:8A:65:VAL:HG13	1.17	1.07
2:3B:61:VAL:HG21	1:4A:287:PHE:CZ	1.72	1.06
2:3B:246:LEU:HD13	1:7A:181:SER:OG	1.52	1.06
2:4B:283:ARG:NH2	1:7A:57:GLY:C	2.08	1.06
1:5A:65:VAL:HG11	1:6A:287:PHE:CE1	1.89	1.06
2:7B:112:LYS:O	3:7C:62:PHE:CG	2.08	1.06
2:2B:115:ASP:CG	3:2C:58:ARG:CB	2.21	1.06
2:8B:119:ASN:ND2	3:8C:55:SER:O	1.87	1.06
2:2B:2:ARG:NH1	1:6A:75:PRO:HG2	1.70	1.06
2:2B:322:LYS:CB	1:6A:225:THR:HG22	1.86	1.06
2:6B:115:ASP:CG	3:6C:58:ARG:HB3	1.76	1.06
2:1B:256:ASN:HD21	1:5A:182:VAL:HG13	1.15	1.06
1:5A:65:VAL:HG11	1:6A:287:PHE:HE1	1.16	1.06
2:5B:112:LYS:O	3:5C:62:PHE:CD2	2.08	1.06
2:1B:256:ASN:CA	1:5A:183:VAL:HG22	1.86	1.05
2:3B:2:ARG:N	1:7A:98:THR:CG2	2.20	1.05
2:3B:56:ARG:HB2	1:4A:286:LYS:HE3	1.31	1.05
2:3B:56:ARG:NE	1:4A:286:LYS:CE	2.20	1.05
2:3B:94:LYS:NZ	3:3C:63:ARG:NH2	2.04	1.05
2:4B:327:ASP:HB3	1:8A:178:GLN:OE1	1.49	1.05
2:1B:112:LYS:O	3:1C:62:PHE:CD2	2.08	1.05
2:4B:88:GLU:HG2	3:4C:24:TYR:HB3	1.33	1.05
1:6A:65:VAL:CG1	1:7A:287:PHE:HE1	1.69	1.05
2:7B:56:ARG:NE	1:8A:286:LYS:CE	2.19	1.05
2:7B:56:ARG:HG3	1:8A:286:LYS:HE2	1.09	1.05
2:2B:348:GLY:C	1:6A:183:VAL:HG12	1.77	1.04
2:4B:324:LYS:HB2	1:8A:224:PRO:HD2	1.12	1.04
2:2B:115:ASP:CG	3:2C:58:ARG:HB3	1.76	1.04
2:5B:283:ARG:HD3	2:8B:56:ARG:CD	1.87	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:115:ASP:CG	3:1C:58:ARG:HB3	1.78	1.04
2:1B:283:ARG:HD3	2:4B:56:ARG:CD	1.87	1.04
2:3B:61:VAL:CG2	1:4A:287:PHE:HE2	1.37	1.04
2:3B:324:LYS:HD2	1:7A:224:PRO:HD2	1.40	1.04
2:4B:350:LYS:HB3	1:8A:183:VAL:HG13	1.39	1.04
1:5A:63:SER:OG	1:6A:286:LYS:NZ	1.91	1.04
2:7B:94:LYS:NZ	3:7C:63:ARG:NH2	2.04	1.04
1:1A:56:LEU:HD12	1:2A:286:LYS:HZ3	0.94	1.03
2:4B:164:ARG:NH2	1:8A:402:TRP:HZ3	1.54	1.03
2:5B:115:ASP:CG	3:5C:58:ARG:HB3	1.78	1.03
2:8B:112:LYS:O	3:8C:62:PHE:CD2	2.11	1.03
1:2A:65:VAL:CG1	1:3A:287:PHE:HE1	1.69	1.03
2:3B:247:ASN:HB3	1:7A:74:GLU:OE2	1.59	1.03
1:5A:56:LEU:HD12	1:6A:286:LYS:HZ3	0.89	1.03
2:7B:56:ARG:HB2	1:8A:286:LYS:HE3	1.31	1.03
2:1B:115:ASP:OD2	3:1C:58:ARG:CB	2.06	1.03
2:3B:259:PRO:O	1:7A:400:ALA:CA	2.04	1.03
2:6B:88:GLU:HG2	3:6C:24:TYR:CG	1.94	1.03
2:7B:61:VAL:CB	1:8A:287:PHE:CZ	2.42	1.03
2:1B:245:LYS:HG2	1:5A:226:VAL:HG23	1.40	1.03
2:2B:343:MET:HA	1:6A:393:LEU:HD21	1.41	1.03
2:3B:247:ASN:CB	1:7A:74:GLU:OE1	2.06	1.03
2:5B:115:ASP:OD2	3:5C:58:ARG:CB	2.06	1.03
2:2B:88:GLU:HG2	3:2C:24:TYR:CG	1.94	1.02
2:2B:247:ASN:OD1	1:6A:77:VAL:HG22	1.59	1.02
2:2B:324:LYS:HD2	1:6A:223:SER:CA	1.83	1.02
2:4B:112:LYS:O	3:4C:62:PHE:CD2	2.11	1.02
2:3B:324:LYS:HA	1:7A:212:PHE:CE2	1.92	1.02
2:1B:259:PRO:O	1:5A:399:PHE:O	1.77	1.02
2:2B:324:LYS:CB	1:6A:224:PRO:C	2.15	1.02
2:3B:115:ASP:CG	3:3C:58:ARG:CB	2.27	1.02
2:4B:2:ARG:HE	1:8A:75:PRO:HD2	1.15	1.02
1:1A:63:SER:OG	1:2A:286:LYS:NZ	1.91	1.02
2:2B:115:ASP:OD2	3:2C:58:ARG:CD	2.07	1.02
2:3B:256:ASN:HD22	1:7A:184:THR:HG23	1.23	1.02
2:6B:94:LYS:HZ3	3:6C:63:ARG:NH2	1.56	1.02
2:3B:324:LYS:NZ	1:7A:216:HIS:HB2	1.75	1.02
2:2B:115:ASP:OD2	3:2C:58:ARG:CG	2.07	1.01
2:3B:61:VAL:CB	1:4A:287:PHE:CZ	2.42	1.01
2:3B:350:LYS:CB	1:7A:183:VAL:HG13	1.90	1.01
2:6B:115:ASP:OD2	3:6C:58:ARG:CG	2.07	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:350:LYS:N	1:7A:183:VAL:HG13	1.75	1.01
2:4B:87:ASP:OD2	3:4C:21:ARG:NH2	1.94	1.01
2:5B:119:ASN:ND2	3:5C:55:SER:C	2.13	1.01
2:6B:115:ASP:CG	3:6C:58:ARG:HD3	1.81	1.01
2:2B:115:ASP:CG	3:2C:58:ARG:HD3	1.81	1.00
2:2B:325:ASP:OD1	1:6A:223:SER:OG	1.77	1.00
2:6B:115:ASP:OD2	3:6C:58:ARG:CD	2.07	1.00
2:4B:344:PRO:HB3	1:8A:389:ASN:ND2	1.72	1.00
2:3B:246:LEU:HD11	1:7A:181:SER:OG	1.54	1.00
2:3B:324:LYS:CD	1:7A:224:PRO:HD2	1.92	1.00
2:4B:324:LYS:HG3	1:8A:224:PRO:CD	1.92	1.00
2:4B:115:ASP:OD2	3:4C:58:ARG:CB	2.09	1.00
2:3B:56:ARG:HG3	1:4A:286:LYS:CE	1.67	1.00
2:7B:94:LYS:HZ1	3:7C:63:ARG:HH21	1.10	1.00
2:4B:255:THR:HG22	1:8A:184:THR:CG2	1.92	0.99
2:7B:122:ASP:OD2	3:7C:52:LYS:HE3	1.62	0.99
1:5A:65:VAL:CG1	1:6A:287:PHE:HE1	1.74	0.99
2:1B:119:ASN:ND2	3:1C:55:SER:C	2.13	0.99
2:3B:247:ASN:HB2	1:7A:74:GLU:OE1	1.61	0.99
2:6B:94:LYS:HZ1	3:6C:63:ARG:HH21	1.02	0.99
2:1B:324:LYS:CD	1:5A:223:SER:HA	1.91	0.99
2:1B:115:ASP:HB2	3:1C:62:PHE:CE2	1.97	0.99
1:5A:56:LEU:CD1	1:6A:286:LYS:HZ3	1.76	0.99
2:1B:2:ARG:NH1	1:5A:76:SER:OG	1.95	0.99
2:3B:324:LYS:CG	1:7A:224:PRO:HD2	1.91	0.99
2:5B:94:LYS:HE3	3:5C:66:GLU:OE2	1.62	0.99
2:6B:119:ASN:ND2	3:6C:55:SER:HB3	1.78	0.99
2:4B:255:THR:CG2	1:8A:184:THR:HG21	1.93	0.99
1:1A:65:VAL:CG1	1:2A:287:PHE:HE1	1.74	0.98
2:4B:246:LEU:HD21	4:8A:501:GDP:H2'	1.45	0.98
2:5B:115:ASP:HB2	3:5C:62:PHE:CE2	1.97	0.98
2:8B:115:ASP:OD2	3:8C:58:ARG:CB	2.09	0.98
2:2B:94:LYS:HZ1	3:2C:63:ARG:NH2	1.58	0.98
2:6B:111:GLU:O	3:6C:62:PHE:CZ	2.17	0.98
1:1A:56:LEU:CD1	1:2A:286:LYS:NZ	2.26	0.98
2:8B:87:ASP:OD2	3:8C:21:ARG:NH2	1.94	0.98
2:3B:88:GLU:CG	3:3C:24:TYR:HD2	1.77	0.98
2:5B:112:LYS:O	3:5C:62:PHE:CG	2.17	0.98
2:7B:115:ASP:CG	3:7C:58:ARG:CB	2.27	0.98
2:1B:112:LYS:O	3:1C:62:PHE:CG	2.17	0.97
2:2B:111:GLU:O	3:2C:62:PHE:CZ	2.17	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7B:88:GLU:CG	3:7C:24:TYR:HD2	1.77	0.97
2:3B:350:LYS:H	1:7A:183:VAL:CG1	1.77	0.97
2:2B:119:ASN:ND2	3:2C:55:SER:HB3	1.78	0.97
2:4B:245:LYS:CE	1:8A:226:VAL:CG2	2.42	0.97
2:3B:94:LYS:HZ1	3:3C:63:ARG:HH21	1.06	0.97
1:5A:56:LEU:CD1	1:6A:286:LYS:NZ	2.26	0.97
2:1B:94:LYS:HE3	3:1C:66:GLU:OE2	1.62	0.97
2:2B:252:GLU:CD	1:6A:102:GLY:HA2	1.84	0.97
2:4B:327:ASP:CB	1:8A:178:GLN:OE1	2.00	0.97
2:6B:122:ASP:OD2	3:6C:52:LYS:HE2	1.61	0.97
2:1B:283:ARG:CD	2:4B:56:ARG:NE	2.27	0.97
2:3B:122:ASP:OD2	3:3C:52:LYS:HE3	1.62	0.97
1:7A:132:ASP:HA	3:7C:68:ARG:CD	1.88	0.97
2:3B:254:VAL:O	1:7A:402:TRP:CE2	2.18	0.97
2:1B:256:ASN:O	1:5A:183:VAL:CG2	2.12	0.96
2:3B:2:ARG:HE	1:7A:75:PRO:CD	1.78	0.96
2:8B:88:GLU:HG2	3:8C:24:TYR:CB	1.95	0.96
2:3B:111:GLU:O	3:3C:62:PHE:CZ	2.18	0.96
2:7B:111:GLU:O	3:7C:62:PHE:CZ	2.18	0.96
2:2B:122:ASP:OD2	3:2C:52:LYS:HE2	1.61	0.96
2:4B:115:ASP:CG	3:4C:58:ARG:CB	2.34	0.96
2:1B:2:ARG:HE	1:5A:75:PRO:CG	1.77	0.96
2:2B:327:ASP:HB3	1:6A:178:GLN:HE22	1.26	0.96
2:4B:88:GLU:HG2	3:4C:24:TYR:CB	1.95	0.96
2:4B:245:LYS:CE	1:8A:226:VAL:HG23	1.96	0.95
2:4B:256:ASN:ND2	1:8A:183:VAL:N	2.14	0.95
2:3B:246:LEU:HD21	4:7A:501:GDP:H2'	1.49	0.95
2:4B:344:PRO:CB	1:8A:389:ASN:HD22	1.74	0.95
1:3A:132:ASP:HA	3:3C:68:ARG:CD	1.88	0.95
2:1B:245:LYS:HG2	1:5A:226:VAL:HG21	1.48	0.95
2:1B:324:LYS:CE	1:5A:216:HIS:ND1	2.30	0.95
2:3B:2:ARG:NE	1:7A:75:PRO:CD	2.29	0.95
2:1B:342:TYR:CD1	1:5A:396:ARG:HD3	1.99	0.95
1:6A:65:VAL:HG11	1:7A:287:PHE:CE1	2.02	0.95
2:7B:88:GLU:HG2	3:7C:24:TYR:HD2	1.10	0.95
2:2B:323:ALA:HB3	1:6A:226:VAL:HG13	1.49	0.94
1:5A:287:PHE:CZ	1:8A:65:VAL:CG1	2.50	0.94
2:8B:115:ASP:CG	3:8C:58:ARG:CB	2.34	0.94
2:3B:84:GLN:HE22	1:4A:284:ARG:CZ	1.59	0.94
1:5A:286:LYS:NZ	1:8A:56:LEU:HD12	1.82	0.94
2:3B:2:ARG:NH1	1:7A:75:PRO:CG	1.79	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5A:65:VAL:CG1	1:6A:287:PHE:CE1	2.50	0.94
1:1A:65:VAL:CG1	1:2A:287:PHE:CE1	2.50	0.94
1:1A:286:LYS:NZ	1:4A:56:LEU:HD12	1.83	0.94
2:4B:324:LYS:CB	1:8A:224:PRO:CD	2.44	0.94
2:1B:245:LYS:CG	1:5A:226:VAL:CG2	2.45	0.94
2:1B:259:PRO:HA	1:5A:399:PHE:HD1	0.78	0.94
2:4B:115:ASP:OD1	3:4C:58:ARG:HD3	1.68	0.94
2:3B:55:VAL:HG11	1:4A:287:PHE:CG	2.00	0.93
2:3B:324:LYS:HZ3	1:7A:216:HIS:HB2	1.27	0.93
2:7B:119:ASN:ND2	3:7C:55:SER:HB3	1.83	0.93
1:1A:287:PHE:CZ	1:4A:65:VAL:CG1	2.50	0.93
2:4B:115:ASP:H	3:4C:62:PHE:HE2	1.14	0.93
2:7B:55:VAL:HG11	1:8A:287:PHE:CG	2.00	0.93
2:8B:115:ASP:OD1	3:8C:58:ARG:HD3	1.68	0.93
2:3B:88:GLU:CG	3:3C:24:TYR:CD2	2.51	0.93
2:4B:245:LYS:HE2	1:8A:226:VAL:CG2	1.96	0.93
2:3B:88:GLU:HG2	3:3C:24:TYR:HD2	1.10	0.93
1:5A:287:PHE:CZ	1:8A:65:VAL:HG12	2.04	0.93
2:3B:254:VAL:C	1:7A:402:TRP:CE2	2.42	0.93
2:3B:350:LYS:N	1:7A:183:VAL:CG1	2.30	0.93
2:1B:56:ARG:CZ	2:2B:283:ARG:CD	2.47	0.93
2:3B:344:PRO:HA	1:7A:392:LYS:HE3	1.49	0.93
2:3B:350:LYS:HB3	1:7A:183:VAL:HG13	1.48	0.93
2:7B:88:GLU:CG	3:7C:24:TYR:CD2	2.51	0.93
2:7B:91:ILE:HG22	3:7C:24:TYR:CE2	2.04	0.93
2:8B:115:ASP:H	3:8C:62:PHE:HE2	1.14	0.92
2:1B:283:ARG:HD3	2:4B:56:ARG:HD3	1.51	0.92
2:2B:347:GLY:CA	1:6A:180:SER:CB	2.42	0.92
2:3B:2:ARG:NE	1:7A:75:PRO:HD2	1.85	0.92
2:4B:246:LEU:CD2	1:8A:181:SER:OG	2.17	0.92
2:4B:344:PRO:HA	1:8A:392:LYS:HE2	0.93	0.92
2:5B:283:ARG:CD	2:8B:56:ARG:NE	2.27	0.92
2:2B:89:SER:HB2	3:2C:21:ARG:NH1	1.85	0.92
2:3B:255:THR:HA	1:7A:402:TRP:CG	2.04	0.92
2:1B:2:ARG:NE	1:5A:75:PRO:HG2	1.82	0.92
2:3B:119:ASN:ND2	3:3C:55:SER:HB3	1.83	0.92
2:3B:344:PRO:HA	1:7A:392:LYS:CD	2.00	0.92
2:1B:259:PRO:O	1:5A:399:PHE:C	2.06	0.92
2:3B:2:ARG:CZ	1:7A:75:PRO:HD2	1.98	0.92
2:6B:122:ASP:OD2	3:6C:52:LYS:HE3	1.69	0.92
2:6B:56:ARG:CZ	2:7B:283:ARG:HD2	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:287:PHE:CZ	1:4A:65:VAL:HG12	2.04	0.92
2:3B:254:VAL:O	1:7A:402:TRP:NE1	2.03	0.92
1:2A:65:VAL:HG11	1:3A:287:PHE:CE1	2.02	0.91
2:5B:283:ARG:HD3	2:8B:56:ARG:HD3	1.51	0.91
2:4B:324:LYS:CG	1:8A:224:PRO:CD	2.48	0.91
2:2B:122:ASP:OD2	3:2C:52:LYS:HE3	1.69	0.91
2:4B:324:LYS:HB2	1:8A:224:PRO:CD	1.99	0.91
2:5B:94:LYS:HZ1	3:5C:63:ARG:HH21	1.13	0.91
2:1B:119:ASN:ND2	3:1C:55:SER:O	2.04	0.91
2:6B:89:SER:HB2	3:6C:21:ARG:NH1	1.85	0.91
1:1A:56:LEU:CD1	1:2A:286:LYS:HZ3	1.81	0.91
2:4B:119:ASN:OD1	3:4C:55:SER:HB3	1.70	0.91
2:2B:56:ARG:CZ	2:3B:283:ARG:HD2	2.00	0.91
2:2B:348:GLY:O	1:6A:183:VAL:HG12	1.69	0.91
2:3B:61:VAL:HG23	1:4A:287:PHE:HZ	1.12	0.91
2:8B:119:ASN:OD1	3:8C:55:SER:HB3	1.70	0.91
2:3B:91:ILE:HG22	3:3C:24:TYR:CE2	2.04	0.91
2:3B:256:ASN:ND2	1:7A:184:THR:HG23	1.86	0.91
2:6B:88:GLU:CB	3:6C:24:TYR:HD2	1.79	0.91
2:1B:342:TYR:CD1	1:5A:396:ARG:CD	2.46	0.91
2:4B:256:ASN:ND2	1:8A:183:VAL:H	1.67	0.90
2:4B:324:LYS:HG3	1:8A:224:PRO:HD2	1.50	0.90
2:5B:56:ARG:CZ	2:6B:283:ARG:CD	2.47	0.90
3:7C:18:GLU:N	1:8A:288:GLU:OE2	2.04	0.90
2:1B:115:ASP:CG	3:1C:58:ARG:HD3	1.91	0.90
2:4B:88:GLU:HG2	3:4C:24:TYR:CG	2.07	0.90
2:1B:344:PRO:HB3	1:5A:389:ASN:ND2	1.86	0.90
2:2B:259:PRO:O	1:6A:399:PHE:C	2.09	0.90
2:5B:119:ASN:ND2	3:5C:55:SER:O	2.04	0.90
2:3B:256:ASN:O	1:7A:399:PHE:CE1	2.25	0.90
2:5B:94:LYS:HE3	3:5C:66:GLU:CG	2.02	0.90
3:7C:18:GLU:HG2	1:8A:288:GLU:OE1	1.72	0.90
2:1B:94:LYS:HE3	3:1C:66:GLU:CG	2.02	0.90
2:4B:87:ASP:CG	3:4C:21:ARG:HH21	1.66	0.90
3:3C:18:GLU:N	1:4A:288:GLU:OE2	2.04	0.90
2:7B:94:LYS:HZ3	3:7C:63:ARG:NH2	1.66	0.90
2:1B:115:ASP:CG	3:1C:58:ARG:CB	2.40	0.90
2:1B:325:ASP:OD1	1:5A:223:SER:OG	1.89	0.90
2:4B:87:ASP:OD1	3:4C:21:ARG:NH2	2.03	0.90
2:1B:94:LYS:HZ1	3:1C:63:ARG:HH21	1.12	0.90
2:1B:327:ASP:OD1	1:5A:212:PHE:CE2	2.07	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:324:LYS:HE2	1:5A:216:HIS:ND1	1.87	0.89
2:4B:322:LYS:NZ	1:8A:222:GLU:O	2.05	0.89
2:5B:115:ASP:CG	3:5C:58:ARG:HD3	1.91	0.89
2:2B:259:PRO:C	1:6A:399:PHE:O	2.10	0.89
2:3B:94:LYS:HZ3	3:3C:63:ARG:NH2	1.70	0.89
2:3B:245:LYS:HA	1:7A:13:GLN:HE22	1.36	0.89
2:8B:87:ASP:CG	3:8C:21:ARG:HH21	1.66	0.89
3:3C:18:GLU:HG2	1:4A:288:GLU:OE1	1.72	0.89
2:6B:88:GLU:HG2	3:6C:24:TYR:CB	2.03	0.89
2:6B:88:GLU:CG	3:6C:24:TYR:HD2	1.80	0.89
2:2B:88:GLU:CG	3:2C:24:TYR:HD2	1.80	0.89
2:6B:88:GLU:HG2	3:6C:24:TYR:HD2	1.37	0.89
1:1A:56:LEU:HD12	1:2A:286:LYS:HZ1	1.35	0.89
2:3B:61:VAL:HB	1:4A:287:PHE:CZ	2.08	0.89
2:3B:247:ASN:HB3	1:7A:74:GLU:CD	1.92	0.89
1:5A:286:LYS:HZ2	1:8A:56:LEU:HD12	1.35	0.89
2:8B:88:GLU:HG2	3:8C:24:TYR:CG	2.07	0.89
2:1B:87:ASP:CG	3:1C:21:ARG:NH2	2.26	0.89
2:7B:61:VAL:HB	1:8A:287:PHE:CZ	2.08	0.89
2:4B:245:LYS:HG3	1:8A:226:VAL:HG21	1.53	0.89
2:5B:56:ARG:CZ	2:6B:283:ARG:HD2	2.03	0.89
2:1B:56:ARG:CZ	2:2B:283:ARG:HD2	2.03	0.88
2:2B:88:GLU:HG2	3:2C:24:TYR:HD2	1.37	0.88
2:3B:2:ARG:HD3	1:7A:98:THR:O	1.73	0.88
2:4B:88:GLU:HG2	3:4C:24:TYR:CD2	2.08	0.88
2:4B:351:LEU:HD11	1:8A:179:VAL:HG21	1.55	0.88
2:8B:87:ASP:OD1	3:8C:21:ARG:NH2	2.03	0.88
1:6A:65:VAL:HG13	1:7A:287:PHE:HE1	1.37	0.88
2:7B:61:VAL:HG23	1:8A:287:PHE:HZ	1.12	0.88
2:2B:88:GLU:HG2	3:2C:24:TYR:CB	2.03	0.88
2:2B:245:LYS:HG3	1:6A:17:GLN:NE2	1.89	0.88
2:8B:119:ASN:CG	3:8C:55:SER:HB3	1.94	0.88
2:2B:259:PRO:C	1:6A:400:ALA:HB2	1.94	0.88
1:4A:132:ASP:OD1	3:4C:68:ARG:HD3	1.73	0.88
1:2A:65:VAL:HG13	1:3A:287:PHE:HE1	1.37	0.88
2:4B:246:LEU:CD2	4:8A:501:GDP:H2'	2.02	0.88
2:8B:87:ASP:OD2	3:8C:21:ARG:CZ	2.22	0.88
2:8B:88:GLU:HG2	3:8C:24:TYR:CD2	2.08	0.88
2:3B:243:PRO:CG	1:7A:76:SER:HB3	2.03	0.88
2:5B:87:ASP:CG	3:5C:21:ARG:NH2	2.26	0.88
2:8B:115:ASP:CG	3:8C:58:ARG:HD3	1.94	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5B:115:ASP:CG	3:5C:58:ARG:CB	2.40	0.87
2:3B:331:ALA:HB2	1:7A:178:GLN:O	1.73	0.87
2:4B:344:PRO:HB2	1:8A:389:ASN:ND2	1.87	0.87
2:1B:347:GLY:HA2	1:5A:180:SER:H	1.37	0.87
2:4B:115:ASP:CG	3:4C:58:ARG:HD3	1.94	0.87
2:1B:327:ASP:OD1	1:5A:212:PHE:HE2	1.57	0.87
2:5B:94:LYS:HE3	3:5C:66:GLU:CD	1.94	0.87
2:1B:247:ASN:H	1:5A:13:GLN:HE22	1.14	0.87
2:2B:322:LYS:HB2	1:6A:225:THR:HG22	0.92	0.87
2:2B:324:LYS:NZ	1:6A:216:HIS:HB2	1.89	0.87
2:2B:259:PRO:HB3	1:6A:399:PHE:CD1	2.10	0.87
2:3B:247:ASN:OD1	1:7A:13:GLN:OE1	1.92	0.87
1:8A:132:ASP:OD1	3:8C:68:ARG:HD3	1.73	0.87
2:6B:119:ASN:HD21	3:6C:56:LEU:N	1.73	0.87
2:1B:256:ASN:CA	1:5A:183:VAL:HG21	2.04	0.86
2:1B:283:ARG:CD	2:4B:56:ARG:CZ	2.52	0.86
2:4B:119:ASN:CG	3:4C:55:SER:HB3	1.94	0.86
2:1B:115:ASP:OD2	3:1C:58:ARG:HD3	1.75	0.86
2:1B:94:LYS:HE3	3:1C:66:GLU:CD	1.94	0.86
2:3B:122:ASP:OD2	3:3C:52:LYS:HG2	1.75	0.86
2:4B:87:ASP:OD2	3:4C:21:ARG:CZ	2.22	0.86
2:7B:61:VAL:CG2	1:8A:287:PHE:HZ	1.58	0.86
1:1A:91:PRO:HD2	1:2A:287:PHE:CD2	2.10	0.86
2:3B:246:LEU:HD13	1:7A:181:SER:HG	1.39	0.86
2:5B:283:ARG:CD	2:8B:56:ARG:CZ	2.52	0.86
2:2B:324:LYS:CD	1:6A:223:SER:HA	1.97	0.86
1:4A:132:ASP:HA	3:4C:68:ARG:CG	2.06	0.86
2:5B:115:ASP:OD2	3:5C:58:ARG:HD3	1.75	0.86
2:7B:122:ASP:OD2	3:7C:52:LYS:HG2	1.75	0.86
2:3B:2:ARG:NH1	1:7A:75:PRO:CD	2.37	0.86
2:7B:84:GLN:HE22	1:8A:284:ARG:CZ	1.59	0.86
2:3B:245:LYS:HG3	1:7A:17:GLN:OE1	1.76	0.85
2:3B:122:ASP:OD2	3:3C:52:LYS:HE2	1.75	0.85
1:5A:91:PRO:HD2	1:6A:287:PHE:CD2	2.10	0.85
2:2B:88:GLU:CB	3:2C:24:TYR:HD2	1.79	0.85
2:2B:255:THR:HG21	1:6A:104:ASN:CB	2.05	0.85
2:4B:130:GLY:HA2	1:8A:98:THR:HG21	1.58	0.85
2:2B:252:GLU:HG2	1:6A:102:GLY:HA3	0.87	0.85
2:3B:343:MET:O	1:7A:392:LYS:HE3	1.76	0.85
2:2B:119:ASN:HD21	3:2C:56:LEU:N	1.73	0.85
2:3B:327:ASP:OD2	1:7A:212:PHE:HD2	1.54	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5B:119:ASN:ND2	3:5C:55:SER:HB3	1.92	0.85
2:3B:2:ARG:HH11	1:7A:75:PRO:HG3	1.38	0.85
2:3B:94:LYS:HZ1	3:3C:63:ARG:NH2	1.68	0.85
2:4B:88:GLU:CG	3:4C:24:TYR:HB3	2.07	0.85
2:4B:322:LYS:HZ1	1:8A:222:GLU:C	1.79	0.85
2:7B:122:ASP:OD2	3:7C:52:LYS:HE2	1.75	0.85
1:8A:132:ASP:HA	3:8C:68:ARG:CG	2.06	0.85
2:8B:88:GLU:CG	3:8C:24:TYR:HB3	2.07	0.84
2:2B:122:ASP:CG	3:2C:52:LYS:HE2	1.98	0.84
2:3B:2:ARG:HH11	1:7A:75:PRO:CD	1.90	0.84
2:1B:256:ASN:ND2	1:5A:182:VAL:HG13	1.92	0.84
2:3B:89:SER:CB	3:3C:21:ARG:NH1	2.40	0.84
2:4B:245:LYS:HG2	1:8A:226:VAL:CB	2.07	0.84
2:2B:260:PHE:HA	1:6A:400:ALA:HB2	1.59	0.84
2:1B:87:ASP:OD2	3:1C:21:ARG:NH2	2.11	0.84
2:3B:259:PRO:O	1:7A:400:ALA:HA	1.78	0.84
2:3B:324:LYS:CA	1:7A:212:PHE:CZ	2.60	0.84
2:5B:87:ASP:OD2	3:5C:21:ARG:NH2	2.11	0.84
2:5B:115:ASP:OD1	3:5C:58:ARG:HD3	1.78	0.84
2:6B:88:GLU:HG2	3:6C:24:TYR:HB3	1.59	0.84
2:8B:115:ASP:CB	3:8C:58:ARG:HB3	2.07	0.84
2:1B:254:VAL:CG1	1:5A:402:TRP:CH2	2.60	0.83
2:1B:119:ASN:ND2	3:1C:55:SER:HB3	1.92	0.83
2:7B:122:ASP:CG	3:7C:52:LYS:CE	2.47	0.83
2:6B:115:ASP:OD1	3:6C:58:ARG:HD3	1.77	0.83
2:4B:115:ASP:CB	3:4C:58:ARG:HB3	2.07	0.83
2:2B:91:ILE:HG22	3:2C:24:TYR:CE2	2.14	0.83
1:5A:56:LEU:HD12	1:6A:286:LYS:HZ1	1.40	0.83
2:7B:94:LYS:HZ1	3:7C:63:ARG:NH2	1.72	0.83
2:2B:88:GLU:HG2	3:2C:24:TYR:HB3	1.59	0.83
2:4B:256:ASN:ND2	1:8A:184:THR:H	1.76	0.83
2:3B:122:ASP:CG	3:3C:52:LYS:CE	2.47	0.83
2:3B:324:LYS:HD2	1:7A:224:PRO:CD	2.07	0.83
2:4B:119:ASN:ND2	3:4C:55:SER:HB3	1.94	0.83
2:6B:122:ASP:CG	3:6C:52:LYS:HE2	1.98	0.83
2:8B:94:LYS:NZ	3:8C:63:ARG:HH21	1.77	0.83
2:1B:56:ARG:NH2	2:2B:283:ARG:HD2	1.94	0.82
2:3B:61:VAL:CG2	1:4A:287:PHE:HZ	1.58	0.82
2:5B:56:ARG:NH2	2:6B:283:ARG:HD2	1.94	0.82
2:3B:247:ASN:CB	1:7A:74:GLU:CD	2.48	0.82
2:4B:344:PRO:HB2	1:8A:389:ASN:HD21	1.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7C:18:GLU:HG3	1:8A:288:GLU:OE2	1.79	0.82
2:7B:89:SER:CB	3:7C:21:ARG:NH1	2.40	0.82
1:1A:286:LYS:HZ2	1:4A:56:LEU:HD12	1.42	0.82
2:2B:115:ASP:CG	3:2C:58:ARG:CD	2.46	0.82
2:2B:115:ASP:OD1	3:2C:58:ARG:HD3	1.77	0.82
2:1B:325:ASP:CG	1:5A:223:SER:OG	2.17	0.82
1:2A:132:ASP:HA	3:2C:68:ARG:CG	2.10	0.82
2:3B:122:ASP:CG	3:3C:52:LYS:HE2	2.00	0.82
2:3B:344:PRO:HD3	1:7A:393:LEU:HG	1.60	0.82
2:4B:2:ARG:NE	1:8A:75:PRO:HD2	1.94	0.82
2:6B:91:ILE:HG22	3:6C:24:TYR:CE2	2.14	0.82
2:7B:122:ASP:CG	3:7C:52:LYS:HE2	2.00	0.82
2:2B:258:VAL:O	1:6A:402:TRP:NE1	2.13	0.81
2:4B:164:ARG:NH2	1:8A:402:TRP:CZ3	2.45	0.81
2:8B:119:ASN:ND2	3:8C:55:SER:HB3	1.94	0.81
1:6A:132:ASP:HA	3:6C:68:ARG:CG	2.10	0.81
2:1B:88:GLU:HG2	3:1C:24:TYR:HB3	1.60	0.81
2:4B:94:LYS:NZ	3:4C:63:ARG:HH21	1.77	0.81
3:3C:18:GLU:HG3	1:4A:288:GLU:OE2	1.79	0.81
2:5B:88:GLU:HG2	3:5C:24:TYR:HB3	1.60	0.81
2:6B:115:ASP:CG	3:6C:58:ARG:CD	2.46	0.81
1:8A:132:ASP:HA	3:8C:68:ARG:CD	2.11	0.81
2:4B:245:LYS:CD	1:8A:226:VAL:HG22	2.10	0.81
2:3B:350:LYS:CA	1:7A:183:VAL:HG13	2.10	0.81
2:4B:256:ASN:HD22	1:8A:183:VAL:CA	1.92	0.81
2:1B:115:ASP:OD1	3:1C:58:ARG:HD3	1.78	0.80
2:2B:2:ARG:CZ	1:6A:75:PRO:CG	2.35	0.80
1:4A:132:ASP:HA	3:4C:68:ARG:CD	2.11	0.80
2:2B:94:LYS:HZ3	3:2C:63:ARG:NH2	1.75	0.80
2:3B:344:PRO:HA	1:7A:392:LYS:HD3	1.61	0.80
2:6B:115:ASP:CG	3:6C:58:ARG:HB2	2.02	0.80
2:2B:2:ARG:HG3	1:6A:98:THR:HG23	1.63	0.80
2:3B:122:ASP:OD2	3:3C:52:LYS:CG	2.30	0.80
2:3B:243:PRO:HG2	1:7A:76:SER:HB3	1.62	0.80
2:3B:331:ALA:CB	1:7A:178:GLN:O	2.30	0.80
2:4B:115:ASP:CB	3:4C:62:PHE:CE2	2.63	0.80
2:4B:245:LYS:HD3	1:8A:226:VAL:HG22	1.63	0.80
2:1B:245:LYS:CG	1:5A:226:VAL:HG21	2.10	0.80
2:3B:256:ASN:CB	1:7A:183:VAL:HG21	1.95	0.80
2:5B:89:SER:HA	3:5C:24:TYR:CZ	1.95	0.80
2:7B:56:ARG:HG3	1:8A:286:LYS:CD	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:259:PRO:O	1:7A:400:ALA:CB	2.30	0.79
2:1B:261:PRO:HG3	1:5A:400:ALA:HB1	1.63	0.79
2:2B:115:ASP:CG	3:2C:58:ARG:HB2	2.02	0.79
2:3B:247:ASN:CB	1:7A:74:GLU:OE2	2.29	0.79
2:3B:256:ASN:CB	1:7A:183:VAL:HG22	1.98	0.79
2:4B:259:PRO:HA	1:8A:399:PHE:HA	1.61	0.79
2:3B:350:LYS:H	1:7A:183:VAL:HG13	1.37	0.79
2:2B:119:ASN:ND2	3:2C:56:LEU:N	2.30	0.79
2:7B:122:ASP:OD2	3:7C:52:LYS:CG	2.30	0.79
2:8B:115:ASP:CB	3:8C:62:PHE:CE2	2.63	0.79
2:2B:259:PRO:HA	1:6A:399:PHE:HB3	1.63	0.79
2:2B:259:PRO:O	1:6A:400:ALA:HB3	1.78	0.79
2:3B:2:ARG:CZ	1:7A:75:PRO:CG	2.61	0.79
2:3B:56:ARG:HG3	1:4A:286:LYS:CD	2.11	0.79
2:3B:56:ARG:NE	1:4A:286:LYS:HE3	1.97	0.79
2:3B:119:ASN:CG	3:3C:55:SER:HB3	2.03	0.79
2:4B:324:LYS:NZ	1:8A:216:HIS:HB3	1.94	0.79
2:1B:56:ARG:HD3	2:2B:283:ARG:HD3	1.63	0.79
2:5B:56:ARG:HD3	2:6B:283:ARG:HD3	1.63	0.79
2:3B:119:ASN:ND2	3:3C:55:SER:O	2.16	0.78
2:2B:252:GLU:OE2	1:6A:102:GLY:HA2	1.82	0.78
2:2B:56:ARG:CD	2:3B:283:ARG:HD3	2.14	0.78
2:2B:327:ASP:CB	1:6A:178:GLN:HE22	1.97	0.78
2:3B:324:LYS:HG2	1:7A:212:PHE:CG	2.18	0.78
2:1B:324:LYS:HZ1	1:5A:216:HIS:HB2	0.63	0.78
2:2B:259:PRO:HB3	1:6A:399:PHE:HD1	1.49	0.78
2:2B:260:PHE:CA	1:6A:400:ALA:HB2	2.14	0.78
2:7B:119:ASN:ND2	3:7C:55:SER:O	2.16	0.78
2:2B:94:LYS:HZ1	3:2C:63:ARG:HH21	0.80	0.78
2:4B:322:LYS:NZ	1:8A:222:GLU:C	2.37	0.78
2:7B:119:ASN:CG	3:7C:55:SER:HB3	2.03	0.77
2:5B:119:ASN:CG	3:5C:55:SER:HB3	2.04	0.77
2:6B:56:ARG:CD	2:7B:283:ARG:HD3	2.14	0.77
2:6B:119:ASN:CG	3:6C:55:SER:HB3	2.04	0.77
2:1B:119:ASN:CG	3:1C:55:SER:HB3	2.04	0.77
2:3B:2:ARG:CZ	1:7A:75:PRO:CD	2.59	0.77
2:3B:259:PRO:O	1:7A:400:ALA:HB2	1.83	0.77
2:3B:245:LYS:HG2	1:7A:226:VAL:HG21	1.66	0.77
2:3B:255:THR:HG23	1:7A:402:TRP:HB3	1.65	0.77
2:4B:2:ARG:HE	1:8A:75:PRO:CD	1.98	0.77
2:8B:89:SER:HA	3:8C:24:TYR:CZ	2.05	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:347:GLY:CA	1:6A:180:SER:HB3	2.15	0.77
2:3B:2:ARG:N	1:7A:98:THR:HG22	1.98	0.77
2:7B:115:ASP:OD1	3:7C:58:ARG:HD3	1.84	0.77
2:2B:119:ASN:HD21	3:2C:55:SER:CB	1.98	0.77
2:3B:256:ASN:CB	1:7A:183:VAL:HG23	2.13	0.77
2:2B:119:ASN:HD21	3:2C:55:SER:CA	1.98	0.76
2:4B:245:LYS:HD3	1:8A:226:VAL:CG2	2.15	0.76
2:2B:119:ASN:CG	3:2C:55:SER:HB3	2.04	0.76
2:4B:2:ARG:HH12	1:8A:76:SER:HG	1.32	0.76
2:6B:119:ASN:HD21	3:6C:55:SER:CA	1.98	0.76
2:1B:87:ASP:CG	3:1C:21:ARG:HH21	1.89	0.76
2:1B:256:ASN:HA	1:5A:183:VAL:HG21	1.57	0.76
2:2B:122:ASP:CG	3:2C:52:LYS:CE	2.53	0.76
2:3B:115:ASP:CG	3:3C:58:ARG:HD3	2.06	0.76
2:4B:130:GLY:CA	1:8A:98:THR:HG21	2.16	0.76
3:1C:92:MET:HE3	3:1C:131:LEU:HG	1.66	0.76
2:3B:115:ASP:OD1	3:3C:58:ARG:HD3	1.84	0.76
2:6B:119:ASN:ND2	3:6C:56:LEU:N	2.30	0.76
2:7B:56:ARG:NE	1:8A:286:LYS:HE3	1.97	0.76
2:2B:324:LYS:CA	1:6A:224:PRO:O	2.34	0.76
1:3A:132:ASP:HA	3:3C:68:ARG:HD3	1.66	0.76
2:6B:119:ASN:HD21	3:6C:55:SER:CB	1.98	0.76
2:1B:324:LYS:HD2	1:5A:224:PRO:HD3	1.62	0.76
2:2B:56:ARG:CZ	2:3B:283:ARG:CD	2.64	0.76
2:4B:115:ASP:N	3:4C:62:PHE:HE2	1.84	0.76
2:6B:119:ASN:ND2	3:6C:55:SER:O	2.18	0.76
2:8B:88:GLU:CG	3:8C:24:TYR:CD2	2.68	0.76
2:4B:119:ASN:HD21	3:4C:55:SER:CA	1.99	0.76
2:7B:119:ASN:HD21	3:7C:56:LEU:N	1.83	0.76
2:1B:259:PRO:CA	1:5A:399:PHE:CD1	2.49	0.75
2:6B:115:ASP:CB	3:6C:58:ARG:CB	2.64	0.75
2:7B:84:GLN:HE21	1:8A:284:ARG:CZ	1.70	0.75
2:3B:324:LYS:HG3	1:7A:224:PRO:HD2	1.68	0.75
2:5B:283:ARG:CD	2:8B:56:ARG:CD	2.64	0.75
2:6B:56:ARG:CZ	2:7B:283:ARG:CD	2.64	0.75
2:1B:254:VAL:HG12	1:5A:402:TRP:CH2	2.20	0.75
2:2B:56:ARG:NE	2:3B:283:ARG:CD	2.50	0.75
2:6B:122:ASP:CG	3:6C:52:LYS:CE	2.53	0.75
2:3B:246:LEU:HD21	4:7A:501:GDP:C2'	2.17	0.75
2:3B:84:GLN:HE21	1:4A:284:ARG:CZ	1.69	0.75
2:4B:88:GLU:CG	3:4C:24:TYR:CD2	2.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7B:115:ASP:CG	3:7C:58:ARG:HD3	2.06	0.75
2:1B:89:SER:HA	3:1C:24:TYR:CZ	1.95	0.75
2:3B:342:TYR:O	1:7A:392:LYS:O	2.04	0.75
2:8B:119:ASN:HD21	3:8C:55:SER:CA	1.99	0.75
2:3B:115:ASP:OD2	3:3C:58:ARG:CG	2.35	0.75
2:3B:119:ASN:HD21	3:3C:56:LEU:N	1.83	0.75
3:8C:92:MET:HE2	3:8C:131:LEU:HD23	1.69	0.75
1:7A:132:ASP:HA	3:7C:68:ARG:HD3	1.66	0.75
2:8B:115:ASP:N	3:8C:62:PHE:HE2	1.84	0.75
2:2B:115:ASP:CB	3:2C:58:ARG:CB	2.64	0.74
2:2B:119:ASN:ND2	3:2C:55:SER:O	2.18	0.74
2:2B:122:ASP:OD2	3:2C:52:LYS:HG2	1.87	0.74
2:1B:283:ARG:CD	2:4B:56:ARG:CD	2.64	0.74
2:7B:115:ASP:OD2	3:7C:58:ARG:CG	2.35	0.74
2:2B:327:ASP:HB3	1:6A:178:GLN:NE2	2.00	0.74
2:6B:122:ASP:OD2	3:6C:52:LYS:HG2	1.87	0.74
2:2B:2:ARG:HE	1:6A:75:PRO:HG3	0.58	0.74
2:2B:259:PRO:O	1:6A:400:ALA:CA	2.34	0.74
2:2B:324:LYS:CG	1:6A:224:PRO:O	2.36	0.74
2:3B:2:ARG:HE	1:7A:75:PRO:HD3	1.50	0.74
2:5B:119:ASN:OD1	3:5C:55:SER:HB3	1.88	0.74
2:6B:56:ARG:NE	2:7B:283:ARG:CD	2.50	0.74
3:3C:18:GLU:CB	1:4A:288:GLU:OE2	2.35	0.74
3:3C:92:MET:HE3	3:3C:131:LEU:HG	1.70	0.74
2:1B:119:ASN:OD1	3:1C:55:SER:HB3	1.88	0.74
2:2B:247:ASN:OD1	1:6A:77:VAL:CG2	2.36	0.74
1:4A:132:ASP:OD1	3:4C:68:ARG:CD	2.35	0.73
2:4B:346:SER:OG	1:8A:178:GLN:O	2.05	0.73
2:8B:87:ASP:OD1	3:8C:21:ARG:NE	2.21	0.73
2:1B:324:LYS:CE	1:5A:224:PRO:HD3	2.14	0.73
2:2B:2:ARG:NH1	1:6A:75:PRO:CG	2.49	0.73
1:8A:132:ASP:OD1	3:8C:68:ARG:CD	2.35	0.73
2:3B:343:MET:SD	1:7A:393:LEU:CD2	2.77	0.73
1:6A:132:ASP:OD1	3:6C:68:ARG:CD	2.36	0.73
3:7C:18:GLU:CB	1:8A:288:GLU:OE2	2.35	0.73
2:1B:324:LYS:CD	1:5A:223:SER:CA	2.67	0.73
2:3B:61:VAL:CB	1:4A:287:PHE:HZ	1.92	0.73
2:3B:344:PRO:CA	1:7A:392:LYS:CE	2.61	0.73
1:4A:132:ASP:HA	3:4C:68:ARG:HG2	1.71	0.73
2:3B:115:ASP:OD2	3:3C:58:ARG:HD3	1.89	0.73
2:5B:115:ASP:H	3:5C:62:PHE:HE2	1.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6A:63:SER:H	1:7A:286:LYS:HZ1	1.36	0.73
1:1A:367:ARG:HH12	1:4A:59:SER:HB3	1.53	0.73
2:3B:122:ASP:OD1	3:3C:52:LYS:HE2	1.89	0.73
2:2B:259:PRO:O	1:6A:400:ALA:N	2.22	0.73
2:3B:344:PRO:HA	1:7A:392:LYS:HE2	1.70	0.73
3:4C:92:MET:HE3	3:4C:131:LEU:HG	1.68	0.73
2:1B:88:GLU:HG2	3:1C:24:TYR:CD2	2.24	0.73
1:8A:132:ASP:HA	3:8C:68:ARG:HG2	1.70	0.73
2:1B:115:ASP:H	3:1C:62:PHE:HE2	1.36	0.72
1:5A:367:ARG:HH12	1:8A:59:SER:HB3	1.53	0.72
2:3B:324:LYS:HB2	1:7A:224:PRO:O	1.89	0.72
2:5B:87:ASP:CG	3:5C:21:ARG:HH21	1.89	0.72
2:6B:115:ASP:CB	3:6C:58:ARG:HB3	2.18	0.72
2:7B:122:ASP:OD1	3:7C:52:LYS:HE2	1.89	0.72
2:4B:87:ASP:OD1	3:4C:21:ARG:NE	2.21	0.72
2:2B:2:ARG:NE	1:6A:75:PRO:CD	2.52	0.72
2:1B:115:ASP:CB	3:1C:58:ARG:HB3	2.19	0.72
2:2B:245:LYS:HG3	1:6A:17:GLN:HE22	1.53	0.72
2:2B:259:PRO:O	1:6A:399:PHE:O	2.06	0.72
2:4B:351:LEU:HD11	1:8A:179:VAL:CG2	2.18	0.72
2:5B:115:ASP:CB	3:5C:58:ARG:HB3	2.19	0.72
2:6B:119:ASN:ND2	3:6C:55:SER:CB	2.52	0.72
2:2B:115:ASP:CB	3:2C:58:ARG:HB3	2.18	0.72
2:4B:2:ARG:HH11	1:8A:75:PRO:HG2	1.55	0.72
2:5B:88:GLU:HG2	3:5C:24:TYR:CD2	2.24	0.72
2:2B:346:SER:OG	1:6A:178:GLN:O	1.93	0.72
2:1B:115:ASP:OD2	3:1C:58:ARG:CG	2.38	0.71
2:7B:115:ASP:OD2	3:7C:58:ARG:HD3	1.89	0.71
1:2A:63:SER:H	1:3A:286:LYS:HZ1	1.39	0.71
2:3B:247:ASN:OD1	1:7A:13:GLN:CD	2.29	0.71
2:3B:255:THR:HA	1:7A:402:TRP:CD2	2.24	0.71
2:4B:89:SER:HA	3:4C:24:TYR:CZ	2.05	0.71
2:5B:94:LYS:NZ	3:5C:63:ARG:HH21	1.89	0.71
3:6C:92:MET:HE3	3:6C:131:LEU:HG	1.71	0.71
3:7C:92:MET:CE	3:7C:131:LEU:HD23	2.21	0.71
3:7C:92:MET:HE2	3:7C:131:LEU:HD23	1.73	0.71
2:8B:87:ASP:CG	3:8C:21:ARG:CZ	2.59	0.71
1:1A:91:PRO:CD	1:2A:287:PHE:CD2	2.73	0.71
2:1B:2:ARG:NH2	1:5A:76:SER:OG	2.24	0.71
2:4B:344:PRO:CA	1:8A:392:LYS:CE	2.56	0.71
2:5B:115:ASP:OD2	3:5C:58:ARG:CD	2.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2C:92:MET:CE	3:2C:131:LEU:HD23	2.21	0.71
2:1B:88:GLU:CB	3:1C:24:TYR:HD2	2.04	0.71
3:4C:92:MET:CE	3:4C:131:LEU:HD23	2.21	0.71
2:2B:245:LYS:C	1:6A:13:GLN:HE22	1.93	0.71
2:3B:119:ASN:HD21	3:3C:55:SER:CB	2.04	0.71
3:5C:92:MET:CE	3:5C:131:LEU:HD23	2.21	0.71
1:4A:132:ASP:HA	3:4C:68:ARG:HD3	1.73	0.70
2:5B:115:ASP:OD2	3:5C:58:ARG:CG	2.38	0.70
2:7B:119:ASN:HD21	3:7C:55:SER:CB	2.04	0.70
2:1B:346:SER:C	1:5A:179:VAL:HA	2.10	0.70
2:3B:119:ASN:HD21	3:3C:55:SER:CA	2.04	0.70
2:3B:122:ASP:CG	3:3C:52:LYS:HE3	2.11	0.70
3:6C:92:MET:CE	3:6C:131:LEU:HD23	2.21	0.70
2:1B:346:SER:HB3	1:5A:177:PRO:O	1.91	0.70
2:3B:324:LYS:HA	1:7A:212:PHE:CE1	2.27	0.70
2:1B:122:ASP:OD2	3:1C:52:LYS:CE	2.39	0.70
2:1B:94:LYS:NZ	3:1C:63:ARG:HH21	1.88	0.70
3:1C:92:MET:CE	3:1C:131:LEU:HD23	2.21	0.70
2:5B:122:ASP:OD2	3:5C:52:LYS:CE	2.39	0.70
2:6B:88:GLU:CB	3:6C:24:TYR:CD2	2.69	0.70
2:7B:119:ASN:HD21	3:7C:55:SER:CA	2.04	0.70
1:2A:132:ASP:OD1	3:2C:68:ARG:HD3	1.91	0.70
3:3C:92:MET:CE	3:3C:131:LEU:HD23	2.21	0.70
3:5C:92:MET:HE3	3:5C:131:LEU:HG	1.71	0.70
1:8A:132:ASP:HA	3:8C:68:ARG:HD3	1.73	0.70
1:5A:91:PRO:CD	1:6A:287:PHE:CD2	2.73	0.70
2:1B:115:ASP:OD2	3:1C:58:ARG:CD	2.39	0.70
3:2C:92:MET:HE2	3:2C:131:LEU:HD23	1.73	0.70
3:7C:92:MET:HE3	3:7C:131:LEU:HG	1.74	0.70
3:8C:92:MET:CE	3:8C:131:LEU:HD23	2.21	0.70
2:8B:122:ASP:OD2	3:8C:52:LYS:HG2	1.92	0.70
2:2B:322:LYS:CB	1:6A:225:THR:CG2	2.59	0.69
2:4B:87:ASP:CG	3:4C:21:ARG:CZ	2.59	0.69
1:6A:132:ASP:OD1	3:6C:68:ARG:HD3	1.91	0.69
1:6A:132:ASP:HA	3:6C:68:ARG:CD	2.22	0.69
2:1B:254:VAL:HG11	1:5A:402:TRP:CH2	2.26	0.69
2:2B:119:ASN:ND2	3:2C:55:SER:CB	2.52	0.69
2:3B:255:THR:OG1	1:7A:402:TRP:CE3	2.43	0.69
2:2B:91:ILE:HG22	3:2C:24:TYR:CZ	2.28	0.69
2:7B:61:VAL:CB	1:8A:287:PHE:HZ	1.92	0.69
3:2C:92:MET:HE3	3:2C:131:LEU:HG	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4B:122:ASP:OD2	3:4C:52:LYS:HG2	1.92	0.69
2:3B:55:VAL:HG12	1:4A:286:LYS:HD3	1.74	0.69
2:3B:88:GLU:HG2	3:3C:24:TYR:CG	2.27	0.69
2:4B:256:ASN:HD21	1:8A:182:VAL:HG12	1.56	0.69
2:7B:88:GLU:HG2	3:7C:24:TYR:CG	2.27	0.69
2:7B:122:ASP:OD2	3:7C:52:LYS:CD	2.41	0.69
2:3B:55:VAL:CG1	1:4A:287:PHE:HA	2.23	0.69
1:6A:65:VAL:HG12	1:7A:287:PHE:CE1	2.28	0.69
2:6B:115:ASP:CB	3:6C:58:ARG:HB2	2.23	0.69
2:7B:55:VAL:CG1	1:8A:287:PHE:HA	2.23	0.69
2:7B:115:ASP:HB2	3:7C:62:PHE:CE2	2.28	0.69
1:2A:132:ASP:HA	3:2C:68:ARG:CD	2.23	0.68
2:4B:115:ASP:OD2	3:4C:58:ARG:HD3	1.92	0.68
2:4B:256:ASN:O	1:8A:399:PHE:CE1	2.46	0.68
2:7B:122:ASP:CG	3:7C:52:LYS:HE3	2.11	0.68
2:1B:247:ASN:H	1:5A:13:GLN:NE2	1.90	0.68
2:4B:115:ASP:OD2	3:4C:58:ARG:CG	2.42	0.68
2:7B:115:ASP:H	3:7C:62:PHE:HE2	1.41	0.68
1:2A:249:PHE:H	1:2A:360:GLU:HG2	1.59	0.68
2:3B:344:PRO:CA	1:7A:392:LYS:HE3	2.20	0.68
2:2B:246:LEU:HD21	4:6A:501:GDP:H8	1.57	0.68
2:3B:122:ASP:OD2	3:3C:52:LYS:CD	2.41	0.68
2:3B:245:LYS:CA	1:7A:13:GLN:HE22	2.06	0.68
2:4B:246:LEU:HD21	4:8A:501:GDP:C2'	2.23	0.68
1:5A:249:PHE:H	1:5A:360:GLU:HG2	1.59	0.68
2:8B:87:ASP:OD1	3:8C:21:ARG:CZ	2.41	0.68
2:5B:88:GLU:HG2	3:5C:24:TYR:CG	2.29	0.68
2:8B:115:ASP:OD2	3:8C:58:ARG:HD3	1.92	0.68
2:1B:256:ASN:O	1:5A:183:VAL:HG11	1.94	0.68
2:2B:348:GLY:O	1:6A:183:VAL:CG1	2.40	0.68
3:3C:92:MET:HE2	3:3C:131:LEU:HD23	1.76	0.68
2:1B:88:GLU:HG2	3:1C:24:TYR:CG	2.29	0.68
2:1B:2:ARG:NH2	1:5A:76:SER:HG	1.91	0.68
2:1B:94:LYS:HE3	3:1C:66:GLU:HG2	1.75	0.68
1:2A:132:ASP:OD1	3:2C:68:ARG:CD	2.36	0.68
2:2B:56:ARG:HD3	2:3B:283:ARG:HD3	1.75	0.68
2:3B:115:ASP:HB2	3:3C:62:PHE:CE2	2.28	0.68
2:6B:91:ILE:HG22	3:6C:24:TYR:CZ	2.28	0.68
2:2B:246:LEU:CA	1:6A:13:GLN:HE22	2.05	0.68
2:4B:87:ASP:OD1	3:4C:21:ARG:CZ	2.41	0.68
2:6B:56:ARG:HD3	2:7B:283:ARG:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7B:55:VAL:CG1	1:8A:286:LYS:HD3	2.24	0.68
3:6C:92:MET:HE2	3:6C:131:LEU:HD23	1.75	0.67
1:7A:249:PHE:H	1:7A:360:GLU:HG2	1.59	0.67
2:1B:245:LYS:HG2	1:5A:226:VAL:HG22	1.69	0.67
2:1B:327:ASP:OD1	1:5A:178:GLN:NE2	2.27	0.67
2:2B:115:ASP:CB	3:2C:58:ARG:HB2	2.24	0.67
2:3B:55:VAL:CG1	1:4A:286:LYS:HD3	2.24	0.67
3:3C:18:GLU:HG3	1:4A:288:GLU:CG	2.20	0.67
1:5A:287:PHE:CE1	1:8A:65:VAL:HG13	2.00	0.67
3:5C:92:MET:HE2	3:5C:131:LEU:HD23	1.75	0.67
1:8A:249:PHE:H	1:8A:360:GLU:HG2	1.59	0.67
2:8B:115:ASP:OD2	3:8C:58:ARG:CG	2.42	0.67
1:4A:249:PHE:H	1:4A:360:GLU:HG2	1.59	0.67
2:7B:55:VAL:HG12	1:8A:286:LYS:HD3	1.74	0.67
2:3B:2:ARG:HG3	1:7A:98:THR:C	2.15	0.67
2:3B:115:ASP:H	3:3C:62:PHE:HE2	1.41	0.67
2:3B:245:LYS:CA	1:7A:13:GLN:NE2	2.48	0.67
2:2B:122:ASP:OD2	3:2C:52:LYS:CD	2.43	0.67
1:1A:286:LYS:HZ1	1:4A:63:SER:H	1.42	0.67
2:2B:87:ASP:OD1	3:2C:21:ARG:NE	2.08	0.67
2:3B:115:ASP:CG	3:3C:58:ARG:HB2	2.15	0.67
2:7B:89:SER:HB2	3:7C:21:ARG:HH12	1.56	0.67
3:7C:18:GLU:HG3	1:8A:288:GLU:CG	2.20	0.67
1:1A:249:PHE:H	1:1A:360:GLU:HG2	1.59	0.67
2:2B:122:ASP:OD2	3:2C:52:LYS:CG	2.43	0.67
2:2B:246:LEU:CA	1:6A:13:GLN:NE2	2.58	0.67
2:4B:115:ASP:CB	3:4C:58:ARG:CB	2.72	0.67
2:4B:252:GLU:HG3	1:8A:102:GLY:CA	2.25	0.67
2:1B:94:LYS:HE2	3:1C:66:GLU:OE2	1.90	0.67
2:3B:245:LYS:HA	1:7A:13:GLN:HE21	1.56	0.67
2:5B:94:LYS:HE3	3:5C:66:GLU:HG2	1.75	0.67
1:6A:249:PHE:H	1:6A:360:GLU:HG2	1.59	0.67
1:3A:249:PHE:H	1:3A:360:GLU:HG2	1.59	0.66
2:3B:2:ARG:HH12	1:7A:75:PRO:HG2	1.48	0.66
2:6B:122:ASP:OD2	3:6C:52:LYS:CD	2.43	0.66
2:2B:88:GLU:CG	3:2C:24:TYR:HB3	2.25	0.66
2:2B:122:ASP:OD1	3:2C:52:LYS:HE2	1.96	0.66
2:2B:256:ASN:O	1:6A:183:VAL:CG2	2.37	0.66
2:5B:89:SER:OG	3:5C:21:ARG:HG3	1.96	0.66
1:3A:329:ASP:HB3	1:3A:332:LEU:HB2	1.78	0.66
2:3B:2:ARG:N	1:7A:98:THR:HG23	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4B:256:ASN:ND2	1:8A:184:THR:N	2.42	0.66
2:4B:343:MET:C	1:8A:392:LYS:HE3	2.16	0.66
2:8B:119:ASN:OD1	3:8C:55:SER:CB	2.43	0.66
1:1A:91:PRO:HD3	1:2A:287:PHE:CE2	2.31	0.66
2:2B:323:ALA:CB	1:6A:226:VAL:HG13	2.23	0.66
2:3B:344:PRO:HB3	1:7A:389:ASN:HD22	1.54	0.66
1:7A:329:ASP:HB3	1:7A:332:LEU:HB2	1.78	0.66
2:1B:89:SER:OG	3:1C:21:ARG:HG3	1.96	0.66
2:6B:94:LYS:HZ1	3:6C:63:ARG:NH2	1.77	0.66
2:1B:87:ASP:OD1	3:1C:21:ARG:NH2	2.28	0.66
2:4B:324:LYS:HG3	1:8A:224:PRO:CG	2.24	0.66
2:1B:119:ASN:HD21	3:1C:55:SER:CA	2.08	0.66
1:4A:329:ASP:HB3	1:4A:332:LEU:HB2	1.78	0.66
2:1B:2:ARG:CZ	1:5A:76:SER:HG	2.09	0.66
2:2B:342:TYR:C	1:6A:393:LEU:HD23	2.07	0.66
2:4B:256:ASN:HD22	1:8A:184:THR:N	1.94	0.66
2:5B:115:ASP:CB	3:5C:62:PHE:CE2	2.78	0.66
2:7B:119:ASN:ND2	3:7C:56:LEU:N	2.42	0.66
2:1B:247:ASN:OD1	1:5A:13:GLN:NE2	2.29	0.66
2:6B:122:ASP:OD2	3:6C:52:LYS:CG	2.43	0.66
2:2B:115:ASP:OD1	3:2C:58:ARG:CD	2.44	0.65
2:2B:342:TYR:O	1:6A:393:LEU:HD21	1.90	0.65
1:8A:329:ASP:HB3	1:8A:332:LEU:HB2	1.78	0.65
2:3B:350:LYS:N	1:7A:183:VAL:HG12	2.11	0.65
2:2B:344:PRO:HD3	1:6A:393:LEU:HD11	1.78	0.65
1:5A:91:PRO:HD3	1:6A:287:PHE:CE2	2.31	0.65
2:7B:55:VAL:HG13	1:8A:287:PHE:HA	1.78	0.65
2:8B:111:GLU:O	3:8C:62:PHE:CZ	2.49	0.65
1:2A:329:ASP:HB3	1:2A:332:LEU:HB2	1.78	0.65
2:4B:111:GLU:O	3:4C:62:PHE:CZ	2.49	0.65
1:5A:132:ASP:OD1	3:5C:68:ARG:HD3	1.97	0.65
1:6A:329:ASP:HB3	1:6A:332:LEU:HB2	1.78	0.65
2:8B:122:ASP:OD2	3:8C:52:LYS:CE	2.45	0.65
2:2B:88:GLU:CB	3:2C:24:TYR:CD2	2.69	0.65
2:2B:255:THR:CG2	1:6A:104:ASN:HB2	2.12	0.65
2:3B:350:LYS:HB3	1:7A:183:VAL:CG1	2.26	0.65
2:6B:115:ASP:OD1	3:6C:58:ARG:CD	2.44	0.65
2:7B:132:GLN:HE22	2:7B:249:ASP:HB2	1.62	0.65
2:1B:132:GLN:HE22	2:1B:249:ASP:HB2	1.62	0.65
1:2A:65:VAL:HG12	1:3A:287:PHE:CE1	2.29	0.65
2:3B:255:THR:HG23	1:7A:402:TRP:CB	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4B:119:ASN:OD1	3:4C:55:SER:CB	2.43	0.65
2:5B:119:ASN:HD21	3:5C:55:SER:CA	2.08	0.65
2:6B:88:GLU:CG	3:6C:24:TYR:HB3	2.25	0.65
2:4B:350:LYS:CB	1:8A:183:VAL:HG13	2.23	0.65
1:1A:329:ASP:HB3	1:1A:332:LEU:HB2	1.78	0.65
3:1C:49:ASP:OD2	3:1C:52:LYS:HD2	1.97	0.65
2:4B:259:PRO:O	1:8A:399:PHE:O	0.66	0.65
1:5A:329:ASP:HB3	1:5A:332:LEU:HB2	1.78	0.65
2:5B:88:GLU:CB	3:5C:24:TYR:HD2	2.04	0.65
2:8B:132:GLN:HE22	2:8B:249:ASP:HB2	1.62	0.65
3:2C:49:ASP:OD2	3:2C:52:LYS:HD2	1.97	0.65
2:3B:254:VAL:C	1:7A:402:TRP:CZ2	2.44	0.65
2:4B:122:ASP:OD2	3:4C:52:LYS:CE	2.45	0.65
2:6B:122:ASP:OD1	3:6C:52:LYS:HE2	1.96	0.65
3:7C:49:ASP:OD2	3:7C:52:LYS:HD2	1.97	0.65
2:1B:56:ARG:NH2	2:2B:283:ARG:CD	2.59	0.64
2:2B:327:ASP:CB	1:6A:178:GLN:NE2	2.59	0.64
3:4C:49:ASP:OD2	3:4C:52:LYS:HD2	1.97	0.64
1:1A:5:ASN:ND2	1:1A:50:SER:O	2.31	0.64
2:3B:350:LYS:HB3	1:7A:183:VAL:H	1.61	0.64
3:3C:18:GLU:HA	1:4A:288:GLU:CD	2.17	0.64
1:5A:72:ASP:HB3	1:5A:78:ILE:HD11	1.79	0.64
1:8A:5:ASN:ND2	1:8A:50:SER:O	2.31	0.64
2:1B:56:ARG:CD	2:2B:283:ARG:HD3	2.28	0.64
2:2B:222:TYR:O	2:2B:226:ASN:ND2	2.31	0.64
2:3B:245:LYS:HE3	1:7A:17:GLN:CD	2.18	0.64
2:4B:132:GLN:HE22	2:4B:249:ASP:HB2	1.62	0.64
1:5A:5:ASN:ND2	1:5A:50:SER:O	2.31	0.64
2:5B:222:TYR:O	2:5B:226:ASN:ND2	2.31	0.64
1:6A:72:ASP:HB3	1:6A:78:ILE:HD11	1.79	0.64
2:1B:256:ASN:C	1:5A:183:VAL:CG2	2.51	0.64
2:2B:260:PHE:CD1	1:6A:399:PHE:O	2.50	0.64
2:6B:132:GLN:HE22	2:6B:249:ASP:HB2	1.62	0.64
3:7C:18:GLU:HA	1:8A:288:GLU:CD	2.17	0.64
2:2B:132:GLN:HE22	2:2B:249:ASP:HB2	1.62	0.64
2:3B:89:SER:HB2	3:3C:21:ARG:HH12	1.56	0.64
3:4C:92:MET:HE2	3:4C:131:LEU:HD23	1.78	0.64
2:5B:88:GLU:HG2	3:5C:24:TYR:CB	2.27	0.64
2:1B:115:ASP:CB	3:1C:62:PHE:CE2	2.78	0.64
2:3B:222:TYR:O	2:3B:226:ASN:ND2	2.31	0.64
3:6C:49:ASP:OD2	3:6C:52:LYS:HD2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:72:ASP:HB3	1:1A:78:ILE:HD11	1.79	0.64
1:1A:351:PRO:HD2	2:1B:388:MET:CE	2.28	0.64
1:3A:72:ASP:HB3	1:3A:78:ILE:HD11	1.79	0.64
2:3B:132:GLN:HE22	2:3B:249:ASP:HB2	1.62	0.64
2:3B:256:ASN:HD22	1:7A:183:VAL:HG23	1.62	0.64
3:3C:195:GLU:OE1	3:3C:195:GLU:N	2.30	0.64
2:7B:115:ASP:CG	3:7C:58:ARG:HB2	2.15	0.64
2:1B:222:TYR:O	2:1B:226:ASN:ND2	2.31	0.64
2:5B:56:ARG:CD	2:6B:283:ARG:HD3	2.28	0.64
1:7A:72:ASP:HB3	1:7A:78:ILE:HD11	1.79	0.64
1:1A:132:ASP:OD1	3:1C:68:ARG:HD3	1.97	0.64
2:1B:111:GLU:O	3:1C:62:PHE:CZ	2.51	0.64
1:2A:351:PRO:HD2	2:2B:388:MET:CE	2.28	0.64
2:3B:115:ASP:OD2	3:3C:58:ARG:CD	2.46	0.64
2:4B:222:TYR:O	2:4B:226:ASN:ND2	2.31	0.64
2:5B:132:GLN:HE22	2:5B:249:ASP:HB2	1.62	0.64
2:8B:115:ASP:CB	3:8C:58:ARG:CB	2.72	0.64
2:8B:222:TYR:O	2:8B:226:ASN:ND2	2.31	0.64
2:1B:256:ASN:CB	1:5A:183:VAL:HG22	2.28	0.64
2:2B:89:SER:HA	3:2C:24:TYR:CE2	2.33	0.64
1:6A:56:LEU:HD12	1:7A:286:LYS:NZ	2.13	0.64
3:7C:195:GLU:OE1	3:7C:195:GLU:N	2.30	0.64
3:8C:92:MET:HE2	3:8C:131:LEU:CD2	2.26	0.64
2:1B:119:ASN:HD21	3:1C:55:SER:CB	2.12	0.63
1:6A:5:ASN:ND2	1:6A:50:SER:O	2.31	0.63
1:6A:351:PRO:HD2	2:6B:388:MET:CE	2.28	0.63
3:8C:49:ASP:OD2	3:8C:52:LYS:HD2	1.97	0.63
3:1C:92:MET:HE3	3:1C:131:LEU:CG	2.28	0.63
2:4B:246:LEU:HD13	1:8A:181:SER:OG	1.99	0.63
2:5B:111:GLU:O	3:5C:62:PHE:CZ	2.51	0.63
2:7B:222:TYR:O	2:7B:226:ASN:ND2	2.31	0.63
2:1B:115:ASP:CG	3:1C:58:ARG:CD	2.66	0.63
2:1B:256:ASN:HD22	1:5A:183:VAL:H	1.46	0.63
1:3A:5:ASN:ND2	1:3A:50:SER:O	2.31	0.63
2:3B:55:VAL:HG13	1:4A:287:PHE:HA	1.78	0.63
1:5A:286:LYS:HZ1	1:8A:63:SER:CB	2.10	0.63
2:5B:87:ASP:OD1	3:5C:21:ARG:NH2	2.28	0.63
2:5B:119:ASN:HD21	3:5C:55:SER:CB	2.11	0.63
2:1B:88:GLU:HG2	3:1C:24:TYR:CB	2.27	0.63
2:1B:324:LYS:CE	1:5A:216:HIS:CG	2.76	0.63
1:2A:56:LEU:HD12	1:3A:286:LYS:NZ	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:346:SER:O	1:6A:179:VAL:HA	1.99	0.63
2:3B:2:ARG:NH1	1:7A:75:PRO:HD2	2.11	0.63
1:4A:5:ASN:ND2	1:4A:50:SER:O	2.31	0.63
3:5C:49:ASP:OD2	3:5C:52:LYS:HD2	1.97	0.63
1:2A:72:ASP:HB3	1:2A:78:ILE:HD11	1.79	0.63
2:2B:347:GLY:C	1:6A:180:SER:OG	2.37	0.63
2:3B:245:LYS:HE3	1:7A:17:GLN:NE2	2.13	0.63
2:1B:322:LYS:HD3	1:5A:223:SER:O	1.99	0.63
1:5A:351:PRO:HD2	2:5B:388:MET:CE	2.28	0.63
2:6B:222:TYR:O	2:6B:226:ASN:ND2	2.31	0.63
2:7B:115:ASP:OD2	3:7C:58:ARG:CD	2.46	0.63
2:2B:115:ASP:HB3	3:2C:58:ARG:HB2	1.80	0.63
2:3B:245:LYS:CG	1:7A:17:GLN:OE1	2.46	0.63
2:6B:115:ASP:HB3	3:6C:58:ARG:HB2	1.80	0.63
2:1B:119:ASN:HD21	3:1C:55:SER:HB3	1.57	0.63
2:1B:324:LYS:NZ	1:5A:216:HIS:CA	2.61	0.63
3:3C:49:ASP:OD2	3:3C:52:LYS:HD2	1.97	0.63
1:4A:72:ASP:HB3	1:4A:78:ILE:HD11	1.79	0.63
1:7A:351:PRO:HD2	2:7B:388:MET:CE	2.28	0.63
1:8A:351:PRO:HD2	2:8B:388:MET:CE	2.28	0.63
1:2A:5:ASN:ND2	1:2A:50:SER:O	2.31	0.63
2:2B:246:LEU:HD21	4:6A:501:GDP:C8	2.34	0.63
2:3B:55:VAL:CG1	1:4A:287:PHE:CG	2.54	0.63
2:3B:243:PRO:CG	1:7A:76:SER:CB	2.75	0.63
2:3B:324:LYS:NZ	1:7A:216:HIS:CB	2.55	0.63
2:6B:89:SER:HA	3:6C:24:TYR:CE2	2.33	0.63
2:7B:115:ASP:CB	3:7C:58:ARG:HB3	2.29	0.63
2:2B:324:LYS:CG	1:6A:224:PRO:C	2.66	0.62
1:8A:72:ASP:HB3	1:8A:78:ILE:HD11	1.79	0.62
1:4A:351:PRO:HD2	2:4B:388:MET:CE	2.28	0.62
2:5B:87:ASP:OD2	3:5C:21:ARG:CZ	2.47	0.62
3:1C:92:MET:HE2	3:1C:131:LEU:HD23	1.80	0.62
2:3B:243:PRO:CB	1:7A:76:SER:HB3	2.29	0.62
1:7A:5:ASN:ND2	1:7A:50:SER:O	2.31	0.62
2:3B:119:ASN:ND2	3:3C:56:LEU:N	2.42	0.62
3:8C:195:GLU:OE1	3:8C:195:GLU:N	2.30	0.62
1:3A:351:PRO:HD2	2:3B:388:MET:CE	2.28	0.62
2:4B:164:ARG:HH21	1:8A:402:TRP:HZ3	1.47	0.62
3:4C:92:MET:HE3	3:4C:131:LEU:CG	2.30	0.62
1:5A:286:LYS:HZ1	1:8A:63:SER:H	1.46	0.62
2:1B:87:ASP:OD2	3:1C:21:ARG:CZ	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:259:PRO:HB3	1:5A:399:PHE:CE1	2.34	0.62
2:3B:324:LYS:HZ1	1:7A:216:HIS:HB2	1.62	0.62
2:7B:122:ASP:OD1	3:7C:52:LYS:CE	2.46	0.62
2:5B:56:ARG:NH2	2:6B:283:ARG:CD	2.59	0.62
2:1B:88:GLU:CB	3:1C:24:TYR:CD2	2.83	0.62
1:5A:367:ARG:HH12	1:8A:59:SER:CB	2.12	0.62
3:8C:92:MET:HE3	3:8C:131:LEU:HG	1.81	0.62
2:4B:256:ASN:ND2	1:8A:183:VAL:CA	2.59	0.62
3:4C:195:GLU:OE1	3:4C:195:GLU:N	2.30	0.62
2:2B:252:GLU:HG3	1:6A:102:GLY:HA3	1.78	0.61
2:5B:88:GLU:CB	3:5C:24:TYR:CD2	2.83	0.61
2:2B:247:ASN:N	1:6A:13:GLN:OE1	2.31	0.61
2:3B:122:ASP:OD1	3:3C:52:LYS:CE	2.46	0.61
1:1A:367:ARG:HH12	1:4A:59:SER:CB	2.12	0.61
2:1B:247:ASN:N	1:5A:13:GLN:HE22	1.94	0.61
1:3A:131:CYS:O	3:3C:68:ARG:HG2	2.01	0.61
2:2B:256:ASN:HD21	1:6A:103:GLY:HA3	1.65	0.61
2:3B:115:ASP:CB	3:3C:58:ARG:HB3	2.29	0.61
2:3B:256:ASN:CA	1:7A:183:VAL:CG2	2.77	0.61
1:4A:136:GLY:HA3	1:4A:256:LEU:HD13	1.82	0.61
2:2B:347:GLY:HA2	1:6A:180:SER:HB3	1.68	0.61
2:6B:111:GLU:O	3:6C:62:PHE:HZ	1.82	0.61
1:8A:136:GLY:HA3	1:8A:256:LEU:HD13	1.82	0.61
1:5A:136:GLY:HA3	1:5A:256:LEU:HD13	1.82	0.61
1:2A:230:ASN:OD1	4:2A:501:GDP:N1	2.32	0.61
1:1A:136:GLY:HA3	1:1A:256:LEU:HD13	1.82	0.60
1:7A:131:CYS:O	3:7C:68:ARG:HG2	2.01	0.60
3:5C:195:GLU:OE1	3:5C:195:GLU:N	2.30	0.60
1:6A:136:GLY:HA3	1:6A:256:LEU:HD13	1.82	0.60
3:6C:20:ARG:HD3	3:6C:59:GLU:OE2	2.02	0.60
2:1B:259:PRO:HB3	1:5A:399:PHE:CD1	2.36	0.60
3:1C:195:GLU:OE1	3:1C:195:GLU:N	2.30	0.60
2:3B:324:LYS:HZ1	1:7A:216:HIS:CB	2.13	0.60
1:4A:243:SER:HB3	1:4A:254:ILE:H	1.67	0.60
3:5C:20:ARG:HD3	3:5C:59:GLU:OE2	2.01	0.60
2:1B:324:LYS:HD2	1:5A:223:SER:CA	2.14	0.60
1:2A:136:GLY:HA3	1:2A:256:LEU:HD13	1.82	0.60
2:3B:327:ASP:OD2	1:7A:212:PHE:HE2	1.78	0.60
2:8B:115:ASP:CG	3:8C:58:ARG:CD	2.68	0.60
1:1A:367:ARG:NH1	1:4A:59:SER:HB3	2.16	0.60
2:1B:346:SER:O	1:5A:179:VAL:CA	2.40	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5A:243:SER:HB3	1:5A:254:ILE:H	1.67	0.60
2:5B:94:LYS:HE2	3:5C:66:GLU:OE2	1.90	0.60
2:3B:88:GLU:CB	3:3C:24:TYR:HD2	2.15	0.60
3:3C:20:ARG:HD3	3:3C:59:GLU:OE2	2.02	0.60
2:5B:115:ASP:CG	3:5C:58:ARG:CD	2.66	0.60
3:7C:20:ARG:HD3	3:7C:59:GLU:OE2	2.02	0.60
2:1B:254:VAL:HG11	1:5A:402:TRP:HH2	1.63	0.60
1:3A:136:GLY:HA3	1:3A:256:LEU:HD13	1.82	0.60
2:4B:119:ASN:HD21	3:4C:55:SER:CB	2.14	0.60
1:7A:136:GLY:HA3	1:7A:256:LEU:HD13	1.82	0.60
1:1A:243:SER:HB3	1:1A:254:ILE:H	1.67	0.60
3:3C:92:MET:HE3	3:3C:131:LEU:CG	2.32	0.60
2:5B:115:ASP:CB	3:5C:58:ARG:CB	2.80	0.60
1:7A:243:SER:HB3	1:7A:254:ILE:H	1.67	0.60
1:8A:243:SER:HB3	1:8A:254:ILE:H	1.67	0.60
1:1A:287:PHE:CE1	1:4A:65:VAL:HG13	2.00	0.60
2:3B:246:LEU:HD21	4:7A:501:GDP:H3'	1.83	0.60
3:8C:20:ARG:HD3	3:8C:59:GLU:OE2	2.02	0.60
3:1C:20:ARG:HD3	3:1C:59:GLU:OE2	2.01	0.59
2:3B:256:ASN:O	1:7A:399:PHE:CD1	2.54	0.59
1:8A:230:ASN:OD1	4:8A:501:GDP:N1	2.32	0.59
2:1B:259:PRO:CB	1:5A:399:PHE:CD1	2.85	0.59
2:2B:259:PRO:C	1:6A:399:PHE:C	2.58	0.59
1:3A:243:SER:HB3	1:3A:254:ILE:H	1.67	0.59
2:3B:115:ASP:CB	3:3C:58:ARG:CB	2.80	0.59
2:2B:254:VAL:O	1:6A:402:TRP:CZ2	2.55	0.59
3:2C:195:GLU:OE1	3:2C:195:GLU:N	2.30	0.59
1:3A:230:ASN:OD1	4:3A:501:GDP:N1	2.32	0.59
2:3B:84:GLN:NE2	1:4A:284:ARG:NH1	0.61	0.59
2:4B:324:LYS:HG3	1:8A:224:PRO:HG2	1.84	0.59
2:4B:115:ASP:CG	3:4C:58:ARG:CD	2.68	0.59
1:8A:141:HIS:NE2	1:8A:170:SER:OG	2.36	0.59
2:1B:115:ASP:CB	3:1C:58:ARG:CB	2.80	0.59
2:2B:2:ARG:HH11	1:6A:75:PRO:HG2	1.64	0.59
2:3B:255:THR:HA	1:7A:402:TRP:CD1	2.37	0.59
1:4A:141:HIS:NE2	1:4A:170:SER:OG	2.36	0.59
2:4B:351:LEU:CD1	1:8A:179:VAL:CG2	2.80	0.59
3:6C:195:GLU:OE1	3:6C:195:GLU:N	2.30	0.59
1:1A:230:ASN:OD1	4:1A:501:GDP:N1	2.32	0.59
3:2C:20:ARG:HD3	3:2C:59:GLU:OE2	2.02	0.59
3:4C:20:ARG:HD3	3:4C:59:GLU:OE2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6A:230:ASN:OD1	4:6A:501:GDP:N1	2.32	0.59
1:6A:243:SER:HB3	1:6A:254:ILE:H	1.67	0.59
2:7B:84:GLN:NE2	1:8A:284:ARG:NH1	0.61	0.59
2:7B:119:ASN:OD1	3:7C:55:SER:HB3	2.02	0.59
2:8B:119:ASN:HD21	3:8C:55:SER:CB	2.14	0.59
1:5A:367:ARG:NH1	1:8A:59:SER:HB3	2.16	0.59
2:3B:74:ILE:HG21	2:3B:91:ILE:HD11	1.85	0.59
2:6B:87:ASP:OD1	3:6C:21:ARG:NE	2.08	0.59
1:7A:141:HIS:NE2	1:7A:170:SER:OG	2.36	0.59
2:7B:74:ILE:HG21	2:7B:91:ILE:HD11	1.85	0.59
1:2A:243:SER:HB3	1:2A:254:ILE:H	1.67	0.59
2:2B:246:LEU:HA	1:6A:13:GLN:OE1	2.03	0.59
2:4B:115:ASP:OD2	3:4C:62:PHE:CZ	2.55	0.59
2:8B:115:ASP:OD2	3:8C:62:PHE:CZ	2.55	0.59
1:2A:141:HIS:NE2	1:2A:170:SER:OG	2.36	0.59
2:2B:74:ILE:HG21	2:2B:91:ILE:HD11	1.85	0.59
2:2B:343:MET:CE	1:6A:399:PHE:CE1	2.86	0.59
2:7B:88:GLU:CB	3:7C:24:TYR:HD2	2.15	0.59
1:1A:56:LEU:CD1	1:2A:286:LYS:HZ1	2.02	0.58
2:1B:74:ILE:HG21	2:1B:91:ILE:HD11	1.85	0.58
2:4B:115:ASP:OD2	3:4C:58:ARG:CD	2.51	0.58
1:6A:141:HIS:NE2	1:6A:170:SER:OG	2.36	0.58
2:6B:74:ILE:HG21	2:6B:91:ILE:HD11	1.85	0.58
1:3A:141:HIS:NE2	1:3A:170:SER:OG	2.36	0.58
2:4B:256:ASN:HD21	1:8A:184:THR:H	1.51	0.58
2:5B:74:ILE:HG21	2:5B:91:ILE:HD11	1.85	0.58
2:2B:56:ARG:NE	2:3B:283:ARG:HD3	2.19	0.58
2:3B:324:LYS:HG3	1:7A:224:PRO:CD	2.33	0.58
2:7B:115:ASP:CB	3:7C:58:ARG:CB	2.80	0.58
3:5C:92:MET:HE3	3:5C:131:LEU:CG	2.34	0.58
2:1B:254:VAL:HG12	1:5A:402:TRP:CZ2	2.38	0.58
1:5A:230:ASN:OD1	4:5A:501:GDP:N1	2.33	0.58
2:3B:344:PRO:HD3	1:7A:393:LEU:CG	2.31	0.58
2:4B:2:ARG:HG3	1:8A:98:THR:O	2.04	0.58
1:1A:141:HIS:NE2	1:1A:170:SER:OG	2.36	0.58
1:1A:286:LYS:HZ1	1:4A:63:SER:CB	2.16	0.58
1:2A:65:VAL:HG12	1:3A:287:PHE:CZ	2.39	0.58
3:6C:92:MET:HE3	3:6C:131:LEU:CG	2.34	0.58
2:8B:70:GLU:HG2	2:8B:97:GLY:HA3	1.86	0.58
2:1B:269:SER:HB3	2:1B:299:PHE:HD1	1.69	0.58
2:1B:346:SER:O	1:5A:179:VAL:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:119:ASN:OD1	3:3C:55:SER:HB3	2.02	0.58
2:3B:246:LEU:HD21	4:7A:501:GDP:C3'	2.34	0.58
2:3B:350:LYS:HB3	1:7A:183:VAL:N	2.19	0.58
2:5B:70:GLU:HG2	2:5B:97:GLY:HA3	1.86	0.58
2:2B:260:PHE:HA	1:6A:400:ALA:CB	2.31	0.58
2:3B:343:MET:SD	1:7A:393:LEU:HD21	2.43	0.58
2:4B:74:ILE:HG21	2:4B:91:ILE:HD11	1.85	0.58
2:6B:269:SER:HB3	2:6B:299:PHE:HD1	1.69	0.58
2:4B:89:SER:OG	3:4C:21:ARG:HG3	2.03	0.58
2:8B:115:ASP:OD2	3:8C:58:ARG:CD	2.51	0.58
2:1B:94:LYS:HZ1	3:1C:63:ARG:NH2	1.93	0.57
3:2C:92:MET:HE2	3:2C:131:LEU:CD2	2.34	0.57
1:5A:141:HIS:NE2	1:5A:170:SER:OG	2.36	0.57
2:8B:74:ILE:HG21	2:8B:91:ILE:HD11	1.85	0.57
2:8B:122:ASP:OD2	3:8C:52:LYS:HE3	2.04	0.57
1:1A:286:LYS:HZ3	1:4A:56:LEU:HD12	1.66	0.57
2:3B:2:ARG:HH11	1:7A:75:PRO:HG2	0.42	0.57
3:3C:18:GLU:CG	1:4A:288:GLU:OE2	2.41	0.57
2:1B:342:TYR:CD1	1:5A:396:ARG:HD2	2.38	0.57
2:2B:112:LYS:HA	3:2C:62:PHE:CE1	2.40	0.57
1:5A:286:LYS:NZ	1:8A:56:LEU:CD1	2.65	0.57
2:6B:112:LYS:HA	3:6C:62:PHE:CE1	2.40	0.57
2:2B:269:SER:HB3	2:2B:299:PHE:HD1	1.69	0.57
2:5B:269:SER:HB3	2:5B:299:PHE:HD1	1.69	0.57
3:7C:92:MET:HE2	3:7C:131:LEU:CD2	2.33	0.57
2:8B:89:SER:OG	3:8C:21:ARG:HG3	2.03	0.57
2:3B:84:GLN:CD	1:4A:284:ARG:HH11	1.80	0.57
2:4B:246:LEU:CD1	1:8A:181:SER:OG	2.52	0.57
1:6A:65:VAL:HG12	1:7A:287:PHE:CZ	2.39	0.57
2:2B:70:GLU:HG2	2:2B:97:GLY:HA3	1.86	0.57
2:2B:111:GLU:O	3:2C:62:PHE:HZ	1.82	0.57
2:4B:70:GLU:HG2	2:4B:97:GLY:HA3	1.86	0.57
2:4B:115:ASP:HB3	3:4C:58:ARG:CB	2.35	0.57
2:4B:122:ASP:OD2	3:4C:52:LYS:HE3	2.05	0.57
2:6B:115:ASP:H	3:6C:62:PHE:HE2	1.53	0.57
2:7B:55:VAL:CG1	1:8A:287:PHE:CG	2.54	0.57
2:3B:247:ASN:CG	1:7A:74:GLU:OE2	2.43	0.57
2:4B:256:ASN:HD21	1:8A:182:VAL:CG1	2.17	0.57
2:2B:63:ARG:NH2	2:2B:128:THR:OG1	2.38	0.57
2:4B:245:LYS:HG2	1:8A:226:VAL:HG21	0.57	0.57
2:6B:56:ARG:NE	2:7B:283:ARG:HD3	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:63:ARG:NH2	2:3B:128:THR:OG1	2.38	0.57
2:4B:269:SER:HB3	2:4B:299:PHE:HD1	1.69	0.57
1:6A:351:PRO:HD2	2:6B:388:MET:HE3	1.87	0.57
2:6B:70:GLU:HG2	2:6B:97:GLY:HA3	1.86	0.57
2:1B:122:ASP:OD2	3:1C:52:LYS:HE3	2.05	0.56
1:4A:277:ALA:HB3	1:4A:370:MET:HB3	1.87	0.56
2:7B:70:GLU:HG2	2:7B:97:GLY:HA3	1.86	0.56
2:7B:269:SER:HB3	2:7B:299:PHE:HD1	1.69	0.56
2:3B:70:GLU:HG2	2:3B:97:GLY:HA3	1.86	0.56
2:1B:70:GLU:HG2	2:1B:97:GLY:HA3	1.86	0.56
2:1B:88:GLU:CG	3:1C:24:TYR:CD2	2.88	0.56
1:2A:63:SER:CB	1:3A:286:LYS:HZ1	2.18	0.56
1:2A:351:PRO:HD2	2:2B:388:MET:HE3	1.87	0.56
2:2B:115:ASP:H	3:2C:62:PHE:HE2	1.53	0.56
2:2B:348:GLY:N	1:6A:180:SER:OG	2.37	0.56
3:2C:92:MET:HE3	3:2C:131:LEU:CG	2.35	0.56
2:3B:115:ASP:CG	3:3C:58:ARG:CD	2.74	0.56
2:4B:283:ARG:NH2	1:7A:57:GLY:O	2.38	0.56
1:7A:230:ASN:OD1	4:7A:501:GDP:N1	2.33	0.56
2:8B:63:ARG:NH2	2:8B:128:THR:OG1	2.38	0.56
2:2B:348:GLY:CA	1:6A:183:VAL:HG12	2.35	0.56
1:3A:239:GLY:HA3	1:3A:371:VAL:HG21	1.88	0.56
3:1C:92:MET:CE	3:1C:131:LEU:CD2	2.84	0.56
3:2C:92:MET:CE	3:2C:131:LEU:CD2	2.84	0.56
2:3B:245:LYS:CG	1:7A:226:VAL:HG21	2.34	0.56
1:4A:239:GLY:HA3	1:4A:371:VAL:HG21	1.88	0.56
2:4B:63:ARG:NH2	2:4B:128:THR:OG1	2.38	0.56
1:5A:277:ALA:HB3	1:5A:370:MET:HB3	1.87	0.56
2:7B:91:ILE:HG22	3:7C:24:TYR:CZ	2.40	0.56
1:8A:239:GLY:HA3	1:8A:371:VAL:HG21	1.88	0.56
2:8B:269:SER:HB3	2:8B:299:PHE:HD1	1.69	0.56
2:1B:2:ARG:HD3	1:5A:75:PRO:HD2	1.87	0.56
2:3B:91:ILE:HG22	3:3C:24:TYR:CZ	2.41	0.56
2:5B:88:GLU:CG	3:5C:24:TYR:HB3	2.35	0.56
1:7A:239:GLY:HA3	1:7A:371:VAL:HG21	1.88	0.56
2:7B:63:ARG:NH2	2:7B:128:THR:OG1	2.38	0.56
2:8B:115:ASP:HB3	3:8C:58:ARG:CB	2.35	0.56
2:1B:63:ARG:NH2	2:1B:128:THR:OG1	2.38	0.56
1:4A:29:GLU:OE2	1:4A:324:ARG:NH1	2.35	0.56
2:5B:94:LYS:HZ1	3:5C:63:ARG:NH2	1.94	0.56
1:1A:19:ALA:HA	1:1A:22:PHE:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:245:LYS:HG3	1:6A:17:GLN:CD	2.25	0.56
2:5B:63:ARG:NH2	2:5B:128:THR:OG1	2.38	0.56
2:5B:88:GLU:CG	3:5C:24:TYR:CD2	2.88	0.56
1:5A:239:GLY:HA3	1:5A:371:VAL:HG21	1.88	0.56
2:6B:63:ARG:NH2	2:6B:128:THR:OG1	2.38	0.56
1:7A:351:PRO:HD2	2:7B:388:MET:HE2	1.86	0.56
1:8A:277:ALA:HB3	1:8A:370:MET:HB3	1.87	0.56
1:1A:239:GLY:HA3	1:1A:371:VAL:HG21	1.88	0.55
1:1A:351:PRO:HD2	2:1B:388:MET:HE3	1.88	0.55
2:2B:2:ARG:HH11	1:6A:75:PRO:CG	2.17	0.55
2:2B:287:PRO:O	2:2B:291:ARG:NH2	2.39	0.55
1:7A:277:ALA:HB3	1:7A:370:MET:HB3	1.87	0.55
1:1A:277:ALA:HB3	1:1A:370:MET:HB3	1.87	0.55
1:2A:239:GLY:HA3	1:2A:371:VAL:HG21	1.88	0.55
2:2B:346:SER:O	1:6A:180:SER:N	2.35	0.55
2:3B:142:GLY:O	2:3B:146:SER:OG	2.24	0.55
2:3B:269:SER:HB3	2:3B:299:PHE:HD1	1.69	0.55
2:1B:122:ASP:OD2	3:1C:52:LYS:HG2	2.07	0.55
2:3B:56:ARG:CD	1:4A:286:LYS:CE	2.48	0.55
2:3B:344:PRO:CB	1:7A:389:ASN:ND2	2.32	0.55
2:4B:245:LYS:HG2	1:8A:226:VAL:CG1	2.35	0.55
3:4C:92:MET:CE	3:4C:131:LEU:CD2	2.84	0.55
2:5B:287:PRO:O	2:5B:291:ARG:NH2	2.39	0.55
3:5C:92:MET:CE	3:5C:131:LEU:CD2	2.84	0.55
3:5C:92:MET:HE2	3:5C:131:LEU:CD2	2.37	0.55
1:6A:239:GLY:HA3	1:6A:371:VAL:HG21	1.88	0.55
2:6B:287:PRO:O	2:6B:291:ARG:NH2	2.39	0.55
3:6C:92:MET:CE	3:6C:131:LEU:CD2	2.84	0.55
3:6C:92:MET:HE2	3:6C:131:LEU:CD2	2.37	0.55
1:3A:277:ALA:HB3	1:3A:370:MET:HB3	1.87	0.55
2:8B:115:ASP:CB	3:8C:62:PHE:HE2	2.19	0.55
2:8B:287:PRO:O	2:8B:291:ARG:NH2	2.39	0.55
2:1B:245:LYS:HB3	1:5A:226:VAL:HG21	1.89	0.55
2:1B:254:VAL:CG1	1:5A:402:TRP:CZ2	2.88	0.55
2:3B:56:ARG:HD3	1:4A:289:GLU:OE1	2.06	0.55
2:3B:343:MET:C	1:7A:392:LYS:HE3	2.27	0.55
2:4B:142:GLY:O	2:4B:146:SER:OG	2.24	0.55
1:5A:19:ALA:HA	1:5A:22:PHE:HB3	1.88	0.55
2:5B:122:ASP:OD2	3:5C:52:LYS:HE3	2.05	0.55
3:7C:92:MET:CE	3:7C:131:LEU:CD2	2.84	0.55
2:1B:287:PRO:O	2:1B:291:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:324:LYS:CA	1:7A:212:PHE:CE1	2.90	0.55
3:3C:92:MET:CE	3:3C:131:LEU:CD2	2.84	0.55
1:4A:19:ALA:HA	1:4A:22:PHE:HB3	1.88	0.55
2:4B:247:ASN:HB2	1:8A:13:GLN:OE1	2.07	0.55
1:8A:356:ILE:HD11	2:8B:176:ILE:CD1	2.37	0.55
2:2B:88:GLU:CD	3:2C:24:TYR:HB3	2.27	0.55
2:2B:139:SER:HA	2:2B:170:VAL:H	1.72	0.55
1:3A:356:ILE:HD11	2:3B:176:ILE:CD1	2.37	0.55
2:3B:89:SER:HB2	3:3C:21:ARG:CZ	2.33	0.55
1:5A:16:ASN:O	1:5A:20:ALA:N	2.39	0.55
2:5B:94:LYS:CE	3:5C:66:GLU:CD	2.59	0.55
2:6B:142:GLY:O	2:6B:146:SER:OG	2.24	0.55
2:7B:56:ARG:HD3	1:8A:289:GLU:OE1	2.06	0.55
1:2A:204:LEU:HD11	1:2A:274:CYS:HB2	1.89	0.55
1:2A:277:ALA:HB3	1:2A:370:MET:HB3	1.87	0.55
2:7B:142:GLY:O	2:7B:146:SER:OG	2.24	0.55
2:1B:324:LYS:CG	1:5A:223:SER:CA	2.72	0.55
1:3A:204:LEU:HD11	1:3A:274:CYS:HB2	1.89	0.55
1:6A:204:LEU:HD11	1:6A:274:CYS:HB2	1.89	0.55
2:7B:139:SER:HA	2:7B:170:VAL:H	1.72	0.55
3:7C:92:MET:HE3	3:7C:131:LEU:CG	2.36	0.55
2:1B:245:LYS:CB	1:5A:226:VAL:HG21	2.37	0.55
1:2A:19:ALA:HA	1:2A:22:PHE:HB3	1.88	0.55
1:3A:29:GLU:OE2	1:3A:324:ARG:NH1	2.35	0.55
1:4A:204:LEU:HD11	1:4A:274:CYS:HB2	1.89	0.55
2:4B:287:PRO:O	2:4B:291:ARG:NH2	2.39	0.55
2:2B:286:PHE:HD1	2:2B:289:LEU:HB3	1.72	0.54
1:5A:204:LEU:HD11	1:5A:274:CYS:HB2	1.89	0.54
1:6A:19:ALA:HA	1:6A:22:PHE:HB3	1.88	0.54
1:6A:277:ALA:HB3	1:6A:370:MET:HB3	1.87	0.54
1:7A:204:LEU:HD11	1:7A:274:CYS:HB2	1.89	0.54
2:7B:287:PRO:O	2:7B:291:ARG:NH2	2.39	0.54
1:8A:204:LEU:HD11	1:8A:274:CYS:HB2	1.89	0.54
1:1A:204:LEU:HD11	1:1A:274:CYS:HB2	1.89	0.54
2:2B:259:PRO:CB	1:6A:399:PHE:HD1	2.19	0.54
1:5A:356:ILE:HD11	2:5B:176:ILE:CD1	2.37	0.54
1:6A:356:ILE:HD11	2:6B:176:ILE:CD1	2.37	0.54
1:7A:356:ILE:HD11	2:7B:176:ILE:CD1	2.37	0.54
2:8B:142:GLY:O	2:8B:146:SER:OG	2.24	0.54
2:2B:142:GLY:O	2:2B:146:SER:OG	2.24	0.54
1:3A:16:ASN:O	1:3A:20:ALA:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3A:19:ALA:HA	1:3A:22:PHE:HB3	1.88	0.54
2:4B:139:SER:HA	2:4B:170:VAL:H	1.72	0.54
2:6B:88:GLU:CD	3:6C:24:TYR:HB3	2.27	0.54
1:7A:19:ALA:HA	1:7A:22:PHE:HB3	1.88	0.54
1:8A:19:ALA:HA	1:8A:22:PHE:HB3	1.88	0.54
2:8B:139:SER:HA	2:8B:170:VAL:H	1.72	0.54
2:3B:84:GLN:HE22	1:4A:284:ARG:NH1	0.70	0.54
2:6B:89:SER:CA	3:6C:24:TYR:CE2	2.91	0.54
1:8A:16:ASN:O	1:8A:20:ALA:N	2.39	0.54
3:8C:92:MET:CE	3:8C:131:LEU:CD2	2.84	0.54
2:3B:139:SER:HA	2:3B:170:VAL:H	1.72	0.54
2:3B:287:PRO:O	2:3B:291:ARG:NH2	2.39	0.54
1:4A:356:ILE:HD11	2:4B:176:ILE:CD1	2.37	0.54
2:5B:203:LEU:HD13	2:5B:229:ILE:HG12	1.90	0.54
1:6A:16:ASN:O	1:6A:20:ALA:N	2.39	0.54
2:6B:286:PHE:HD1	2:6B:289:LEU:HB3	1.72	0.54
2:1B:142:GLY:O	2:1B:146:SER:OG	2.24	0.54
2:1B:203:LEU:HD13	2:1B:229:ILE:HG12	1.90	0.54
2:2B:89:SER:CA	3:2C:24:TYR:CE2	2.91	0.54
2:4B:115:ASP:CB	3:4C:62:PHE:HE2	2.19	0.54
2:4B:351:LEU:CD1	1:8A:179:VAL:HG22	2.38	0.54
2:5B:286:PHE:HD1	2:5B:289:LEU:HB3	1.72	0.54
2:6B:139:SER:HA	2:6B:170:VAL:H	1.72	0.54
2:1B:286:PHE:HD1	2:1B:289:LEU:HB3	1.72	0.54
2:2B:52:PHE:HB3	2:2B:60:TYR:HB3	1.90	0.54
2:3B:256:ASN:ND2	1:7A:184:THR:CG2	2.66	0.54
1:4A:230:ASN:OD1	4:4A:501:GDP:N1	2.32	0.54
2:7B:115:ASP:CG	3:7C:58:ARG:CD	2.74	0.54
2:1B:139:SER:HA	2:1B:170:VAL:H	1.72	0.54
2:3B:351:LEU:CD1	1:7A:180:SER:O	2.55	0.54
1:4A:391:ASP:OD2	1:4A:417:ARG:NH1	2.41	0.54
2:4B:52:PHE:HB3	2:4B:60:TYR:HB3	1.90	0.54
1:5A:351:PRO:HD2	2:5B:388:MET:HE3	1.88	0.54
2:5B:122:ASP:OD2	3:5C:52:LYS:HG2	2.07	0.54
2:5B:139:SER:HA	2:5B:170:VAL:H	1.72	0.54
2:8B:52:PHE:HB3	2:8B:60:TYR:HB3	1.90	0.54
2:1B:322:LYS:HB2	1:5A:225:THR:CG2	2.38	0.54
2:3B:88:GLU:HG2	3:3C:24:TYR:CB	2.38	0.54
2:6B:52:PHE:HB3	2:6B:60:TYR:HB3	1.90	0.54
2:7B:211:ILE:HG22	2:7B:273:MET:HE1	1.90	0.54
1:1A:356:ILE:HD11	2:1B:176:ILE:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:88:GLU:CG	3:1C:24:TYR:HB3	2.35	0.54
1:2A:29:GLU:OE2	1:2A:324:ARG:NH1	2.35	0.54
2:3B:256:ASN:C	1:7A:183:VAL:HG21	2.28	0.54
2:5B:52:PHE:HB3	2:5B:60:TYR:HB3	1.90	0.54
1:7A:391:ASP:OD2	1:7A:417:ARG:NH1	2.41	0.54
1:1A:29:GLU:OE2	1:1A:324:ARG:NH1	2.35	0.53
2:2B:322:LYS:HD3	1:6A:225:THR:CG2	2.38	0.53
2:3B:52:PHE:HB3	2:3B:60:TYR:HB3	1.90	0.53
2:4B:164:ARG:CZ	1:8A:402:TRP:HZ3	2.17	0.53
2:7B:52:PHE:HB3	2:7B:60:TYR:HB3	1.90	0.53
2:1B:52:PHE:HB3	2:1B:60:TYR:HB3	1.90	0.53
2:1B:255:THR:CB	1:5A:102:GLY:O	2.56	0.53
1:2A:356:ILE:HD11	2:2B:176:ILE:CD1	2.37	0.53
2:3B:255:THR:CA	1:7A:402:TRP:CD2	2.91	0.53
1:5A:391:ASP:OD2	1:5A:417:ARG:NH1	2.41	0.53
1:8A:391:ASP:OD2	1:8A:417:ARG:NH1	2.41	0.53
2:8B:203:LEU:HD13	2:8B:229:ILE:HG12	1.90	0.53
1:1A:287:PHE:CD1	1:4A:56:LEU:HG	2.44	0.53
2:1B:324:LYS:CE	1:5A:216:HIS:HB2	2.37	0.53
1:3A:351:PRO:HD2	2:3B:388:MET:HE2	1.89	0.53
1:4A:132:ASP:OD1	3:4C:68:ARG:NE	2.35	0.53
1:6A:65:VAL:CG1	1:7A:287:PHE:CZ	2.91	0.53
2:1B:259:PRO:O	1:5A:399:PHE:CA	2.57	0.53
1:2A:132:ASP:HA	3:2C:68:ARG:HG2	1.91	0.53
2:4B:203:LEU:HD13	2:4B:229:ILE:HG12	1.90	0.53
2:7B:84:GLN:CD	1:8A:284:ARG:HH12	1.84	0.53
2:8B:127:LYS:HE3	3:8C:17:GLU:OE1	2.08	0.53
1:1A:91:PRO:CD	1:2A:287:PHE:CE2	2.92	0.53
1:1A:286:LYS:NZ	1:4A:56:LEU:CD1	2.65	0.53
2:2B:2:ARG:HD3	1:6A:98:THR:O	2.08	0.53
2:3B:286:PHE:HD1	2:3B:289:LEU:HB3	1.72	0.53
2:3B:324:LYS:CG	1:7A:212:PHE:CD1	2.92	0.53
1:5A:56:LEU:CD1	1:6A:286:LYS:HZ1	2.07	0.53
1:5A:287:PHE:CD1	1:8A:56:LEU:HG	2.44	0.53
2:2B:194:LEU:HD22	2:2B:418:LEU:HD22	1.91	0.53
2:2B:203:LEU:HD13	2:2B:229:ILE:HG12	1.90	0.53
2:2B:245:LYS:HA	1:6A:17:GLN:HE22	1.73	0.53
2:3B:324:LYS:HG3	1:7A:224:PRO:CG	2.39	0.53
1:2A:391:ASP:OD2	1:2A:417:ARG:NH1	2.41	0.53
2:2B:343:MET:HE3	1:6A:399:PHE:CE1	2.44	0.53
1:6A:391:ASP:OD2	1:6A:417:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6B:194:LEU:HD22	2:6B:418:LEU:HD22	1.91	0.53
2:6B:203:LEU:HD13	2:6B:229:ILE:HG12	1.90	0.53
1:3A:391:ASP:OD2	1:3A:417:ARG:NH1	2.41	0.53
2:4B:324:LYS:NZ	1:8A:216:HIS:ND1	2.50	0.53
2:4B:344:PRO:N	1:8A:392:LYS:HE3	2.23	0.53
1:1A:16:ASN:O	1:1A:20:ALA:N	2.39	0.53
1:1A:391:ASP:OD2	1:1A:417:ARG:NH1	2.41	0.53
2:2B:2:ARG:HG3	1:6A:98:THR:CG2	2.37	0.53
2:3B:256:ASN:CA	1:7A:183:VAL:HG21	2.39	0.53
2:3B:330:MET:HG3	1:7A:179:VAL:HG21	1.90	0.53
2:4B:94:LYS:NZ	3:4C:63:ARG:NH2	2.52	0.53
2:4B:247:ASN:CB	1:8A:13:GLN:OE1	2.57	0.53
2:5B:142:GLY:O	2:5B:146:SER:OG	2.24	0.53
1:6A:29:GLU:OE2	1:6A:324:ARG:NH1	2.35	0.53
2:8B:94:LYS:NZ	3:8C:63:ARG:NH2	2.52	0.53
2:8B:205:ASN:HD21	4:8B:501:GDP:H1'	1.74	0.53
2:3B:205:ASN:HD21	4:3B:501:GDP:H1'	1.74	0.53
2:7B:286:PHE:HD1	2:7B:289:LEU:HB3	1.72	0.53
2:8B:211:ILE:HG22	2:8B:273:MET:HE1	1.91	0.53
2:8B:286:PHE:HD1	2:8B:289:LEU:HB3	1.72	0.53
2:3B:344:PRO:HD3	1:7A:393:LEU:CD2	2.39	0.52
2:4B:286:PHE:HD1	2:4B:289:LEU:HB3	1.72	0.52
1:6A:63:SER:CB	1:7A:286:LYS:HZ1	2.22	0.52
2:7B:88:GLU:HG2	3:7C:24:TYR:CB	2.38	0.52
1:2A:16:ASN:O	1:2A:20:ALA:N	2.39	0.52
2:3B:203:LEU:HD13	2:3B:229:ILE:HG12	1.90	0.52
2:7B:203:LEU:HD13	2:7B:229:ILE:HG12	1.90	0.52
3:7C:14:ARG:NH1	1:8A:294:GLU:OE1	2.43	0.52
2:2B:66:LEU:HB2	2:2B:91:ILE:HG13	1.92	0.52
2:6B:211:ILE:HG22	2:6B:273:MET:HE1	1.91	0.52
1:5A:91:PRO:CD	1:6A:287:PHE:CE2	2.92	0.52
2:5B:116:GLN:CG	3:5C:63:ARG:NH1	2.51	0.52
2:8B:194:LEU:HD22	2:8B:418:LEU:HD22	1.91	0.52
2:3B:112:LYS:C	3:3C:62:PHE:CD2	2.78	0.52
2:4B:127:LYS:HE3	3:4C:17:GLU:OE1	2.08	0.52
2:4B:194:LEU:HD22	2:4B:418:LEU:HD22	1.91	0.52
1:7A:193:LEU:HD11	1:7A:383:LEU:HD22	1.92	0.52
2:7B:194:LEU:HD22	2:7B:418:LEU:HD22	1.91	0.52
1:8A:29:GLU:OE2	1:8A:324:ARG:NH1	2.35	0.52
3:8C:228:ASP:O	3:8C:232:ARG:HG3	2.10	0.52
2:1B:205:ASN:HD21	4:1B:501:GDP:H1'	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:252:GLU:HG2	1:5A:102:GLY:HA2	1.91	0.52
2:1B:255:THR:HB	1:5A:102:GLY:O	2.10	0.52
2:3B:194:LEU:HD22	2:3B:418:LEU:HD22	1.91	0.52
3:3C:92:MET:HE2	3:3C:131:LEU:CD2	2.39	0.52
1:4A:351:PRO:HD2	2:4B:388:MET:HE2	1.91	0.52
2:4B:256:ASN:HD22	1:8A:183:VAL:C	2.13	0.52
2:6B:66:LEU:HB2	2:6B:91:ILE:HG13	1.92	0.52
2:7B:84:GLN:CD	1:8A:284:ARG:HH11	1.80	0.52
2:7B:205:ASN:HD21	4:7B:501:GDP:H1'	1.74	0.52
2:1B:66:LEU:HB2	2:1B:91:ILE:HG13	1.92	0.52
2:2B:205:ASN:HD21	4:2B:501:GDP:H1'	1.74	0.52
1:3A:193:LEU:HD11	1:3A:383:LEU:HD22	1.92	0.52
1:4A:16:ASN:O	1:4A:20:ALA:N	2.39	0.52
3:4C:228:ASP:O	3:4C:232:ARG:HG3	2.10	0.52
1:7A:29:GLU:OE2	1:7A:324:ARG:NH1	2.35	0.52
3:7C:228:ASP:O	3:7C:232:ARG:HG3	2.10	0.52
1:8A:351:PRO:HD2	2:8B:388:MET:HE2	1.89	0.52
2:3B:324:LYS:NZ	1:7A:224:PRO:HG2	2.25	0.52
3:3C:228:ASP:O	3:3C:232:ARG:HG3	2.10	0.52
2:4B:205:ASN:HD21	4:4B:501:GDP:H1'	1.74	0.52
2:5B:66:LEU:HB2	2:5B:91:ILE:HG13	1.92	0.52
3:1C:92:MET:HE3	3:1C:131:LEU:CD2	2.39	0.52
1:2A:193:LEU:HD11	1:2A:383:LEU:HD22	1.92	0.52
2:2B:122:ASP:CG	3:2C:52:LYS:HE3	2.25	0.52
1:6A:193:LEU:HD11	1:6A:383:LEU:HD22	1.92	0.52
1:1A:193:LEU:HD11	1:1A:383:LEU:HD22	1.92	0.52
2:1B:322:LYS:HB2	1:5A:225:THR:HG22	1.92	0.52
2:1B:347:GLY:HA2	1:5A:180:SER:N	2.15	0.52
1:5A:193:LEU:HD11	1:5A:383:LEU:HD22	1.92	0.52
2:4B:119:ASN:ND2	3:4C:56:LEU:N	2.58	0.51
2:6B:205:ASN:HD21	4:6B:501:GDP:H1'	1.74	0.51
2:1B:88:GLU:HB3	3:1C:24:TYR:HD2	1.75	0.51
3:3C:14:ARG:NH1	1:4A:294:GLU:OE1	2.43	0.51
1:5A:29:GLU:OE2	1:5A:324:ARG:NH1	2.35	0.51
2:5B:194:LEU:HD22	2:5B:418:LEU:HD22	1.91	0.51
2:5B:205:ASN:HD21	4:5B:501:GDP:H1'	1.74	0.51
2:6B:94:LYS:HZ3	3:6C:63:ARG:HH22	1.52	0.51
2:1B:194:LEU:HD22	2:1B:418:LEU:HD22	1.91	0.51
2:1B:261:PRO:HD3	1:5A:400:ALA:HB2	1.92	0.51
2:2B:324:LYS:HA	1:6A:212:PHE:CE1	2.45	0.51
3:2C:228:ASP:O	3:2C:232:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7B:66:LEU:HB2	2:7B:91:ILE:HG13	1.92	0.51
2:1B:211:ILE:HG22	2:1B:273:MET:HE1	1.92	0.51
2:1B:324:LYS:HD2	1:5A:223:SER:HA	1.67	0.51
2:3B:66:LEU:HB2	2:3B:91:ILE:HG13	1.92	0.51
2:3B:211:ILE:HG22	2:3B:273:MET:HE1	1.93	0.51
2:3B:324:LYS:CB	1:7A:224:PRO:HD2	2.39	0.51
2:5B:211:ILE:HG22	2:5B:273:MET:HE1	1.92	0.51
1:5A:143:ILE:HG22	1:5A:189:THR:HA	1.92	0.51
2:7B:89:SER:HB2	3:7C:21:ARG:CZ	2.33	0.51
2:3B:322:LYS:CB	1:7A:225:THR:HG22	2.40	0.51
2:4B:324:LYS:HD2	1:8A:222:GLU:O	2.10	0.51
2:6B:89:SER:OG	3:6C:21:ARG:HG3	2.11	0.51
1:7A:143:ILE:HG22	1:7A:189:THR:HA	1.92	0.51
1:1A:143:ILE:HG22	1:1A:189:THR:HA	1.92	0.51
2:4B:252:GLU:HG2	1:8A:102:GLY:C	2.31	0.51
2:6B:115:ASP:HB2	3:6C:62:PHE:CE2	2.45	0.51
1:8A:265:PRO:HG3	1:8A:317:LEU:HD22	1.93	0.51
1:4A:193:LEU:HD11	1:4A:383:LEU:HD22	1.92	0.51
1:4A:265:PRO:HG3	1:4A:317:LEU:HD22	1.93	0.51
1:4A:351:PRO:HD2	2:4B:388:MET:HE3	1.91	0.51
2:4B:343:MET:C	1:8A:392:LYS:CE	2.78	0.51
1:7A:132:ASP:HA	3:7C:68:ARG:CG	2.40	0.51
1:8A:193:LEU:HD11	1:8A:383:LEU:HD22	1.92	0.51
1:3A:18:ILE:O	1:3A:22:PHE:N	2.44	0.51
2:4B:344:PRO:N	1:8A:392:LYS:CE	2.74	0.51
2:5B:283:ARG:HD2	2:8B:56:ARG:NH2	2.23	0.51
1:3A:143:ILE:HG22	1:3A:189:THR:HA	1.92	0.51
2:3B:256:ASN:ND2	1:7A:183:VAL:HG23	2.25	0.51
2:5B:115:ASP:HB2	3:5C:62:PHE:HE2	1.68	0.51
1:6A:18:ILE:O	1:6A:22:PHE:N	2.44	0.51
2:3B:324:LYS:CD	1:7A:224:PRO:CD	2.74	0.50
2:4B:66:LEU:HB2	2:4B:91:ILE:HG13	1.92	0.50
3:5C:228:ASP:O	3:5C:232:ARG:HG3	2.10	0.50
1:7A:18:ILE:O	1:7A:22:PHE:N	2.44	0.50
1:1A:286:LYS:HZ1	1:4A:63:SER:N	2.08	0.50
2:2B:2:ARG:HD3	1:6A:75:PRO:CD	2.41	0.50
2:2B:89:SER:OG	3:2C:21:ARG:HG3	2.11	0.50
2:3B:2:ARG:N	1:7A:98:THR:HG21	2.20	0.50
1:4A:143:ILE:HG22	1:4A:189:THR:HA	1.92	0.50
2:4B:211:ILE:HG22	2:4B:273:MET:HE1	1.94	0.50
3:6C:228:ASP:O	3:6C:232:ARG:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:8B:66:LEU:HB2	2:8B:91:ILE:HG13	1.92	0.50
2:2B:115:ASP:HB2	3:2C:62:PHE:CE2	2.45	0.50
2:3B:56:ARG:HG3	1:4A:286:LYS:HD3	1.90	0.50
2:5B:115:ASP:N	3:5C:62:PHE:HE2	2.06	0.50
1:7A:265:PRO:HG3	1:7A:317:LEU:HD22	1.93	0.50
1:1A:351:PRO:HD2	2:1B:388:MET:HE2	1.94	0.50
2:1B:116:GLN:CG	3:1C:63:ARG:NH1	2.51	0.50
2:2B:350:LYS:HA	1:6A:181:SER:O	2.11	0.50
1:3A:265:PRO:HG3	1:3A:317:LEU:HD22	1.93	0.50
1:3A:351:PRO:HD2	2:3B:388:MET:HE3	1.93	0.50
1:3A:380:ALA:O	1:3A:384:ASP:N	2.45	0.50
1:4A:18:ILE:O	1:4A:22:PHE:N	2.44	0.50
1:2A:56:LEU:HD12	1:3A:286:LYS:HZ2	1.76	0.50
2:4B:164:ARG:CZ	1:8A:402:TRP:CZ3	2.94	0.50
1:5A:380:ALA:O	1:5A:384:ASP:N	2.45	0.50
1:6A:63:SER:CB	1:7A:286:LYS:NZ	2.74	0.50
2:7B:84:GLN:HE22	1:8A:284:ARG:NH1	0.70	0.50
1:1A:182:VAL:HB	1:1A:185:GLU:HB2	1.94	0.50
1:2A:143:ILE:HG22	1:2A:189:THR:HA	1.92	0.50
1:2A:182:VAL:HB	1:2A:185:GLU:HB2	1.94	0.50
2:3B:259:PRO:C	1:7A:400:ALA:HB2	2.31	0.50
2:5B:88:GLU:HB3	3:5C:24:TYR:HD2	1.75	0.50
1:8A:143:ILE:HG22	1:8A:189:THR:HA	1.92	0.50
1:1A:380:ALA:O	1:1A:384:ASP:N	2.45	0.50
2:1B:283:ARG:HD2	2:4B:56:ARG:NH2	2.23	0.50
1:6A:132:ASP:HA	3:6C:68:ARG:HG2	1.91	0.50
1:7A:380:ALA:O	1:7A:384:ASP:N	2.45	0.50
2:1B:256:ASN:O	1:5A:183:VAL:CG1	2.58	0.50
1:3A:132:ASP:HA	3:3C:68:ARG:CG	2.40	0.50
1:6A:143:ILE:HG22	1:6A:189:THR:HA	1.92	0.50
1:7A:16:ASN:O	1:7A:20:ALA:N	2.39	0.50
2:3B:324:LYS:HZ2	1:7A:224:PRO:HG2	1.76	0.50
1:5A:265:PRO:HG3	1:5A:317:LEU:HD22	1.93	0.50
2:5B:127:LYS:HE3	3:5C:17:GLU:OE1	2.12	0.50
3:7C:200:PRO:HB2	3:7C:237:MET:CE	2.42	0.50
1:1A:265:PRO:HG3	1:1A:317:LEU:HD22	1.93	0.49
3:1C:228:ASP:O	3:1C:232:ARG:HG3	2.10	0.49
1:2A:18:ILE:O	1:2A:22:PHE:N	2.44	0.49
1:5A:182:VAL:HB	1:5A:185:GLU:HB2	1.94	0.49
2:7B:119:ASN:HD21	3:7C:55:SER:HB3	1.55	0.49
2:1B:324:LYS:HE2	1:5A:216:HIS:CE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:349:LEU:O	1:6A:180:SER:O	2.28	0.49
2:7B:115:ASP:OD1	3:7C:58:ARG:CD	2.59	0.49
2:3B:179:SER:HB3	2:3B:182:GLU:HB2	1.94	0.49
2:4B:91:ILE:HG22	3:4C:24:TYR:CE2	2.47	0.49
2:6B:89:SER:CB	3:6C:21:ARG:NH1	2.69	0.49
2:7B:119:ASN:ND2	3:7C:55:SER:CB	2.60	0.49
1:1A:18:ILE:O	1:1A:22:PHE:N	2.44	0.49
2:2B:211:ILE:HG22	2:2B:273:MET:HE1	1.94	0.49
3:3C:200:PRO:HB2	3:3C:237:MET:CE	2.42	0.49
1:4A:380:ALA:O	1:4A:384:ASP:N	2.45	0.49
1:8A:351:PRO:HD2	2:8B:388:MET:HE3	1.93	0.49
1:4A:174:LEU:N	1:4A:206:PHE:O	2.44	0.49
3:4C:92:MET:HE3	3:4C:131:LEU:CD2	2.43	0.49
1:5A:299:LEU:HD11	1:5A:370:MET:HG2	1.94	0.49
2:5B:122:ASP:OD2	3:5C:52:LYS:HE2	2.12	0.49
3:5C:200:PRO:HB2	3:5C:237:MET:CE	2.42	0.49
2:8B:91:ILE:HG22	3:8C:24:TYR:CE2	2.47	0.49
2:1B:94:LYS:CE	3:1C:66:GLU:CD	2.59	0.49
1:2A:265:PRO:HG3	1:2A:317:LEU:HD22	1.93	0.49
2:3B:344:PRO:HD2	1:7A:393:LEU:HD21	1.95	0.49
1:4A:182:VAL:HB	1:4A:185:GLU:HB2	1.94	0.49
1:6A:131:CYS:O	3:6C:68:ARG:HG2	2.13	0.49
1:6A:182:VAL:HB	1:6A:185:GLU:HB2	1.94	0.49
2:7B:55:VAL:CG1	1:8A:287:PHE:CA	2.90	0.49
1:8A:380:ALA:O	1:8A:384:ASP:N	2.45	0.49
2:1B:127:LYS:HE3	3:1C:17:GLU:OE1	2.12	0.49
1:3A:182:VAL:HB	1:3A:185:GLU:HB2	1.94	0.49
2:3B:2:ARG:HE	1:7A:75:PRO:CG	2.23	0.49
3:4C:200:PRO:HB2	3:4C:237:MET:CE	2.43	0.49
1:6A:265:PRO:HG3	1:6A:317:LEU:HD22	1.93	0.49
2:6B:122:ASP:CG	3:6C:52:LYS:HE3	2.25	0.49
2:7B:179:SER:HB3	2:7B:182:GLU:HB2	1.94	0.49
2:2B:245:LYS:C	1:6A:13:GLN:NE2	2.59	0.49
2:3B:244:GLY:O	1:7A:13:GLN:NE2	2.46	0.49
1:4A:13:GLN:HB3	4:4A:501:GDP:O1A	2.13	0.49
2:4B:115:ASP:HB3	3:4C:58:ARG:HB2	1.95	0.49
1:6A:13:GLN:HB3	4:6A:501:GDP:O1A	2.13	0.49
3:6C:200:PRO:HB2	3:6C:237:MET:CE	2.43	0.49
2:1B:344:PRO:CB	1:5A:389:ASN:ND2	2.70	0.49
3:1C:200:PRO:HB2	3:1C:237:MET:CE	2.42	0.49
2:2B:119:ASN:OD1	3:2C:55:SER:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4B:263:ASN:O	2:4B:370:ASN:ND2	2.43	0.49
1:5A:9:VAL:HG13	1:5A:69:ILE:HG23	1.95	0.49
1:5A:351:PRO:HD2	2:5B:388:MET:HE2	1.94	0.49
1:7A:13:GLN:HB3	4:7A:501:GDP:O1A	2.13	0.49
1:1A:299:LEU:HD11	1:1A:370:MET:HG2	1.94	0.49
2:1B:3:GLU:HA	2:1B:50:VAL:HA	1.95	0.49
2:1B:261:PRO:HG3	1:5A:400:ALA:CB	2.40	0.49
2:1B:263:ASN:O	2:1B:370:ASN:ND2	2.43	0.49
1:2A:131:CYS:O	3:2C:68:ARG:HG2	2.13	0.49
1:2A:380:ALA:O	1:2A:384:ASP:N	2.45	0.49
2:2B:2:ARG:CD	1:6A:75:PRO:CD	2.91	0.49
3:2C:200:PRO:HB2	3:2C:237:MET:CE	2.43	0.49
3:4C:92:MET:HE2	3:4C:131:LEU:CD2	2.42	0.49
2:5B:3:GLU:HA	2:5B:50:VAL:HA	1.95	0.49
1:6A:380:ALA:O	1:6A:384:ASP:N	2.45	0.49
2:8B:179:SER:HB3	2:8B:182:GLU:HB2	1.94	0.49
1:2A:299:LEU:HD11	1:2A:370:MET:HG2	1.94	0.48
2:3B:330:MET:CG	1:7A:179:VAL:HG21	2.43	0.48
2:4B:179:SER:HB3	2:4B:182:GLU:HB2	1.94	0.48
1:5A:65:VAL:CG1	1:6A:287:PHE:CZ	2.97	0.48
1:6A:299:LEU:HD11	1:6A:370:MET:HG2	1.94	0.48
1:8A:182:VAL:HB	1:8A:185:GLU:HB2	1.94	0.48
2:1B:115:ASP:HB2	3:1C:62:PHE:HE2	1.68	0.48
2:1B:115:ASP:N	3:1C:62:PHE:HE2	2.06	0.48
1:2A:351:PRO:HD2	2:2B:388:MET:HE2	1.95	0.48
1:3A:13:GLN:HB3	4:3A:501:GDP:O1A	2.13	0.48
2:3B:322:LYS:HB2	1:7A:225:THR:HG22	1.95	0.48
1:5A:13:GLN:HB3	4:5A:501:GDP:O1A	2.13	0.48
1:5A:18:ILE:O	1:5A:22:PHE:N	2.44	0.48
1:6A:9:VAL:HG13	1:6A:69:ILE:HG23	1.95	0.48
2:6B:179:SER:HB3	2:6B:182:GLU:HB2	1.94	0.48
1:7A:299:LEU:HD11	1:7A:370:MET:HG2	1.94	0.48
1:8A:9:VAL:HG13	1:8A:69:ILE:HG23	1.95	0.48
1:8A:13:GLN:HB3	4:8A:501:GDP:O1A	2.13	0.48
2:1B:179:SER:HB3	2:1B:182:GLU:HB2	1.94	0.48
2:2B:164:ARG:HD2	2:2B:254:VAL:HG21	1.96	0.48
2:2B:179:SER:HB3	2:2B:182:GLU:HB2	1.94	0.48
2:3B:247:ASN:CG	1:7A:13:GLN:OE1	2.51	0.48
2:3B:324:LYS:HG2	1:7A:212:PHE:CD1	2.49	0.48
2:4B:3:GLU:HA	2:4B:50:VAL:HA	1.95	0.48
2:5B:164:ARG:HD2	2:5B:254:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7A:258:GLU:O	1:7A:262:ASN:ND2	2.47	0.48
1:4A:258:GLU:O	1:4A:262:ASN:ND2	2.47	0.48
1:6A:258:GLU:O	1:6A:262:ASN:ND2	2.47	0.48
1:7A:182:VAL:HB	1:7A:185:GLU:HB2	1.94	0.48
2:8B:3:GLU:HA	2:8B:50:VAL:HA	1.95	0.48
2:8B:115:ASP:HB3	3:8C:58:ARG:HB2	1.95	0.48
1:1A:174:LEU:N	1:1A:206:PHE:O	2.44	0.48
2:1B:164:ARG:HD2	2:1B:254:VAL:HG21	1.96	0.48
2:2B:346:SER:CB	1:6A:178:GLN:O	2.61	0.48
1:3A:299:LEU:HD11	1:3A:370:MET:HG2	1.94	0.48
2:3B:164:ARG:HD2	2:3B:254:VAL:HG21	1.96	0.48
1:4A:299:LEU:HD11	1:4A:370:MET:HG2	1.94	0.48
2:4B:164:ARG:HD2	2:4B:254:VAL:HG21	1.96	0.48
2:6B:164:ARG:HD2	2:6B:254:VAL:HG21	1.96	0.48
2:7B:164:ARG:HD2	2:7B:254:VAL:HG21	1.96	0.48
2:8B:164:ARG:HD2	2:8B:254:VAL:HG21	1.96	0.48
2:8B:382:ILE:HD12	2:8B:412:ARG:HG2	1.96	0.48
3:8C:200:PRO:HB2	3:8C:237:MET:CE	2.42	0.48
1:1A:258:GLU:O	1:1A:262:ASN:ND2	2.47	0.48
1:2A:9:VAL:HG13	1:2A:69:ILE:HG23	1.95	0.48
1:3A:258:GLU:O	1:3A:262:ASN:ND2	2.47	0.48
2:3B:55:VAL:CG1	1:4A:287:PHE:CA	2.90	0.48
2:5B:382:ILE:HD12	2:5B:412:ARG:HG2	1.96	0.48
2:7B:56:ARG:HG3	1:8A:286:LYS:HD3	1.90	0.48
1:1A:13:GLN:HB3	4:1A:501:GDP:O1A	2.13	0.48
1:1A:286:LYS:HZ3	1:4A:56:LEU:CD1	2.25	0.48
2:2B:261:PRO:HD3	1:6A:400:ALA:HB1	1.95	0.48
1:5A:258:GLU:O	1:5A:262:ASN:ND2	2.47	0.48
1:7A:9:VAL:HG13	1:7A:69:ILE:HG23	1.95	0.48
2:7B:382:ILE:HD12	2:7B:412:ARG:HG2	1.96	0.48
1:8A:18:ILE:O	1:8A:22:PHE:N	2.44	0.48
1:8A:258:GLU:O	1:8A:262:ASN:ND2	2.47	0.48
1:8A:299:LEU:HD11	1:8A:370:MET:HG2	1.94	0.48
1:8A:157:GLU:HG3	1:8A:195:THR:HG23	1.96	0.48
1:2A:258:GLU:O	1:2A:262:ASN:ND2	2.47	0.48
2:4B:69:LEU:HD12	2:4B:98:ALA:HB2	1.96	0.48
2:7B:263:ASN:O	2:7B:370:ASN:ND2	2.43	0.48
1:8A:174:LEU:N	1:8A:206:PHE:O	2.44	0.48
2:8B:69:LEU:HD12	2:8B:98:ALA:HB2	1.96	0.48
2:8B:119:ASN:ND2	3:8C:56:LEU:N	2.58	0.48
2:1B:256:ASN:HD22	1:5A:183:VAL:HG22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:13:GLN:HB3	4:2A:501:GDP:O1A	2.13	0.48
2:3B:69:LEU:HD12	2:3B:98:ALA:HB2	1.96	0.48
2:3B:243:PRO:HB3	1:7A:76:SER:CB	2.44	0.48
2:3B:323:ALA:O	1:7A:212:PHE:CZ	2.67	0.47
2:4B:190:LEU:HD23	2:4B:193:ILE:HD12	1.96	0.47
2:4B:252:GLU:CG	1:8A:102:GLY:C	2.82	0.47
2:5B:119:ASN:HD21	3:5C:55:SER:HB3	1.57	0.47
2:6B:3:GLU:HA	2:6B:50:VAL:HA	1.95	0.47
2:6B:119:ASN:OD1	3:6C:55:SER:HB3	2.13	0.47
2:6B:382:ILE:HD12	2:6B:412:ARG:HG2	1.96	0.47
2:7B:69:LEU:HD12	2:7B:98:ALA:HB2	1.96	0.47
2:8B:115:ASP:OD1	3:8C:58:ARG:CD	2.53	0.47
2:1B:2:ARG:NE	1:5A:75:PRO:CG	2.60	0.47
2:1B:382:ILE:HD12	2:1B:412:ARG:HG2	1.96	0.47
1:3A:400:ALA:HB3	1:3A:402:TRP:CD1	2.49	0.47
2:3B:61:VAL:HG23	1:4A:287:PHE:CE2	1.95	0.47
1:4A:400:ALA:HB3	1:4A:402:TRP:CD1	2.49	0.47
1:5A:157:GLU:HG3	1:5A:195:THR:HG23	1.96	0.47
2:5B:268:ALA:HB2	2:5B:368:LEU:HD23	1.97	0.47
1:6A:56:LEU:HD12	1:7A:286:LYS:HZ3	1.79	0.47
2:8B:190:LEU:HD23	2:8B:193:ILE:HD12	1.96	0.47
2:8B:268:ALA:HB2	2:8B:368:LEU:HD23	1.97	0.47
1:1A:9:VAL:HG13	1:1A:69:ILE:HG23	1.95	0.47
2:1B:260:PHE:HA	1:5A:399:PHE:O	2.14	0.47
2:2B:3:GLU:HA	2:2B:50:VAL:HA	1.95	0.47
1:3A:9:VAL:HG13	1:3A:69:ILE:HG23	1.95	0.47
1:3A:176:SER:HB3	1:3A:208:ASN:HB2	1.96	0.47
2:3B:2:ARG:HG3	1:7A:98:THR:HG22	1.95	0.47
2:3B:344:PRO:CA	1:7A:392:LYS:HD3	2.37	0.47
1:7A:176:SER:HB3	1:7A:208:ASN:HB2	1.96	0.47
2:7B:190:LEU:HD23	2:7B:193:ILE:HD12	1.96	0.47
1:1A:400:ALA:HB3	1:1A:402:TRP:CD1	2.49	0.47
2:2B:346:SER:CB	1:6A:178:GLN:C	2.68	0.47
2:3B:190:LEU:HD23	2:3B:193:ILE:HD12	1.96	0.47
3:3C:222:LYS:HD2	3:3C:222:LYS:HA	1.62	0.47
1:5A:174:LEU:N	1:5A:206:PHE:O	2.44	0.47
2:5B:179:SER:HB3	2:5B:182:GLU:HB2	1.94	0.47
2:1B:256:ASN:ND2	1:5A:182:VAL:CG1	2.70	0.47
1:3A:212:PHE:CD1	1:3A:229:LEU:HD21	2.50	0.47
1:3A:367:ARG:HD3	1:3A:368:LYS:HG3	1.97	0.47
2:3B:3:GLU:HA	2:3B:50:VAL:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:340:ALA:C	1:7A:396:ARG:NH2	2.68	0.47
2:3B:350:LYS:CG	1:7A:183:VAL:HG13	2.44	0.47
1:4A:212:PHE:CD1	1:4A:229:LEU:HD21	2.50	0.47
2:4B:268:ALA:HB2	2:4B:368:LEU:HD23	1.97	0.47
1:6A:400:ALA:HB3	1:6A:402:TRP:CD1	2.49	0.47
1:7A:367:ARG:HD3	1:7A:368:LYS:HG3	1.97	0.47
2:7B:119:ASN:OD1	3:7C:55:SER:CB	2.62	0.47
1:1A:157:GLU:HG3	1:1A:195:THR:HG23	1.96	0.47
1:2A:65:VAL:CG1	1:3A:287:PHE:CZ	2.91	0.47
1:2A:400:ALA:HB3	1:2A:402:TRP:CD1	2.50	0.47
2:2B:382:ILE:HD12	2:2B:412:ARG:HG2	1.96	0.47
2:3B:89:SER:OG	3:3C:21:ARG:HG3	2.15	0.47
2:4B:130:GLY:CA	1:8A:98:THR:CG2	2.91	0.47
1:6A:212:PHE:CD1	1:6A:229:LEU:HD21	2.50	0.47
1:7A:400:ALA:HB3	1:7A:402:TRP:CD1	2.50	0.47
1:8A:212:PHE:CD1	1:8A:229:LEU:HD21	2.50	0.47
3:8C:92:MET:HE3	3:8C:131:LEU:CG	2.43	0.47
1:1A:212:PHE:CD1	1:1A:229:LEU:HD21	2.50	0.47
2:1B:268:ALA:HB2	2:1B:368:LEU:HD23	1.97	0.47
2:1B:324:LYS:NZ	1:5A:216:HIS:HA	2.30	0.47
2:2B:69:LEU:HD12	2:2B:98:ALA:HB2	1.96	0.47
2:2B:268:ALA:HB2	2:2B:368:LEU:HD23	1.97	0.47
2:3B:268:ALA:HB2	2:3B:368:LEU:HD23	1.97	0.47
2:3B:382:ILE:HD12	2:3B:412:ARG:HG2	1.96	0.47
1:4A:9:VAL:HG13	1:4A:69:ILE:HG23	1.95	0.47
1:4A:157:GLU:HG3	1:4A:195:THR:HG23	1.96	0.47
2:4B:237:THR:HG22	2:4B:250:LEU:HD11	1.97	0.47
2:4B:382:ILE:HD12	2:4B:412:ARG:HG2	1.96	0.47
2:5B:69:LEU:HD12	2:5B:98:ALA:HB2	1.96	0.47
1:6A:351:PRO:HD2	2:6B:388:MET:HE2	1.95	0.47
1:7A:157:GLU:HG3	1:7A:195:THR:HG23	1.96	0.47
2:7B:3:GLU:HA	2:7B:50:VAL:HA	1.95	0.47
2:7B:89:SER:OG	3:7C:21:ARG:HG3	2.15	0.47
1:8A:176:SER:HB3	1:8A:208:ASN:HB2	1.96	0.47
2:8B:237:THR:HG22	2:8B:250:LEU:HD11	1.97	0.47
2:1B:119:ASN:OD1	3:1C:55:SER:CB	2.60	0.47
2:2B:122:ASP:OD1	3:2C:52:LYS:CE	2.61	0.47
2:3B:344:PRO:HB3	1:7A:389:ASN:HA	1.97	0.47
1:4A:176:SER:HB3	1:4A:208:ASN:HB2	1.96	0.47
2:7B:268:ALA:HB2	2:7B:368:LEU:HD23	1.97	0.47
2:1B:237:THR:HG22	2:1B:250:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:119:ASN:OD1	3:3C:55:SER:CB	2.62	0.47
1:4A:367:ARG:HD3	1:4A:368:LYS:HG3	1.97	0.47
2:6B:69:LEU:HD12	2:6B:98:ALA:HB2	1.96	0.47
2:6B:268:ALA:HB2	2:6B:368:LEU:HD23	1.97	0.47
2:7B:112:LYS:C	3:7C:62:PHE:CD2	2.78	0.47
1:8A:367:ARG:HD3	1:8A:368:LYS:HG3	1.97	0.47
1:8A:400:ALA:HB3	1:8A:402:TRP:CD1	2.49	0.47
2:1B:69:LEU:HD12	2:1B:98:ALA:HB2	1.96	0.47
2:1B:327:ASP:CG	1:5A:178:GLN:HE22	2.16	0.47
3:4C:222:LYS:HD2	3:4C:222:LYS:HA	1.62	0.47
1:5A:400:ALA:HB3	1:5A:402:TRP:CD1	2.49	0.47
2:6B:190:LEU:HD23	2:6B:193:ILE:HD12	1.96	0.47
1:7A:212:PHE:CD1	1:7A:229:LEU:HD21	2.50	0.47
2:7B:237:THR:HG22	2:7B:250:LEU:HD11	1.97	0.47
2:8B:122:ASP:OD2	3:8C:52:LYS:CG	2.62	0.47
2:3B:237:THR:HG22	2:3B:250:LEU:HD11	1.97	0.46
2:3B:350:LYS:HB3	1:7A:183:VAL:HG22	1.98	0.46
2:4B:122:ASP:OD2	3:4C:52:LYS:CG	2.62	0.46
1:5A:286:LYS:HZ1	1:8A:63:SER:N	2.11	0.46
2:1B:94:LYS:NZ	3:1C:63:ARG:NH2	2.58	0.46
2:1B:190:LEU:HD23	2:1B:193:ILE:HD12	1.96	0.46
1:3A:157:GLU:HG3	1:3A:195:THR:HG23	1.96	0.46
2:3B:115:ASP:OD1	3:3C:58:ARG:CD	2.59	0.46
1:5A:212:PHE:CD1	1:5A:229:LEU:HD21	2.50	0.46
2:5B:205:ASN:HA	2:5B:208:LEU:HB2	1.97	0.46
2:5B:237:THR:HG22	2:5B:250:LEU:HD11	1.97	0.46
1:1A:132:ASP:OD1	3:1C:68:ARG:CD	2.63	0.46
2:1B:257:LEU:HD21	2:1B:314:SER:HB2	1.98	0.46
2:1B:260:PHE:HD1	1:5A:399:PHE:O	1.98	0.46
2:2B:190:LEU:HD23	2:2B:193:ILE:HD12	1.96	0.46
2:2B:347:GLY:HA3	1:6A:180:SER:CB	2.40	0.46
1:3A:174:LEU:N	1:3A:206:PHE:O	2.44	0.46
1:3A:356:ILE:HD11	2:3B:176:ILE:HD11	1.98	0.46
2:4B:324:LYS:CE	1:8A:216:HIS:CG	2.90	0.46
1:6A:157:GLU:HG3	1:6A:195:THR:HG23	1.96	0.46
1:7A:351:PRO:HD2	2:7B:388:MET:HE3	1.96	0.46
1:1A:65:VAL:CG1	1:2A:287:PHE:CZ	2.97	0.46
2:2B:237:THR:HG22	2:2B:250:LEU:HD11	1.97	0.46
2:3B:91:ILE:CG2	3:3C:24:TYR:CE2	2.90	0.46
2:3B:344:PRO:CD	1:7A:393:LEU:HD21	2.45	0.46
1:4A:356:ILE:HD11	2:4B:176:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4B:252:GLU:CG	1:8A:102:GLY:CA	2.92	0.46
1:5A:149:SER:OG	1:5A:188:ASN:O	2.34	0.46
2:5B:257:LEU:HD21	2:5B:314:SER:HB2	1.98	0.46
1:7A:174:LEU:N	1:7A:206:PHE:O	2.44	0.46
2:1B:205:ASN:HA	2:1B:208:LEU:HB2	1.97	0.46
1:2A:157:GLU:HG3	1:2A:195:THR:HG23	1.96	0.46
1:2A:367:ARG:HD3	1:2A:368:LYS:HG3	1.97	0.46
2:5B:119:ASN:OD1	3:5C:55:SER:CB	2.60	0.46
2:5B:190:LEU:HD23	2:5B:193:ILE:HD12	1.96	0.46
1:6A:367:ARG:HD3	1:6A:368:LYS:HG3	1.97	0.46
2:6B:237:THR:HG22	2:6B:250:LEU:HD11	1.97	0.46
2:8B:89:SER:HB2	3:8C:21:ARG:NH1	2.31	0.46
2:8B:257:LEU:HD21	2:8B:314:SER:HB2	1.97	0.46
1:1A:54:SER:HB3	1:1A:65:VAL:HG23	1.97	0.46
1:1A:367:ARG:HD3	1:1A:368:LYS:HG3	1.97	0.46
2:1B:255:THR:HG21	1:5A:102:GLY:O	2.16	0.46
1:2A:176:SER:HB3	1:2A:208:ASN:HB2	1.96	0.46
1:2A:212:PHE:CD1	1:2A:229:LEU:HD21	2.50	0.46
2:3B:84:GLN:CD	1:4A:284:ARG:HH12	1.84	0.46
2:3B:111:GLU:O	3:3C:62:PHE:CE1	2.69	0.46
2:3B:351:LEU:HD13	1:7A:181:SER:HA	1.98	0.46
1:5A:367:ARG:HD3	1:5A:368:LYS:HG3	1.97	0.46
1:1A:65:VAL:HG12	1:2A:287:PHE:CZ	2.50	0.46
2:1B:104:ARG:HA	2:1B:108:VAL:HB	1.98	0.46
1:2A:149:SER:OG	1:2A:188:ASN:O	2.34	0.46
2:2B:246:LEU:CD2	4:6A:501:GDP:H8	2.28	0.46
2:2B:341:SER:O	1:6A:396:ARG:NH1	2.38	0.46
2:3B:104:ARG:HA	2:3B:108:VAL:HB	1.98	0.46
2:4B:89:SER:HB2	3:4C:21:ARG:NH1	2.31	0.46
2:4B:256:ASN:CG	1:8A:183:VAL:H	2.16	0.46
2:4B:257:LEU:HD21	2:4B:314:SER:HB2	1.97	0.46
1:5A:65:VAL:HG12	1:6A:287:PHE:CZ	2.50	0.46
1:5A:356:ILE:HD11	2:5B:176:ILE:HD11	1.98	0.46
2:5B:115:ASP:OD2	3:5C:62:PHE:CZ	2.69	0.46
2:5B:115:ASP:OD1	3:5C:58:ARG:CD	2.58	0.46
1:6A:327:MET:HG2	1:6A:329:ASP:H	1.81	0.46
1:7A:356:ILE:HD11	2:7B:176:ILE:HD11	1.98	0.46
1:1A:176:SER:HB3	1:1A:208:ASN:HB2	1.96	0.46
3:3C:92:MET:HE3	3:3C:131:LEU:CD2	2.46	0.46
2:4B:104:ARG:HA	2:4B:108:VAL:HB	1.98	0.46
1:5A:54:SER:HB3	1:5A:65:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5A:176:SER:HB3	1:5A:208:ASN:HB2	1.96	0.46
1:5A:327:MET:HG2	1:5A:329:ASP:H	1.81	0.46
1:6A:176:SER:HB3	1:6A:208:ASN:HB2	1.97	0.46
1:7A:327:MET:HG2	1:7A:329:ASP:H	1.81	0.46
1:1A:287:PHE:HZ	1:4A:65:VAL:HG12	1.71	0.46
1:1A:356:ILE:CD1	2:1B:176:ILE:HD11	2.46	0.46
1:2A:327:MET:HG2	1:2A:329:ASP:H	1.81	0.46
2:2B:104:ARG:HA	2:2B:108:VAL:HB	1.98	0.46
2:2B:346:SER:CB	1:6A:177:PRO:O	2.64	0.46
2:3B:2:ARG:NE	1:7A:75:PRO:CG	2.74	0.46
1:5A:278:PRO:HD3	1:5A:369:SER:HA	1.98	0.46
1:6A:356:ILE:CD1	2:6B:176:ILE:HD11	2.46	0.46
2:6B:257:LEU:HD21	2:6B:314:SER:HB2	1.97	0.46
3:6C:198:MET:HE1	3:6C:203:LEU:HB2	1.98	0.46
3:7C:18:GLU:CG	1:8A:288:GLU:OE2	2.41	0.46
3:7C:198:MET:HE1	3:7C:203:LEU:HB2	1.98	0.46
2:8B:205:ASN:HA	2:8B:208:LEU:HB2	1.97	0.46
1:1A:278:PRO:HD3	1:1A:369:SER:HA	1.98	0.46
1:1A:356:ILE:HD11	2:1B:176:ILE:HD11	1.98	0.46
1:2A:187:TYR:OH	1:2A:393:LEU:O	2.26	0.46
2:2B:260:PHE:N	1:6A:400:ALA:HB2	2.30	0.46
1:3A:327:MET:HG2	1:3A:329:ASP:H	1.81	0.46
2:6B:187:ILE:HD11	2:6B:381:LEU:HB3	1.98	0.46
2:6B:238:ALA:HA	2:6B:241:ARG:HG2	1.98	0.46
2:1B:238:ALA:HA	2:1B:241:ARG:HG2	1.98	0.45
2:2B:257:LEU:HD21	2:2B:314:SER:HB2	1.97	0.45
1:3A:278:PRO:HD3	1:3A:369:SER:HA	1.99	0.45
2:4B:187:ILE:HD11	2:4B:381:LEU:HB3	1.98	0.45
1:5A:89:PHE:O	1:6A:287:PHE:CE2	2.69	0.45
2:5B:87:ASP:OD1	3:5C:21:ARG:NE	2.49	0.45
2:7B:115:ASP:CB	3:7C:58:ARG:HB2	2.46	0.45
1:1A:287:PHE:CE1	1:4A:56:LEU:HG	2.51	0.45
2:1B:87:ASP:OD1	3:1C:21:ARG:NE	2.49	0.45
2:1B:122:ASP:OD2	3:1C:52:LYS:HE2	2.12	0.45
2:2B:238:ALA:HA	2:2B:241:ARG:HG2	1.98	0.45
1:3A:132:ASP:OD1	3:3C:68:ARG:NE	2.40	0.45
2:3B:246:LEU:CD2	4:7A:501:GDP:H3'	2.45	0.45
1:4A:327:MET:HG2	1:4A:329:ASP:H	1.81	0.45
1:5A:356:ILE:CD1	2:5B:176:ILE:HD11	2.46	0.45
2:5B:238:ALA:HA	2:5B:241:ARG:HG2	1.98	0.45
1:8A:327:MET:HG2	1:8A:329:ASP:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:115:ASP:HB3	3:1C:58:ARG:CB	2.47	0.45
1:2A:356:ILE:CD1	2:2B:176:ILE:HD11	2.46	0.45
2:3B:245:LYS:CD	1:7A:226:VAL:HG21	2.47	0.45
1:5A:287:PHE:CE1	1:8A:56:LEU:HG	2.51	0.45
1:6A:174:LEU:N	1:6A:206:PHE:O	2.44	0.45
1:6A:278:PRO:HD3	1:6A:369:SER:HA	1.98	0.45
1:7A:356:ILE:CD1	2:7B:176:ILE:HD11	2.46	0.45
2:7B:187:ILE:HD11	2:7B:381:LEU:HB3	1.98	0.45
1:8A:54:SER:HB3	1:8A:65:VAL:HG23	1.97	0.45
1:8A:149:SER:OG	1:8A:188:ASN:O	2.34	0.45
3:1C:141:TYR:HB3	3:1C:166:LEU:HG	1.99	0.45
1:2A:275:ALA:HB3	1:2A:372:LEU:HB3	1.99	0.45
2:2B:243:PRO:CB	1:6A:76:SER:HB3	2.25	0.45
2:3B:256:ASN:CA	1:7A:183:VAL:HG23	2.42	0.45
2:3B:259:PRO:CB	1:7A:399:PHE:HA	2.46	0.45
1:4A:149:SER:OG	1:4A:188:ASN:O	2.34	0.45
2:4B:324:LYS:NZ	1:8A:216:HIS:CD2	2.66	0.45
1:5A:132:ASP:OD1	3:5C:68:ARG:CD	2.63	0.45
2:5B:104:ARG:HA	2:5B:108:VAL:HB	1.98	0.45
2:5B:187:ILE:HD11	2:5B:381:LEU:HB3	1.98	0.45
1:6A:275:ALA:HB3	1:6A:372:LEU:HB3	1.99	0.45
1:6A:356:ILE:HD11	2:6B:176:ILE:HD11	1.98	0.45
1:7A:54:SER:HB3	1:7A:65:VAL:HG23	1.97	0.45
2:7B:257:LEU:HD21	2:7B:314:SER:HB2	1.97	0.45
1:8A:69:ILE:HD12	1:8A:123:ARG:HB2	1.99	0.45
2:8B:187:ILE:HD11	2:8B:381:LEU:HB3	1.98	0.45
1:1A:327:MET:HG2	1:1A:329:ASP:H	1.81	0.45
2:1B:115:ASP:OD2	3:1C:62:PHE:CZ	2.69	0.45
2:1B:187:ILE:HD11	2:1B:381:LEU:HB3	1.98	0.45
1:2A:54:SER:HB3	1:2A:65:VAL:HG23	1.97	0.45
2:2B:322:LYS:HD3	1:6A:225:THR:HG22	1.99	0.45
2:2B:348:GLY:C	1:6A:183:VAL:CG1	2.68	0.45
3:3C:141:TYR:HB3	3:3C:166:LEU:HG	1.99	0.45
1:4A:54:SER:HB3	1:4A:65:VAL:HG23	1.97	0.45
2:5B:94:LYS:NZ	3:5C:63:ARG:NH2	2.58	0.45
1:1A:275:ALA:HB3	1:1A:372:LEU:HB3	1.99	0.45
1:2A:278:PRO:HD3	1:2A:369:SER:HA	1.98	0.45
2:2B:205:ASN:HA	2:2B:208:LEU:HB2	1.97	0.45
2:2B:322:LYS:HD3	1:6A:225:THR:HG23	1.99	0.45
2:3B:205:ASN:HA	2:3B:208:LEU:HB2	1.97	0.45
2:3B:238:ALA:HA	2:3B:241:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:324:LYS:HA	1:7A:212:PHE:CD2	2.48	0.45
1:4A:356:ILE:CD1	2:4B:176:ILE:HD11	2.46	0.45
3:5C:141:TYR:HB3	3:5C:166:LEU:HG	1.99	0.45
1:6A:63:SER:N	1:7A:286:LYS:HZ1	2.11	0.45
1:7A:275:ALA:HB3	1:7A:372:LEU:HB3	1.99	0.45
1:7A:278:PRO:HD3	1:7A:369:SER:HA	1.99	0.45
3:7C:141:TYR:HB3	3:7C:166:LEU:HG	1.99	0.45
1:8A:278:PRO:HD3	1:8A:369:SER:HA	1.99	0.45
1:8A:356:ILE:HD11	2:8B:176:ILE:HD11	1.98	0.45
1:4A:278:PRO:HD3	1:4A:369:SER:HA	1.99	0.45
2:4B:205:ASN:HA	2:4B:208:LEU:HB2	1.98	0.45
3:4C:141:TYR:HB3	3:4C:166:LEU:HG	1.99	0.45
1:5A:69:ILE:HD12	1:5A:123:ARG:HB2	1.99	0.45
2:6B:263:ASN:O	2:6B:370:ASN:ND2	2.43	0.45
1:7A:69:ILE:HD12	1:7A:123:ARG:HB2	1.99	0.45
2:7B:205:ASN:HA	2:7B:208:LEU:HB2	1.97	0.45
3:7C:222:LYS:HD2	3:7C:222:LYS:HA	1.62	0.45
1:2A:356:ILE:HD11	2:2B:176:ILE:HD11	1.98	0.45
3:2C:141:TYR:HB3	3:2C:166:LEU:HG	1.99	0.45
1:5A:425:GLN:HA	1:5A:428:GLN:HB2	1.99	0.45
1:6A:149:SER:OG	1:6A:188:ASN:O	2.34	0.45
2:6B:104:ARG:HA	2:6B:108:VAL:HB	1.98	0.45
3:6C:141:TYR:HB3	3:6C:166:LEU:HG	1.99	0.45
3:6C:222:LYS:HD2	3:6C:222:LYS:HA	1.62	0.45
2:7B:238:ALA:HA	2:7B:241:ARG:HG2	1.99	0.45
1:8A:132:ASP:OD1	3:8C:68:ARG:NE	2.35	0.45
1:1A:89:PHE:O	1:2A:287:PHE:CE2	2.69	0.45
1:3A:149:SER:OG	1:3A:188:ASN:O	2.34	0.45
1:3A:425:GLN:HA	1:3A:428:GLN:HB2	1.99	0.45
2:3B:243:PRO:CB	1:7A:76:SER:CB	2.95	0.45
2:7B:84:GLN:HE21	1:8A:284:ARG:NH1	0.83	0.45
2:8B:88:GLU:CD	3:8C:24:TYR:HB3	2.37	0.45
3:8C:141:TYR:HB3	3:8C:166:LEU:HG	1.99	0.45
1:2A:12:GLY:O	1:2A:16:ASN:ND2	2.50	0.45
1:2A:425:GLN:HA	1:2A:428:GLN:HB2	1.99	0.45
2:4B:350:LYS:HB3	1:8A:183:VAL:CG1	2.29	0.45
1:5A:12:GLY:O	1:5A:16:ASN:ND2	2.50	0.45
1:6A:54:SER:HB3	1:6A:65:VAL:HG23	1.97	0.45
1:6A:425:GLN:HA	1:6A:428:GLN:HB2	1.99	0.45
2:7B:61:VAL:HG21	1:8A:287:PHE:HE2	0.62	0.45
2:7B:88:GLU:HG2	3:7C:24:TYR:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7B:104:ARG:HA	2:7B:108:VAL:HB	1.98	0.45
2:7B:111:GLU:O	3:7C:62:PHE:CE1	2.69	0.45
1:8A:12:GLY:O	1:8A:16:ASN:ND2	2.50	0.45
1:1A:4:ASN:ND2	2:1B:70:GLU:OE2	2.50	0.44
1:1A:12:GLY:O	1:1A:16:ASN:ND2	2.50	0.44
1:1A:69:ILE:HD12	1:1A:123:ARG:HB2	1.99	0.44
2:1B:344:PRO:HB3	1:5A:389:ASN:HD22	1.78	0.44
1:2A:4:ASN:ND2	2:2B:70:GLU:OE2	2.50	0.44
2:3B:263:ASN:O	2:3B:370:ASN:ND2	2.43	0.44
1:4A:69:ILE:HD12	1:4A:123:ARG:HB2	1.99	0.44
2:4B:115:ASP:OD1	3:4C:58:ARG:CD	2.53	0.44
1:5A:4:ASN:ND2	2:5B:70:GLU:OE2	2.50	0.44
2:5B:115:ASP:HB3	3:5C:58:ARG:CB	2.47	0.44
2:5B:263:ASN:O	2:5B:370:ASN:ND2	2.43	0.44
2:6B:205:ASN:HA	2:6B:208:LEU:HB2	1.97	0.44
1:7A:4:ASN:ND2	2:7B:70:GLU:OE2	2.50	0.44
1:8A:4:ASN:ND2	2:8B:70:GLU:OE2	2.50	0.44
2:8B:104:ARG:HA	2:8B:108:VAL:HB	1.98	0.44
1:1A:425:GLN:HA	1:1A:428:GLN:HB2	1.99	0.44
2:1B:252:GLU:CG	1:5A:102:GLY:HA2	2.47	0.44
2:1B:324:LYS:HZ3	1:5A:216:HIS:CB	1.94	0.44
1:2A:174:LEU:N	1:2A:206:PHE:O	2.44	0.44
1:3A:275:ALA:HB3	1:3A:372:LEU:HB3	1.99	0.44
2:3B:115:ASP:CB	3:3C:58:ARG:HB2	2.46	0.44
2:3B:257:LEU:HD21	2:3B:314:SER:HB2	1.98	0.44
2:4B:88:GLU:CD	3:4C:24:TYR:HB3	2.37	0.44
1:5A:275:ALA:HB3	1:5A:372:LEU:HB3	1.99	0.44
1:7A:425:GLN:HA	1:7A:428:GLN:HB2	1.99	0.44
1:1A:10:SER:HB2	1:1A:70:MET:HG2	1.99	0.44
1:1A:22:PHE:HA	1:1A:234:THR:HG23	1.99	0.44
2:2B:184:TYR:OH	2:2B:388:MET:O	2.34	0.44
1:3A:12:GLY:O	1:3A:16:ASN:ND2	2.50	0.44
1:3A:54:SER:HB3	1:3A:65:VAL:HG23	1.97	0.44
2:3B:2:ARG:NE	1:7A:98:THR:O	2.48	0.44
1:4A:22:PHE:HA	1:4A:234:THR:HG23	1.99	0.44
1:4A:425:GLN:HA	1:4A:428:GLN:HB2	1.99	0.44
2:4B:238:ALA:HA	2:4B:241:ARG:HG2	1.98	0.44
1:5A:10:SER:HB2	1:5A:70:MET:HG2	1.99	0.44
1:6A:12:GLY:O	1:6A:16:ASN:ND2	2.50	0.44
2:6B:122:ASP:OD1	3:6C:52:LYS:CE	2.61	0.44
1:7A:12:GLY:O	1:7A:16:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:149:SER:OG	1:1A:188:ASN:O	2.34	0.44
2:1B:324:LYS:NZ	1:5A:224:PRO:HD3	2.32	0.44
2:2B:187:ILE:HD11	2:2B:381:LEU:HB3	1.98	0.44
2:2B:327:ASP:CG	1:6A:178:GLN:NE2	2.71	0.44
3:2C:198:MET:HE1	3:2C:203:LEU:HB2	2.00	0.44
1:3A:22:PHE:HA	1:3A:234:THR:HG23	1.99	0.44
1:4A:12:GLY:O	1:4A:16:ASN:ND2	2.50	0.44
1:6A:4:ASN:ND2	2:6B:70:GLU:OE2	2.50	0.44
1:7A:149:SER:OG	1:7A:188:ASN:O	2.34	0.44
2:7B:61:VAL:HG23	1:8A:287:PHE:CE2	1.95	0.44
1:8A:425:GLN:HA	1:8A:428:GLN:HB2	1.99	0.44
1:1A:381:ARG:NH1	1:1A:431:GLU:OE1	2.51	0.44
2:2B:2:ARG:CD	1:6A:75:PRO:CG	2.85	0.44
2:2B:256:ASN:ND2	1:6A:182:VAL:HG13	2.33	0.44
2:3B:88:GLU:HG2	3:3C:24:TYR:HB3	1.98	0.44
1:6A:69:ILE:HD12	1:6A:123:ARG:HB2	1.99	0.44
1:7A:22:PHE:HA	1:7A:234:THR:HG23	1.99	0.44
1:8A:22:PHE:HA	1:8A:234:THR:HG23	1.99	0.44
2:8B:238:ALA:HA	2:8B:241:ARG:HG2	1.99	0.44
2:2B:16:ILE:O	2:2B:20:PHE:N	2.43	0.44
1:3A:356:ILE:CD1	2:3B:176:ILE:HD11	2.46	0.44
2:4B:382:ILE:O	2:4B:386:ASP:N	2.51	0.44
2:5B:382:ILE:O	2:5B:386:ASP:N	2.51	0.44
2:1B:205:ASN:ND2	4:1B:501:GDP:H1'	2.33	0.44
2:2B:246:LEU:HA	1:6A:13:GLN:CD	2.38	0.44
1:5A:381:ARG:NH1	1:5A:431:GLU:OE1	2.51	0.44
1:6A:56:LEU:HD12	1:7A:286:LYS:HZ2	1.80	0.44
2:7B:205:ASN:ND2	4:7B:501:GDP:H1'	2.33	0.44
1:8A:275:ALA:HB3	1:8A:372:LEU:HB3	1.99	0.44
2:1B:119:ASN:ND2	3:1C:56:LEU:N	2.66	0.44
1:2A:381:ARG:NH1	1:2A:431:GLU:OE1	2.51	0.44
2:3B:187:ILE:HD11	2:3B:381:LEU:HB3	1.98	0.44
2:3B:343:MET:O	1:7A:392:LYS:CE	2.56	0.44
1:4A:275:ALA:HB3	1:4A:372:LEU:HB3	1.99	0.44
1:6A:65:VAL:HG13	1:7A:287:PHE:CE1	2.23	0.44
1:8A:356:ILE:CD1	2:8B:176:ILE:HD11	2.47	0.44
3:1C:222:LYS:HA	3:1C:222:LYS:HD2	1.62	0.44
1:2A:22:PHE:HA	1:2A:234:THR:HG23	2.00	0.44
2:2B:112:LYS:HA	3:2C:62:PHE:CD1	2.53	0.44
2:2B:205:ASN:ND2	4:2B:501:GDP:H1'	2.33	0.44
2:2B:247:ASN:H	1:6A:13:GLN:CD	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3A:4:ASN:ND2	2:3B:70:GLU:OE2	2.50	0.44
1:3A:69:ILE:HD12	1:3A:123:ARG:HB2	1.99	0.44
2:8B:263:ASN:O	2:8B:370:ASN:ND2	2.43	0.44
1:4A:4:ASN:ND2	2:4B:70:GLU:OE2	2.50	0.43
1:6A:10:SER:HB2	1:6A:70:MET:HG2	1.99	0.43
1:6A:22:PHE:HA	1:6A:234:THR:HG23	1.99	0.43
1:7A:381:ARG:NH1	1:7A:431:GLU:OE1	2.51	0.43
1:8A:381:ARG:NH1	1:8A:431:GLU:OE1	2.51	0.43
2:1B:324:LYS:HD3	1:5A:223:SER:HA	1.92	0.43
2:3B:205:ASN:ND2	4:3B:501:GDP:H1'	2.33	0.43
3:3C:198:MET:HE1	3:3C:203:LEU:HB2	2.01	0.43
1:5A:22:PHE:HA	1:5A:234:THR:HG23	2.00	0.43
2:1B:261:PRO:CG	1:5A:400:ALA:HB1	2.40	0.43
1:2A:10:SER:HB2	1:2A:70:MET:HG2	2.00	0.43
2:4B:334:ARG:NH1	2:4B:344:PRO:O	2.52	0.43
2:6B:205:ASN:ND2	4:6B:501:GDP:H1'	2.33	0.43
1:7A:10:SER:HB2	1:7A:70:MET:HG2	1.99	0.43
2:8B:382:ILE:O	2:8B:386:ASP:N	2.51	0.43
1:2A:69:ILE:HD12	1:2A:123:ARG:HB2	1.99	0.43
1:3A:337:LEU:HA	1:3A:340:MET:HB2	2.01	0.43
2:3B:84:GLN:HE21	1:4A:284:ARG:CD	2.31	0.43
1:4A:381:ARG:NH1	1:4A:431:GLU:OE1	2.51	0.43
2:5B:184:TYR:OH	2:5B:388:MET:O	2.34	0.43
2:5B:334:ARG:NH1	2:5B:344:PRO:O	2.52	0.43
1:6A:381:ARG:NH1	1:6A:431:GLU:OE1	2.51	0.43
3:6C:92:MET:HE3	3:6C:131:LEU:CD2	2.48	0.43
2:7B:55:VAL:HG11	1:8A:287:PHE:CA	2.48	0.43
2:2B:324:LYS:HB3	1:6A:223:SER:C	2.37	0.43
1:3A:381:ARG:NH1	1:3A:431:GLU:OE1	2.51	0.43
2:4B:252:GLU:HG3	1:8A:102:GLY:HA2	1.99	0.43
2:5B:115:ASP:HB3	3:5C:58:ARG:HB2	2.00	0.43
2:7B:222:TYR:HB3	4:7B:501:GDP:C6	2.54	0.43
1:8A:10:SER:HB2	1:8A:70:MET:HG2	1.99	0.43
1:8A:337:LEU:HA	1:8A:340:MET:HB2	2.01	0.43
2:8B:205:ASN:ND2	4:8B:501:GDP:H1'	2.33	0.43
2:1B:21:TRP:CZ2	2:1B:64:ALA:HB2	2.54	0.43
2:1B:115:ASP:HB3	3:1C:58:ARG:HB2	2.00	0.43
2:3B:119:ASN:ND2	3:3C:55:SER:CB	2.60	0.43
1:4A:10:SER:HB2	1:4A:70:MET:HG2	1.99	0.43
2:5B:112:LYS:O	3:5C:62:PHE:CE2	2.66	0.43
2:6B:21:TRP:CZ2	2:6B:64:ALA:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6B:112:LYS:HA	3:6C:62:PHE:CD1	2.53	0.43
2:8B:334:ARG:NH1	2:8B:344:PRO:O	2.52	0.43
2:1B:382:ILE:O	2:1B:386:ASP:N	2.51	0.43
3:1C:92:MET:HE2	3:1C:131:LEU:CD2	2.45	0.43
2:3B:55:VAL:HG11	1:4A:287:PHE:CA	2.48	0.43
2:3B:61:VAL:HG21	1:4A:287:PHE:HE2	0.62	0.43
2:5B:205:ASN:ND2	4:5B:501:GDP:H1'	2.33	0.43
2:6B:222:TYR:HB3	4:6B:501:GDP:C6	2.54	0.43
1:1A:63:SER:HG	1:2A:286:LYS:NZ	2.09	0.43
2:1B:334:ARG:NH1	2:1B:344:PRO:O	2.52	0.43
1:4A:337:LEU:HA	1:4A:340:MET:HB2	2.01	0.43
2:4B:91:ILE:HG22	3:4C:24:TYR:CZ	2.54	0.43
2:4B:222:TYR:HB3	4:4B:501:GDP:C6	2.54	0.43
1:6A:337:LEU:HA	1:6A:340:MET:HB2	2.01	0.43
1:7A:328:GLU:OE1	1:7A:368:LYS:NZ	2.45	0.43
2:8B:21:TRP:CZ2	2:8B:64:ALA:HB2	2.54	0.43
2:8B:115:ASP:HB2	3:8C:62:PHE:CD2	2.49	0.43
2:2B:382:ILE:O	2:2B:386:ASP:N	2.51	0.43
1:3A:10:SER:HB2	1:3A:70:MET:HG2	1.99	0.43
2:8B:4:ILE:HG21	2:8B:135:LEU:HG	2.01	0.43
2:1B:222:TYR:HB3	4:1B:501:GDP:C6	2.54	0.43
2:3B:222:TYR:HB3	4:3B:501:GDP:C6	2.54	0.43
2:4B:205:ASN:ND2	4:4B:501:GDP:H1'	2.33	0.43
1:5A:132:ASP:HA	3:5C:68:ARG:CG	2.49	0.43
2:5B:222:TYR:HB3	4:5B:501:GDP:C6	2.54	0.43
1:6A:45:PRO:HG3	1:6A:64:TYR:HE2	1.84	0.43
2:7B:56:ARG:CD	1:8A:286:LYS:HG2	2.13	0.43
1:1A:45:PRO:HG3	1:1A:64:TYR:HE2	1.84	0.42
2:3B:21:TRP:CZ2	2:3B:64:ALA:HB2	2.54	0.42
2:4B:4:ILE:HG21	2:4B:135:LEU:HG	2.01	0.42
2:4B:21:TRP:CZ2	2:4B:64:ALA:HB2	2.54	0.42
2:5B:375:ALA:O	2:5B:379:GLU:N	2.46	0.42
2:6B:101:ASN:H	2:6B:143:GLY:HA3	1.84	0.42
2:6B:382:ILE:O	2:6B:386:ASP:N	2.51	0.42
2:7B:4:ILE:HG21	2:7B:135:LEU:HG	2.01	0.42
2:7B:56:ARG:CD	1:8A:286:LYS:CE	2.48	0.42
3:8C:222:LYS:HD2	3:8C:222:LYS:HA	1.62	0.42
2:1B:91:ILE:HD13	2:1B:91:ILE:HG21	1.85	0.42
2:1B:324:LYS:HG2	1:5A:224:PRO:HD2	0.62	0.42
1:2A:56:LEU:HD12	1:3A:286:LYS:HZ3	1.83	0.42
2:2B:222:TYR:HB3	4:2B:501:GDP:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:115:ASP:HB3	3:3C:58:ARG:HB2	2.01	0.42
2:3B:256:ASN:CG	1:7A:183:VAL:CG2	2.83	0.42
2:7B:382:ILE:O	2:7B:386:ASP:N	2.51	0.42
1:8A:187:TYR:OH	1:8A:393:LEU:O	2.26	0.42
1:1A:337:LEU:HA	1:1A:340:MET:HB2	2.01	0.42
2:1B:4:ILE:HG21	2:1B:135:LEU:HG	2.01	0.42
2:3B:324:LYS:N	1:7A:212:PHE:CZ	2.87	0.42
2:4B:256:ASN:O	1:8A:399:PHE:HE1	1.99	0.42
1:5A:45:PRO:HG3	1:5A:64:TYR:HE2	1.84	0.42
1:6A:182:VAL:HG12	1:6A:184:THR:H	1.84	0.42
2:6B:125:VAL:HB	2:6B:131:LEU:HD22	2.01	0.42
2:7B:21:TRP:CZ2	2:7B:64:ALA:HB2	2.54	0.42
2:7B:91:ILE:CG2	3:7C:24:TYR:CE2	2.90	0.42
2:7B:101:ASN:H	2:7B:143:GLY:HA3	1.84	0.42
2:7B:115:ASP:HB3	3:7C:58:ARG:HB2	2.01	0.42
2:8B:222:TYR:HB3	4:8B:501:GDP:C6	2.54	0.42
2:2B:21:TRP:CZ2	2:2B:64:ALA:HB2	2.54	0.42
2:2B:334:ARG:NH1	2:2B:344:PRO:O	2.52	0.42
1:3A:45:PRO:HG3	1:3A:64:TYR:HE2	1.84	0.42
2:3B:4:ILE:HG21	2:3B:135:LEU:HG	2.01	0.42
1:5A:182:VAL:HG12	1:5A:184:THR:H	1.84	0.42
2:5B:4:ILE:HG21	2:5B:135:LEU:HG	2.01	0.42
2:5B:21:TRP:HZ3	2:5B:51:PHE:HB3	1.85	0.42
1:7A:182:VAL:HG12	1:7A:184:THR:H	1.84	0.42
1:8A:182:VAL:HG12	1:8A:184:THR:H	1.84	0.42
2:1B:101:ASN:H	2:1B:143:GLY:HA3	1.84	0.42
1:2A:45:PRO:HG3	1:2A:64:TYR:HE2	1.84	0.42
1:2A:63:SER:CB	1:3A:286:LYS:NZ	2.74	0.42
1:2A:182:VAL:HG12	1:2A:184:THR:H	1.84	0.42
2:3B:101:ASN:H	2:3B:143:GLY:HA3	1.84	0.42
2:3B:382:ILE:O	2:3B:386:ASP:N	2.51	0.42
1:5A:328:GLU:OE1	1:5A:368:LYS:NZ	2.45	0.42
2:5B:21:TRP:CZ2	2:5B:64:ALA:HB2	2.54	0.42
2:5B:101:ASN:H	2:5B:143:GLY:HA3	1.84	0.42
2:5B:125:VAL:HB	2:5B:131:LEU:HD22	2.01	0.42
2:5B:269:SER:HB3	2:5B:299:PHE:CD1	2.53	0.42
3:5C:198:MET:HE1	3:5C:203:LEU:HB2	2.02	0.42
1:7A:337:LEU:HA	1:7A:340:MET:HB2	2.01	0.42
1:8A:139:VAL:HG12	1:8A:141:HIS:HD2	1.85	0.42
2:3B:269:SER:HB3	2:3B:299:PHE:CD1	2.53	0.42
2:3B:340:ALA:O	1:7A:396:ARG:NH2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4A:45:PRO:HG3	1:4A:64:TYR:HE2	1.84	0.42
2:4B:16:ILE:O	2:4B:20:PHE:N	2.44	0.42
1:6A:139:VAL:HG12	1:6A:141:HIS:HD2	1.85	0.42
1:7A:139:VAL:HG12	1:7A:141:HIS:HD2	1.85	0.42
2:7B:84:GLN:HE21	1:8A:284:ARG:CD	2.31	0.42
1:1A:132:ASP:HA	3:1C:68:ARG:CG	2.49	0.42
2:1B:16:ILE:O	2:1B:20:PHE:N	2.44	0.42
2:1B:74:ILE:O	2:1B:78:GLU:N	2.42	0.42
2:1B:375:ALA:O	2:1B:379:GLU:N	2.46	0.42
1:3A:139:VAL:HG12	1:3A:141:HIS:HD2	1.85	0.42
2:3B:247:ASN:HB3	1:7A:74:GLU:OE1	1.92	0.42
2:3B:323:ALA:C	1:7A:212:PHE:CZ	2.93	0.42
1:4A:182:VAL:HG12	1:4A:184:THR:H	1.84	0.42
2:4B:101:ASN:H	2:4B:143:GLY:HA3	1.84	0.42
2:4B:130:GLY:HA3	1:8A:98:THR:HG21	1.97	0.42
2:4B:246:LEU:HD23	4:8A:501:GDP:H2'	1.91	0.42
1:5A:139:VAL:HG12	1:5A:141:HIS:HD2	1.85	0.42
2:6B:74:ILE:O	2:6B:78:GLU:N	2.42	0.42
1:8A:314:GLY:HA3	1:8A:378:GLU:HG2	2.02	0.42
2:1B:98:ALA:O	2:1B:100:ASN:N	2.53	0.42
1:4A:139:VAL:HG12	1:4A:141:HIS:HD2	1.85	0.42
3:5C:222:LYS:HA	3:5C:222:LYS:HD2	1.62	0.42
1:7A:45:PRO:HG3	1:7A:64:TYR:HE2	1.84	0.42
2:8B:74:ILE:O	2:8B:78:GLU:N	2.42	0.42
2:8B:91:ILE:HG22	3:8C:24:TYR:CZ	2.54	0.42
1:1A:182:VAL:HG12	1:1A:184:THR:H	1.84	0.42
2:1B:21:TRP:HZ3	2:1B:51:PHE:HB3	1.85	0.42
2:2B:4:ILE:HG21	2:2B:135:LEU:HG	2.01	0.42
2:2B:88:GLU:HB3	3:2C:24:TYR:HD2	1.76	0.42
2:2B:89:SER:CB	3:2C:21:ARG:NH1	2.69	0.42
2:2B:344:PRO:HB3	1:6A:389:ASN:HB3	2.01	0.42
2:4B:98:ALA:O	2:4B:100:ASN:N	2.53	0.42
1:5A:286:LYS:HZ3	1:8A:56:LEU:CD1	2.32	0.42
2:6B:21:TRP:HZ3	2:6B:51:PHE:HB3	1.85	0.42
2:6B:334:ARG:NH1	2:6B:344:PRO:O	2.52	0.42
2:8B:98:ALA:O	2:8B:100:ASN:N	2.53	0.42
2:1B:256:ASN:O	1:5A:183:VAL:CB	2.67	0.42
1:2A:337:LEU:HA	1:2A:340:MET:HB2	2.01	0.42
2:2B:98:ALA:O	2:2B:100:ASN:N	2.53	0.42
2:3B:256:ASN:ND2	1:7A:183:VAL:CG2	2.83	0.42
2:3B:334:ARG:NH1	2:3B:344:PRO:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4B:252:GLU:HG2	1:8A:102:GLY:O	2.20	0.42
2:4B:283:ARG:HE	1:7A:59:SER:HB3	1.27	0.42
2:5B:30:LEU:HD22	2:5B:36:LEU:HA	2.02	0.42
2:7B:334:ARG:NH1	2:7B:344:PRO:O	2.52	0.42
2:8B:101:ASN:H	2:8B:143:GLY:HA3	1.84	0.42
2:8B:125:VAL:HB	2:8B:131:LEU:HD22	2.01	0.42
2:1B:30:LEU:HD22	2:1B:36:LEU:HA	2.02	0.41
1:3A:182:VAL:HG12	1:3A:184:THR:H	1.84	0.41
2:3B:98:ALA:O	2:3B:100:ASN:N	2.53	0.41
2:3B:125:VAL:HB	2:3B:131:LEU:HD22	2.01	0.41
2:4B:91:ILE:HD13	2:4B:91:ILE:HG21	1.84	0.41
3:5C:92:MET:HE3	3:5C:131:LEU:CD2	2.48	0.41
2:6B:4:ILE:HG21	2:6B:135:LEU:HG	2.01	0.41
1:1A:240:ILE:HG13	1:1A:241:THR:HG23	2.03	0.41
2:2B:101:ASN:H	2:2B:143:GLY:HA3	1.84	0.41
2:2B:125:VAL:HB	2:2B:131:LEU:HD22	2.01	0.41
2:3B:344:PRO:C	1:7A:392:LYS:HE2	2.41	0.41
1:4A:171:CYS:HA	1:4A:204:LEU:HB3	2.02	0.41
2:6B:98:ALA:O	2:6B:100:ASN:N	2.53	0.41
2:7B:61:VAL:CB	1:8A:287:PHE:CE2	2.81	0.41
2:7B:98:ALA:O	2:7B:100:ASN:N	2.53	0.41
2:7B:125:VAL:HB	2:7B:131:LEU:HD22	2.01	0.41
1:8A:45:PRO:HG3	1:8A:64:TYR:HE2	1.84	0.41
1:8A:171:CYS:HA	1:8A:204:LEU:HB3	2.02	0.41
2:8B:21:TRP:HZ3	2:8B:51:PHE:HB3	1.85	0.41
2:8B:184:TYR:OH	2:8B:388:MET:O	2.34	0.41
2:1B:261:PRO:HD3	1:5A:400:ALA:CB	2.51	0.41
1:3A:171:CYS:HA	1:3A:204:LEU:HB3	2.02	0.41
2:3B:8:HIS:CG	2:3B:17:ALA:HB2	2.56	0.41
2:3B:184:TYR:OH	2:3B:388:MET:O	2.34	0.41
1:4A:314:GLY:HA3	1:4A:378:GLU:HG2	2.02	0.41
2:4B:125:VAL:HB	2:4B:131:LEU:HD22	2.01	0.41
1:5A:286:LYS:HZ3	1:8A:56:LEU:HD12	1.73	0.41
2:5B:74:ILE:HB	2:5B:93:ARG:HH21	1.86	0.41
2:6B:8:HIS:CG	2:6B:17:ALA:HB2	2.56	0.41
1:7A:52:PHE:CD2	1:7A:245:ARG:HD3	2.56	0.41
1:1A:139:VAL:HG12	1:1A:141:HIS:HD2	1.85	0.41
2:2B:21:TRP:HZ3	2:2B:51:PHE:HB3	1.85	0.41
2:3B:351:LEU:HD12	1:7A:180:SER:O	2.19	0.41
1:4A:387:CYS:SG	1:4A:417:ARG:NH2	2.94	0.41
1:5A:240:ILE:HG13	1:5A:241:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7A:314:GLY:HA3	1:7A:378:GLU:HG2	2.02	0.41
1:1A:156:ILE:HG23	1:1A:168:VAL:HG11	2.02	0.41
1:2A:52:PHE:CD2	1:2A:245:ARG:HD3	2.56	0.41
1:3A:52:PHE:CD2	1:3A:245:ARG:HD3	2.56	0.41
2:3B:245:LYS:HD3	1:7A:226:VAL:HG21	2.03	0.41
1:5A:262:ASN:HA	2:5B:180:ALA:HB3	2.03	0.41
2:5B:219:SER:HA	2:5B:220:PRO:HD3	1.92	0.41
2:6B:219:SER:HA	2:6B:220:PRO:HD3	1.92	0.41
1:7A:171:CYS:HA	1:7A:204:LEU:HB3	2.02	0.41
2:7B:8:HIS:CG	2:7B:17:ALA:HB2	2.56	0.41
1:8A:156:ILE:HG23	1:8A:168:VAL:HG11	2.02	0.41
1:2A:240:ILE:HG13	1:2A:241:THR:HG23	2.03	0.41
2:2B:74:ILE:HB	2:2B:93:ARG:HH21	1.85	0.41
1:3A:314:GLY:HA3	1:3A:378:GLU:HG2	2.02	0.41
2:3B:324:LYS:HG3	1:7A:224:PRO:HG2	2.01	0.41
2:4B:30:LEU:HD22	2:4B:36:LEU:HA	2.02	0.41
2:4B:343:MET:O	1:8A:392:LYS:CE	2.69	0.41
1:5A:156:ILE:HG23	1:5A:168:VAL:HG11	2.02	0.41
1:5A:337:LEU:HA	1:5A:340:MET:HB2	2.01	0.41
1:5A:387:CYS:SG	1:5A:417:ARG:NH2	2.94	0.41
1:6A:240:ILE:HG13	1:6A:241:THR:HG23	2.03	0.41
2:7B:74:ILE:HB	2:7B:93:ARG:HH21	1.85	0.41
2:7B:134:PHE:CG	2:7B:156:LEU:HD21	2.56	0.41
2:1B:125:VAL:HB	2:1B:131:LEU:HD22	2.01	0.41
1:2A:51:SER:HB3	1:2A:245:ARG:HG2	2.03	0.41
2:3B:74:ILE:HB	2:3B:93:ARG:HH21	1.86	0.41
1:4A:156:ILE:HG23	1:4A:168:VAL:HG11	2.02	0.41
2:4B:74:ILE:HB	2:4B:93:ARG:HH21	1.85	0.41
1:5A:155:LEU:HD12	1:5A:155:LEU:HA	1.90	0.41
2:6B:30:LEU:HD22	2:6B:36:LEU:HA	2.02	0.41
2:6B:134:PHE:CG	2:6B:156:LEU:HD21	2.56	0.41
1:2A:63:SER:N	1:3A:286:LYS:HZ1	2.12	0.41
1:2A:139:VAL:HG12	1:2A:141:HIS:HD2	1.85	0.41
1:2A:262:ASN:HA	2:2B:180:ALA:HB3	2.03	0.41
2:4B:375:ALA:O	2:4B:379:GLU:N	2.46	0.41
1:6A:51:SER:HB3	1:6A:245:ARG:HG2	2.03	0.41
1:6A:52:PHE:CD2	1:6A:245:ARG:HD3	2.56	0.41
1:7A:387:CYS:SG	1:7A:417:ARG:NH2	2.94	0.41
2:7B:102:TRP:CD1	2:7B:147:GLY:HA2	2.56	0.41
3:8C:198:MET:HE3	3:8C:202:ASP:HB2	2.02	0.41
1:1A:52:PHE:CD2	1:1A:245:ARG:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:262:ASN:HA	2:1B:180:ALA:HB3	2.03	0.41
1:1A:301:ASP:HB2	1:1A:304:SER:HB2	2.03	0.41
1:1A:387:CYS:SG	1:1A:417:ARG:NH2	2.94	0.41
2:1B:115:ASP:CB	3:1C:62:PHE:HE2	2.29	0.41
2:1B:134:PHE:CG	2:1B:156:LEU:HD21	2.56	0.41
2:2B:30:LEU:HD22	2:2B:36:LEU:HA	2.02	0.41
1:3A:262:ASN:HA	2:3B:180:ALA:HB3	2.03	0.41
1:3A:387:CYS:SG	1:3A:417:ARG:NH2	2.94	0.41
2:3B:256:ASN:CG	1:7A:183:VAL:HG22	2.38	0.41
2:3B:331:ALA:HB1	1:7A:178:GLN:O	2.15	0.41
2:4B:8:HIS:CG	2:4B:17:ALA:HB2	2.56	0.41
2:4B:23:LEU:HD23	2:4B:26:ARG:HD3	2.03	0.41
2:4B:102:TRP:CD1	2:4B:147:GLY:HA2	2.56	0.41
1:5A:171:CYS:HA	1:5A:204:LEU:HB3	2.02	0.41
2:5B:89:SER:HA	3:5C:24:TYR:OH	2.15	0.41
2:5B:98:ALA:O	2:5B:100:ASN:N	2.53	0.41
1:6A:262:ASN:HA	2:6B:180:ALA:HB3	2.03	0.41
1:6A:301:ASP:HB2	1:6A:304:SER:HB2	2.03	0.41
1:6A:387:CYS:SG	1:6A:417:ARG:NH2	2.94	0.41
2:7B:21:TRP:HZ3	2:7B:51:PHE:HB3	1.85	0.41
2:8B:30:LEU:HD22	2:8B:36:LEU:HA	2.02	0.41
2:8B:375:ALA:O	2:8B:379:GLU:N	2.46	0.41
1:1A:171:CYS:HA	1:1A:204:LEU:HB3	2.02	0.41
2:1B:89:SER:HA	3:1C:24:TYR:OH	2.15	0.41
1:2A:301:ASP:HB2	1:2A:304:SER:HB2	2.03	0.41
1:2A:387:CYS:SG	1:2A:417:ARG:NH2	2.94	0.41
2:2B:309:VAL:HG12	2:2B:338:ASN:HB3	2.03	0.41
2:2B:343:MET:SD	1:6A:399:PHE:CZ	3.14	0.41
1:3A:132:ASP:CA	3:3C:68:ARG:HD3	2.44	0.41
2:3B:84:GLN:HE21	1:4A:284:ARG:NH1	0.83	0.41
2:3B:134:PHE:CG	2:3B:156:LEU:HD21	2.56	0.41
2:3B:309:VAL:HG12	2:3B:338:ASN:HB3	2.03	0.41
2:4B:21:TRP:HZ3	2:4B:51:PHE:HB3	1.85	0.41
2:4B:245:LYS:HG2	1:8A:226:VAL:HG11	2.00	0.41
2:5B:102:TRP:CD1	2:5B:147:GLY:HA2	2.56	0.41
2:5B:115:ASP:CB	3:5C:62:PHE:HE2	2.28	0.41
1:7A:8:VAL:HB	1:7A:23:TRP:HZ2	1.86	0.41
1:7A:262:ASN:HA	2:7B:180:ALA:HB3	2.03	0.41
2:7B:16:ILE:O	2:7B:20:PHE:N	2.44	0.41
2:7B:23:LEU:HD23	2:7B:26:ARG:HD3	2.03	0.41
1:8A:240:ILE:HG13	1:8A:241:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8A:387:CYS:SG	1:8A:417:ARG:NH2	2.94	0.41
1:1A:8:VAL:HB	1:1A:23:TRP:HZ2	1.86	0.40
2:1B:8:HIS:CG	2:1B:17:ALA:HB2	2.56	0.40
2:1B:74:ILE:HB	2:1B:93:ARG:HH21	1.86	0.40
2:2B:8:HIS:CG	2:2B:17:ALA:HB2	2.56	0.40
1:3A:156:ILE:HG23	1:3A:168:VAL:HG11	2.02	0.40
1:3A:240:ILE:HG13	1:3A:241:THR:HG23	2.03	0.40
2:3B:23:LEU:HD23	2:3B:26:ARG:HD3	2.03	0.40
1:4A:262:ASN:HA	2:4B:180:ALA:HB3	2.03	0.40
1:5A:301:ASP:HB2	1:5A:304:SER:HB2	2.03	0.40
2:5B:8:HIS:CG	2:5B:17:ALA:HB2	2.56	0.40
2:6B:102:TRP:CD1	2:6B:147:GLY:HA2	2.56	0.40
1:7A:184:THR:HG22	1:7A:399:PHE:CD2	2.57	0.40
1:7A:240:ILE:HG13	1:7A:241:THR:HG23	2.03	0.40
2:7B:112:LYS:O	3:7C:62:PHE:CB	2.66	0.40
2:7B:269:SER:HB3	2:7B:299:PHE:CD1	2.53	0.40
1:8A:184:THR:HG22	1:8A:399:PHE:CD2	2.56	0.40
2:8B:23:LEU:HD23	2:8B:26:ARG:HD3	2.03	0.40
2:2B:102:TRP:CD1	2:2B:147:GLY:HA2	2.56	0.40
1:4A:240:ILE:HG13	1:4A:241:THR:HG23	2.02	0.40
1:6A:314:GLY:HA3	1:6A:378:GLU:HG2	2.02	0.40
1:7A:156:ILE:HG23	1:7A:168:VAL:HG11	2.02	0.40
1:8A:262:ASN:HA	2:8B:180:ALA:HB3	2.03	0.40
2:8B:102:TRP:CD1	2:8B:147:GLY:HA2	2.56	0.40
1:1A:51:SER:HB3	1:1A:245:ARG:HG2	2.03	0.40
1:1A:314:GLY:HA3	1:1A:378:GLU:HG2	2.02	0.40
2:1B:102:TRP:CD1	2:1B:147:GLY:HA2	2.56	0.40
3:1C:198:MET:HE1	3:1C:203:LEU:HB2	2.03	0.40
1:2A:137:ILE:HG21	1:2A:159:LEU:HD21	2.04	0.40
1:2A:314:GLY:HA3	1:2A:378:GLU:HG2	2.02	0.40
2:2B:23:LEU:HD23	2:2B:26:ARG:HD3	2.03	0.40
2:2B:119:ASN:OD1	3:2C:55:SER:CB	2.70	0.40
2:2B:134:PHE:CG	2:2B:156:LEU:HD21	2.56	0.40
2:2B:255:THR:HB	1:6A:102:GLY:O	2.21	0.40
1:3A:189:THR:O	1:3A:193:LEU:N	2.53	0.40
1:4A:52:PHE:CD2	1:4A:245:ARG:HD3	2.56	0.40
2:4B:115:ASP:HB2	3:4C:62:PHE:CD2	2.49	0.40
2:5B:119:ASN:ND2	3:5C:56:LEU:N	2.66	0.40
2:5B:134:PHE:CG	2:5B:156:LEU:HD21	2.56	0.40
1:6A:156:ILE:HG23	1:6A:168:VAL:HG11	2.02	0.40
1:6A:184:THR:HG22	1:6A:399:PHE:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6B:23:LEU:HD23	2:6B:26:ARG:HD3	2.03	0.40
1:8A:52:PHE:CD2	1:8A:245:ARG:HD3	2.56	0.40
2:8B:269:SER:HB3	2:8B:299:PHE:CD1	2.53	0.40
2:1B:23:LEU:HD23	2:1B:26:ARG:HD3	2.03	0.40
2:1B:219:SER:HA	2:1B:220:PRO:HD3	1.92	0.40
1:2A:156:ILE:HG23	1:2A:168:VAL:HG11	2.02	0.40
1:2A:194:ASN:HB2	1:2A:416:LEU:HD22	2.03	0.40
2:2B:259:PRO:CB	1:6A:399:PHE:HA	2.51	0.40
1:3A:8:VAL:HB	1:3A:23:TRP:HZ2	1.86	0.40
1:3A:194:ASN:HB2	1:3A:416:LEU:HD22	2.03	0.40
1:3A:425:GLN:O	1:3A:429:VAL:N	2.45	0.40
2:3B:21:TRP:HZ3	2:3B:51:PHE:HB3	1.85	0.40
2:3B:30:LEU:HD22	2:3B:36:LEU:HA	2.02	0.40
2:3B:102:TRP:CD1	2:3B:147:GLY:HA2	2.56	0.40
1:5A:8:VAL:HB	1:5A:23:TRP:HZ2	1.86	0.40
1:5A:52:PHE:CD2	1:5A:245:ARG:HD3	2.56	0.40
1:5A:287:PHE:HZ	1:8A:65:VAL:HG12	1.72	0.40
2:5B:23:LEU:HD23	2:5B:26:ARG:HD3	2.03	0.40
1:6A:171:CYS:HA	1:6A:204:LEU:HB3	2.02	0.40
2:7B:30:LEU:HD22	2:7B:36:LEU:HA	2.02	0.40
2:8B:8:HIS:CG	2:8B:17:ALA:HB2	2.56	0.40
2:8B:134:PHE:CG	2:8B:156:LEU:HD21	2.56	0.40
1:1A:184:THR:HG22	1:1A:399:PHE:CD2	2.56	0.40
2:1B:69:LEU:HB3	2:1B:97:GLY:HA2	2.04	0.40
1:2A:8:VAL:HB	1:2A:23:TRP:HZ2	1.85	0.40
2:2B:3:GLU:N	2:2B:130:GLY:O	2.55	0.40
2:2B:246:LEU:CA	1:6A:13:GLN:OE1	2.68	0.40
2:2B:343:MET:HE1	1:6A:399:PHE:CE1	2.56	0.40
2:4B:112:LYS:O	3:4C:62:PHE:CD1	2.69	0.40
2:5B:309:VAL:HG12	2:5B:338:ASN:HB3	2.03	0.40
1:6A:8:VAL:HB	1:6A:23:TRP:HZ2	1.85	0.40
1:6A:137:ILE:HG21	1:6A:159:LEU:HD21	2.04	0.40
2:6B:69:LEU:HB3	2:6B:97:GLY:HA2	2.04	0.40
2:6B:74:ILE:HB	2:6B:93:ARG:HH21	1.86	0.40
2:6B:119:ASN:OD1	3:6C:55:SER:CB	2.70	0.40
1:7A:51:SER:HB3	1:7A:245:ARG:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	431/433 (100%)	395 (92%)	32 (7%)	4 (1%)	17	57
1	2A	431/433 (100%)	395 (92%)	32 (7%)	4 (1%)	17	57
1	3A	431/433 (100%)	395 (92%)	32 (7%)	4 (1%)	17	57
1	4A	431/433 (100%)	395 (92%)	32 (7%)	4 (1%)	17	57
1	5A	431/433 (100%)	395 (92%)	32 (7%)	4 (1%)	17	57
1	6A	431/433 (100%)	395 (92%)	32 (7%)	4 (1%)	17	57
1	7A	431/433 (100%)	395 (92%)	32 (7%)	4 (1%)	17	57
1	8A	431/433 (100%)	395 (92%)	32 (7%)	4 (1%)	17	57
2	1B	404/426 (95%)	373 (92%)	29 (7%)	2 (0%)	29	68
2	2B	404/426 (95%)	373 (92%)	29 (7%)	2 (0%)	29	68
2	3B	404/426 (95%)	374 (93%)	28 (7%)	2 (0%)	29	68
2	4B	404/426 (95%)	373 (92%)	29 (7%)	2 (0%)	29	68
2	5B	404/426 (95%)	373 (92%)	29 (7%)	2 (0%)	29	68
2	6B	404/426 (95%)	374 (93%)	28 (7%)	2 (0%)	29	68
2	7B	404/426 (95%)	374 (93%)	28 (7%)	2 (0%)	29	68
2	8B	404/426 (95%)	373 (92%)	29 (7%)	2 (0%)	29	68
3	1C	236/238 (99%)	226 (96%)	7 (3%)	3 (1%)	12	50
3	2C	236/238 (99%)	226 (96%)	7 (3%)	3 (1%)	12	50
3	3C	236/238 (99%)	226 (96%)	7 (3%)	3 (1%)	12	50
3	4C	236/238 (99%)	226 (96%)	7 (3%)	3 (1%)	12	50
3	5C	236/238 (99%)	226 (96%)	7 (3%)	3 (1%)	12	50
3	6C	236/238 (99%)	226 (96%)	7 (3%)	3 (1%)	12	50
3	7C	236/238 (99%)	226 (96%)	7 (3%)	3 (1%)	12	50
3	8C	236/238 (99%)	226 (96%)	7 (3%)	3 (1%)	12	50
All	All	8568/8776 (98%)	7955 (93%)	541 (6%)	72 (1%)	24	59

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	399	PHE
3	1C	196	GLY
1	2A	399	PHE
3	2C	196	GLY
1	3A	399	PHE
3	3C	196	GLY
1	4A	399	PHE
3	4C	196	GLY
1	5A	399	PHE
3	5C	196	GLY
1	6A	399	PHE
3	6C	196	GLY
1	7A	399	PHE
3	7C	196	GLY
1	8A	399	PHE
3	8C	196	GLY
1	1A	349	TRP
1	1A	398	ALA
1	1A	401	ASN
2	1B	99	ALA
3	1C	112	GLU
3	1C	195	GLU
1	2A	349	TRP
1	2A	398	ALA
1	2A	401	ASN
2	2B	99	ALA
3	2C	112	GLU
3	2C	195	GLU
1	3A	349	TRP
1	3A	398	ALA
1	3A	401	ASN
2	3B	99	ALA
3	3C	112	GLU
3	3C	195	GLU
1	4A	349	TRP
1	4A	398	ALA
1	4A	401	ASN
2	4B	99	ALA
3	4C	112	GLU
3	4C	195	GLU
1	5A	349	TRP
1	5A	398	ALA

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Mol	Chain	Res	Type
1	5A	401	ASN
2	5B	99	ALA
3	5C	112	GLU
3	5C	195	GLU
1	6A	349	TRP
1	6A	398	ALA
1	6A	401	ASN
2	6B	99	ALA
3	6C	112	GLU
3	6C	195	GLU
1	7A	349	TRP
1	7A	398	ALA
1	7A	401	ASN
2	7B	99	ALA
3	7C	112	GLU
3	7C	195	GLU
1	8A	349	TRP
1	8A	398	ALA
1	8A	401	ASN
2	8B	99	ALA
3	8C	112	GLU
3	8C	195	GLU
2	1B	287	PRO
2	2B	287	PRO
2	3B	287	PRO
2	4B	287	PRO
2	5B	287	PRO
2	6B	287	PRO
2	7B	287	PRO
2	8B	287	PRO

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1A	358/358 (100%)	351 (98%)	7 (2%)	55 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2A	358/358 (100%)	351 (98%)	7 (2%)	55	79
1	3A	358/358 (100%)	351 (98%)	7 (2%)	55	79
1	4A	358/358 (100%)	351 (98%)	7 (2%)	55	79
1	5A	358/358 (100%)	351 (98%)	7 (2%)	55	79
1	6A	358/358 (100%)	351 (98%)	7 (2%)	55	79
1	7A	358/358 (100%)	351 (98%)	7 (2%)	55	79
1	8A	358/358 (100%)	351 (98%)	7 (2%)	55	79
2	1B	333/341 (98%)	325 (98%)	8 (2%)	49	75
2	2B	333/341 (98%)	325 (98%)	8 (2%)	49	75
2	3B	333/341 (98%)	325 (98%)	8 (2%)	49	75
2	4B	333/341 (98%)	325 (98%)	8 (2%)	49	75
2	5B	333/341 (98%)	325 (98%)	8 (2%)	49	75
2	6B	333/341 (98%)	325 (98%)	8 (2%)	49	75
2	7B	333/341 (98%)	325 (98%)	8 (2%)	49	75
2	8B	333/341 (98%)	325 (98%)	8 (2%)	49	75
3	1C	191/193 (99%)	182 (95%)	9 (5%)	26	61
3	2C	191/193 (99%)	182 (95%)	9 (5%)	26	61
3	3C	191/193 (99%)	182 (95%)	9 (5%)	26	61
3	4C	191/193 (99%)	182 (95%)	9 (5%)	26	61
3	5C	191/193 (99%)	182 (95%)	9 (5%)	26	61
3	6C	191/193 (99%)	182 (95%)	9 (5%)	26	61
3	7C	191/193 (99%)	182 (95%)	9 (5%)	26	61
3	8C	191/193 (99%)	182 (95%)	9 (5%)	26	61
All	All	7056/7136 (99%)	6864 (97%)	192 (3%)	48	73

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	110	LEU
1	1A	197	ARG
1	1A	317	LEU
1	1A	324	ARG
1	1A	367	ARG
1	1A	376	ASN

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Mol	Chain	Res	Type
1	1A	417	ARG
2	1B	47	ASN
2	1B	76	ARG
2	1B	107	ASN
2	1B	217	ASN
2	1B	218	ARG
2	1B	298	ASN
2	1B	322	LYS
2	1B	334	ARG
3	1C	22	LEU
3	1C	68	ARG
3	1C	104	LYS
3	1C	115	ASP
3	1C	174	MET
3	1C	199	ASP
3	1C	222	LYS
3	1C	228	ASP
3	1C	232	ARG
1	2A	110	LEU
1	2A	197	ARG
1	2A	317	LEU
1	2A	324	ARG
1	2A	367	ARG
1	2A	376	ASN
1	2A	417	ARG
2	2B	47	ASN
2	2B	76	ARG
2	2B	107	ASN
2	2B	217	ASN
2	2B	218	ARG
2	2B	298	ASN
2	2B	322	LYS
2	2B	334	ARG
3	2C	22	LEU
3	2C	68	ARG
3	2C	104	LYS
3	2C	115	ASP
3	2C	174	MET
3	2C	199	ASP
3	2C	222	LYS
3	2C	228	ASP
3	2C	232	ARG

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Mol	Chain	Res	Type
1	3A	110	LEU
1	3A	197	ARG
1	3A	317	LEU
1	3A	324	ARG
1	3A	367	ARG
1	3A	376	ASN
1	3A	417	ARG
2	3B	47	ASN
2	3B	76	ARG
2	3B	107	ASN
2	3B	217	ASN
2	3B	218	ARG
2	3B	298	ASN
2	3B	322	LYS
2	3B	334	ARG
3	3C	22	LEU
3	3C	68	ARG
3	3C	104	LYS
3	3C	115	ASP
3	3C	174	MET
3	3C	199	ASP
3	3C	222	LYS
3	3C	228	ASP
3	3C	232	ARG
1	4A	110	LEU
1	4A	197	ARG
1	4A	317	LEU
1	4A	324	ARG
1	4A	367	ARG
1	4A	376	ASN
1	4A	417	ARG
2	4B	47	ASN
2	4B	76	ARG
2	4B	107	ASN
2	4B	217	ASN
2	4B	218	ARG
2	4B	298	ASN
2	4B	322	LYS
2	4B	334	ARG
3	4C	22	LEU
3	4C	68	ARG
3	4C	104	LYS

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Mol	Chain	Res	Type
3	4C	115	ASP
3	4C	174	MET
3	4C	199	ASP
3	4C	222	LYS
3	4C	228	ASP
3	4C	232	ARG
1	5A	110	LEU
1	5A	197	ARG
1	5A	317	LEU
1	5A	324	ARG
1	5A	367	ARG
1	5A	376	ASN
1	5A	417	ARG
2	5B	47	ASN
2	5B	76	ARG
2	5B	107	ASN
2	5B	217	ASN
2	5B	218	ARG
2	5B	298	ASN
2	5B	322	LYS
2	5B	334	ARG
3	5C	22	LEU
3	5C	68	ARG
3	5C	104	LYS
3	5C	115	ASP
3	5C	174	MET
3	5C	199	ASP
3	5C	222	LYS
3	5C	228	ASP
3	5C	232	ARG
1	6A	110	LEU
1	6A	197	ARG
1	6A	317	LEU
1	6A	324	ARG
1	6A	367	ARG
1	6A	376	ASN
1	6A	417	ARG
2	6B	47	ASN
2	6B	76	ARG
2	6B	107	ASN
2	6B	217	ASN
2	6B	218	ARG

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Mol	Chain	Res	Type
2	6B	298	ASN
2	6B	322	LYS
2	6B	334	ARG
3	6C	22	LEU
3	6C	68	ARG
3	6C	104	LYS
3	6C	115	ASP
3	6C	174	MET
3	6C	199	ASP
3	6C	222	LYS
3	6C	228	ASP
3	6C	232	ARG
1	7A	110	LEU
1	7A	197	ARG
1	7A	317	LEU
1	7A	324	ARG
1	7A	367	ARG
1	7A	376	ASN
1	7A	417	ARG
2	7B	47	ASN
2	7B	76	ARG
2	7B	107	ASN
2	7B	217	ASN
2	7B	218	ARG
2	7B	298	ASN
2	7B	322	LYS
2	7B	334	ARG
3	7C	22	LEU
3	7C	68	ARG
3	7C	104	LYS
3	7C	115	ASP
3	7C	174	MET
3	7C	199	ASP
3	7C	222	LYS
3	7C	228	ASP
3	7C	232	ARG
1	8A	110	LEU
1	8A	197	ARG
1	8A	317	LEU
1	8A	324	ARG
1	8A	367	ARG
1	8A	376	ASN

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Mol	Chain	Res	Type
1	8A	417	ARG
2	8B	47	ASN
2	8B	76	ARG
2	8B	107	ASN
2	8B	217	ASN
2	8B	218	ARG
2	8B	298	ASN
2	8B	322	LYS
2	8B	334	ARG
3	8C	22	LEU
3	8C	68	ARG
3	8C	104	LYS
3	8C	115	ASP
3	8C	174	MET
3	8C	199	ASP
3	8C	222	LYS
3	8C	228	ASP
3	8C	232	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	16	ASN
1	1A	17	GLN
1	1A	208	ASN
2	1B	15	GLN
2	1B	47	ASN
2	1B	107	ASN
2	1B	119	ASN
2	1B	196	ASN
2	1B	217	ASN
2	1B	227	ASN
2	1B	256	ASN
1	2A	16	ASN
1	2A	17	GLN
1	2A	208	ASN
2	2B	15	GLN
2	2B	47	ASN
2	2B	107	ASN
2	2B	119	ASN
2	2B	196	ASN
2	2B	217	ASN

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Mol	Chain	Res	Type
2	2B	227	ASN
2	2B	256	ASN
1	3A	16	ASN
1	3A	17	GLN
1	3A	208	ASN
2	3B	15	GLN
2	3B	47	ASN
2	3B	84	GLN
2	3B	107	ASN
2	3B	119	ASN
2	3B	196	ASN
2	3B	217	ASN
2	3B	227	ASN
2	3B	256	ASN
1	4A	16	ASN
1	4A	17	GLN
1	4A	208	ASN
2	4B	15	GLN
2	4B	47	ASN
2	4B	107	ASN
2	4B	119	ASN
2	4B	196	ASN
2	4B	217	ASN
2	4B	227	ASN
2	4B	256	ASN
1	5A	13	GLN
1	5A	16	ASN
1	5A	178	GLN
1	5A	208	ASN
1	5A	389	ASN
2	5B	15	GLN
2	5B	47	ASN
2	5B	107	ASN
2	5B	119	ASN
2	5B	196	ASN
2	5B	217	ASN
2	5B	227	ASN
1	6A	16	ASN
1	6A	17	GLN
1	6A	178	GLN
1	6A	208	ASN
1	6A	389	ASN

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Mol	Chain	Res	Type
2	6B	15	GLN
2	6B	47	ASN
2	6B	107	ASN
2	6B	119	ASN
2	6B	196	ASN
2	6B	217	ASN
2	6B	227	ASN
1	7A	16	ASN
1	7A	208	ASN
1	7A	389	ASN
1	7A	421	GLN
2	7B	15	GLN
2	7B	47	ASN
2	7B	84	GLN
2	7B	107	ASN
2	7B	119	ASN
2	7B	196	ASN
2	7B	217	ASN
2	7B	227	ASN
1	8A	16	ASN
1	8A	208	ASN
1	8A	389	ASN
1	8A	421	GLN
2	8B	15	GLN
2	8B	47	ASN
2	8B	107	ASN
2	8B	119	ASN
2	8B	196	ASN
2	8B	217	ASN
2	8B	227	ASN
3	8C	36	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GDP	1A	501	-	24,30,30	1.13	0	30,47,47	1.38	4 (13%)
4	GDP	1B	501	-	24,30,30	1.25	3 (12%)	30,47,47	1.55	4 (13%)
4	GDP	2A	501	-	24,30,30	1.13	0	30,47,47	1.38	4 (13%)
4	GDP	3A	501	-	24,30,30	1.13	0	30,47,47	1.38	4 (13%)
4	GDP	3B	501	-	24,30,30	1.25	3 (12%)	30,47,47	1.55	4 (13%)
4	GDP	5A	501	-	24,30,30	1.13	0	30,47,47	1.38	4 (13%)
4	GDP	6B	501	-	24,30,30	1.25	3 (12%)	30,47,47	1.55	4 (13%)
4	GDP	6A	501	-	24,30,30	1.13	0	30,47,47	1.38	4 (13%)
4	GDP	7A	501	-	24,30,30	1.13	1 (4%)	30,47,47	1.38	4 (13%)
4	GDP	8B	501	-	24,30,30	1.26	3 (12%)	30,47,47	1.55	4 (13%)
4	GDP	4A	501	-	24,30,30	1.12	1 (4%)	30,47,47	1.38	4 (13%)
4	GDP	7B	501	-	24,30,30	1.25	3 (12%)	30,47,47	1.55	4 (13%)
4	GDP	5B	501	-	24,30,30	1.25	3 (12%)	30,47,47	1.55	4 (13%)
4	GDP	4B	501	-	24,30,30	1.26	3 (12%)	30,47,47	1.55	4 (13%)
4	GDP	2B	501	-	24,30,30	1.25	3 (12%)	30,47,47	1.55	4 (13%)
4	GDP	8A	501	-	24,30,30	1.13	1 (4%)	30,47,47	1.38	4 (13%)

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
4	GDP	1A	501	-	-	5/12/32/32	0/3/3/3
4	GDP	1B	501	-	-	3/12/32/32	0/3/3/3
4	GDP	2A	501	-	-	5/12/32/32	0/3/3/3
4	GDP	3A	501	-	-	5/12/32/32	0/3/3/3
4	GDP	3B	501	-	-	3/12/32/32	0/3/3/3
4	GDP	5A	501	-	-	5/12/32/32	0/3/3/3
4	GDP	6B	501	-	-	3/12/32/32	0/3/3/3
4	GDP	6A	501	-	-	5/12/32/32	0/3/3/3
4	GDP	7A	501	-	-	5/12/32/32	0/3/3/3
4	GDP	8B	501	-	-	3/12/32/32	0/3/3/3
4	GDP	4A	501	-	-	5/12/32/32	0/3/3/3
4	GDP	7B	501	-	-	3/12/32/32	0/3/3/3
4	GDP	5B	501	-	-	3/12/32/32	0/3/3/3
4	GDP	4B	501	-	-	3/12/32/32	0/3/3/3
4	GDP	2B	501	-	-	3/12/32/32	0/3/3/3
4	GDP	8A	501	-	-	5/12/32/32	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	8B	501	GDP	O4'-C1'	2.55	1.44	1.41
4	4B	501	GDP	O4'-C1'	2.53	1.44	1.41
4	7B	501	GDP	O4'-C1'	2.51	1.44	1.41
4	2B	501	GDP	O4'-C1'	2.49	1.44	1.41
4	3B	501	GDP	O4'-C1'	2.49	1.44	1.41
4	6B	501	GDP	O4'-C1'	2.48	1.44	1.41
4	1B	501	GDP	O4'-C1'	2.46	1.44	1.41
4	2B	501	GDP	C6-N1	-2.45	1.34	1.37
4	6B	501	GDP	C6-N1	-2.45	1.34	1.37
4	8B	501	GDP	C6-N1	-2.44	1.34	1.37
4	4B	501	GDP	C6-N1	-2.44	1.34	1.37
4	3B	501	GDP	C6-N1	-2.43	1.34	1.37
4	1B	501	GDP	C6-N1	-2.43	1.34	1.37
4	5B	501	GDP	C6-N1	-2.42	1.34	1.37
4	7B	501	GDP	C6-N1	-2.42	1.34	1.37
4	5B	501	GDP	O4'-C1'	2.42	1.44	1.41
4	5B	501	GDP	C5-C4	2.41	1.49	1.43
4	1B	501	GDP	C5-C4	2.41	1.49	1.43
4	7B	501	GDP	C5-C4	2.39	1.49	1.43
4	6B	501	GDP	C5-C4	2.38	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3B	501	GDP	C5-C4	2.38	1.49	1.43
4	4B	501	GDP	C5-C4	2.37	1.49	1.43
4	2B	501	GDP	C5-C4	2.37	1.49	1.43
4	8B	501	GDP	C5-C4	2.36	1.49	1.43
4	8A	501	GDP	C6-N1	-2.03	1.34	1.37
4	4A	501	GDP	C6-N1	-2.03	1.34	1.37
4	7A	501	GDP	C6-N1	-2.03	1.34	1.37

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	8B	501	GDP	PA-O3A-PB	-4.31	118.02	132.83
4	4B	501	GDP	PA-O3A-PB	-4.31	118.04	132.83
4	2B	501	GDP	PA-O3A-PB	-4.31	118.04	132.83
4	7B	501	GDP	PA-O3A-PB	-4.31	118.05	132.83
4	6B	501	GDP	PA-O3A-PB	-4.31	118.05	132.83
4	3B	501	GDP	PA-O3A-PB	-4.30	118.07	132.83
4	5B	501	GDP	PA-O3A-PB	-4.30	118.07	132.83
4	1B	501	GDP	PA-O3A-PB	-4.30	118.09	132.83
4	3B	501	GDP	C3'-C2'-C1'	3.11	105.66	100.98
4	7B	501	GDP	C3'-C2'-C1'	3.11	105.66	100.98
4	8B	501	GDP	C3'-C2'-C1'	3.10	105.65	100.98
4	4B	501	GDP	C3'-C2'-C1'	3.10	105.64	100.98
4	1B	501	GDP	C3'-C2'-C1'	3.09	105.62	100.98
4	5B	501	GDP	C3'-C2'-C1'	3.08	105.62	100.98
4	6B	501	GDP	C3'-C2'-C1'	3.07	105.61	100.98
4	2B	501	GDP	C3'-C2'-C1'	3.06	105.59	100.98
4	7A	501	GDP	PA-O3A-PB	-2.76	123.36	132.83
4	5A	501	GDP	PA-O3A-PB	-2.76	123.37	132.83
4	4A	501	GDP	PA-O3A-PB	-2.75	123.37	132.83
4	8A	501	GDP	PA-O3A-PB	-2.75	123.38	132.83
4	1A	501	GDP	PA-O3A-PB	-2.75	123.38	132.83
4	6A	501	GDP	PA-O3A-PB	-2.75	123.38	132.83
4	3A	501	GDP	PA-O3A-PB	-2.75	123.38	132.83
4	2A	501	GDP	PA-O3A-PB	-2.75	123.39	132.83
4	8A	501	GDP	C3'-C2'-C1'	2.64	104.95	100.98
4	4A	501	GDP	C3'-C2'-C1'	2.63	104.94	100.98
4	1A	501	GDP	C3'-C2'-C1'	2.63	104.94	100.98
4	6A	501	GDP	C3'-C2'-C1'	2.63	104.94	100.98
4	2A	501	GDP	C3'-C2'-C1'	2.63	104.94	100.98
4	5A	501	GDP	C3'-C2'-C1'	2.61	104.91	100.98
4	3A	501	GDP	C3'-C2'-C1'	2.61	104.90	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	7A	501	GDP	C3'-C2'-C1'	2.59	104.88	100.98
4	7A	501	GDP	C2'-C3'-C4'	2.46	107.42	102.64
4	1A	501	GDP	C2'-C3'-C4'	2.45	107.41	102.64
4	5A	501	GDP	C2'-C3'-C4'	2.45	107.40	102.64
4	3A	501	GDP	C2'-C3'-C4'	2.45	107.40	102.64
4	2A	501	GDP	C2'-C3'-C4'	2.43	107.36	102.64
4	6A	501	GDP	C2'-C3'-C4'	2.43	107.36	102.64
4	4A	501	GDP	C2'-C3'-C4'	2.42	107.34	102.64
4	8A	501	GDP	C2'-C3'-C4'	2.42	107.34	102.64
4	6B	501	GDP	O6-C6-C5	-2.32	119.84	124.37
4	2B	501	GDP	O6-C6-C5	-2.32	119.84	124.37
4	5B	501	GDP	O6-C6-C5	-2.32	119.85	124.37
4	3B	501	GDP	C5-C6-N1	2.32	118.04	113.95
4	1B	501	GDP	O6-C6-C5	-2.31	119.86	124.37
4	4B	501	GDP	C5-C6-N1	2.31	118.03	113.95
4	1B	501	GDP	C5-C6-N1	2.31	118.03	113.95
4	8B	501	GDP	C5-C6-N1	2.31	118.03	113.95
4	8B	501	GDP	O6-C6-C5	-2.30	119.87	124.37
4	5B	501	GDP	C5-C6-N1	2.30	118.02	113.95
4	4B	501	GDP	O6-C6-C5	-2.30	119.88	124.37
4	7B	501	GDP	C5-C6-N1	2.30	118.01	113.95
4	3B	501	GDP	O6-C6-C5	-2.30	119.89	124.37
4	7B	501	GDP	O6-C6-C5	-2.29	119.89	124.37
4	6B	501	GDP	C5-C6-N1	2.28	117.98	113.95
4	2B	501	GDP	C5-C6-N1	2.28	117.98	113.95
4	3A	501	GDP	O3B-PB-O2B	2.08	115.59	107.64
4	7A	501	GDP	O3B-PB-O2B	2.08	115.59	107.64
4	1A	501	GDP	O3B-PB-O2B	2.08	115.57	107.64
4	4A	501	GDP	O3B-PB-O2B	2.07	115.56	107.64
4	8A	501	GDP	O3B-PB-O2B	2.07	115.55	107.64
4	6A	501	GDP	O3B-PB-O2B	2.07	115.54	107.64
4	5A	501	GDP	O3B-PB-O2B	2.07	115.54	107.64
4	2A	501	GDP	O3B-PB-O2B	2.07	115.53	107.64

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	1A	501	GDP	C5'-O5'-PA-O2A
4	1B	501	GDP	C5'-O5'-PA-O1A
4	1B	501	GDP	C5'-O5'-PA-O2A
4	2A	501	GDP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
4	2B	501	GDP	C5'-O5'-PA-O1A
4	2B	501	GDP	C5'-O5'-PA-O2A
4	3A	501	GDP	C5'-O5'-PA-O2A
4	3B	501	GDP	C5'-O5'-PA-O1A
4	3B	501	GDP	C5'-O5'-PA-O2A
4	4A	501	GDP	C5'-O5'-PA-O2A
4	4B	501	GDP	C5'-O5'-PA-O1A
4	4B	501	GDP	C5'-O5'-PA-O2A
4	5A	501	GDP	C5'-O5'-PA-O2A
4	5B	501	GDP	C5'-O5'-PA-O1A
4	5B	501	GDP	C5'-O5'-PA-O2A
4	6A	501	GDP	C5'-O5'-PA-O2A
4	6B	501	GDP	C5'-O5'-PA-O1A
4	6B	501	GDP	C5'-O5'-PA-O2A
4	7A	501	GDP	C5'-O5'-PA-O2A
4	7B	501	GDP	C5'-O5'-PA-O1A
4	7B	501	GDP	C5'-O5'-PA-O2A
4	8A	501	GDP	C5'-O5'-PA-O2A
4	8B	501	GDP	C5'-O5'-PA-O1A
4	8B	501	GDP	C5'-O5'-PA-O2A
4	1A	501	GDP	C5'-O5'-PA-O3A
4	2A	501	GDP	C5'-O5'-PA-O3A
4	3A	501	GDP	C5'-O5'-PA-O3A
4	4A	501	GDP	C5'-O5'-PA-O3A
4	5A	501	GDP	C5'-O5'-PA-O3A
4	6A	501	GDP	C5'-O5'-PA-O3A
4	7A	501	GDP	C5'-O5'-PA-O3A
4	8A	501	GDP	C5'-O5'-PA-O3A
4	1A	501	GDP	C5'-O5'-PA-O1A
4	2A	501	GDP	C5'-O5'-PA-O1A
4	3A	501	GDP	C5'-O5'-PA-O1A
4	4A	501	GDP	C5'-O5'-PA-O1A
4	5A	501	GDP	C5'-O5'-PA-O1A
4	6A	501	GDP	C5'-O5'-PA-O1A
4	7A	501	GDP	C5'-O5'-PA-O1A
4	8A	501	GDP	C5'-O5'-PA-O1A
4	1A	501	GDP	O4'-C4'-C5'-O5'
4	2A	501	GDP	O4'-C4'-C5'-O5'
4	4A	501	GDP	O4'-C4'-C5'-O5'
4	5A	501	GDP	O4'-C4'-C5'-O5'
4	6A	501	GDP	O4'-C4'-C5'-O5'
4	8A	501	GDP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	3A	501	GDP	O4'-C4'-C5'-O5'
4	7A	501	GDP	O4'-C4'-C5'-O5'
4	1B	501	GDP	C5'-O5'-PA-O3A
4	2B	501	GDP	C5'-O5'-PA-O3A
4	3B	501	GDP	C5'-O5'-PA-O3A
4	4B	501	GDP	C5'-O5'-PA-O3A
4	5B	501	GDP	C5'-O5'-PA-O3A
4	6B	501	GDP	C5'-O5'-PA-O3A
4	7B	501	GDP	C5'-O5'-PA-O3A
4	8B	501	GDP	C5'-O5'-PA-O3A
4	1A	501	GDP	C3'-C4'-C5'-O5'
4	2A	501	GDP	C3'-C4'-C5'-O5'
4	3A	501	GDP	C3'-C4'-C5'-O5'
4	4A	501	GDP	C3'-C4'-C5'-O5'
4	5A	501	GDP	C3'-C4'-C5'-O5'
4	6A	501	GDP	C3'-C4'-C5'-O5'
4	7A	501	GDP	C3'-C4'-C5'-O5'
4	8A	501	GDP	C3'-C4'-C5'-O5'

There are no ring outliers.

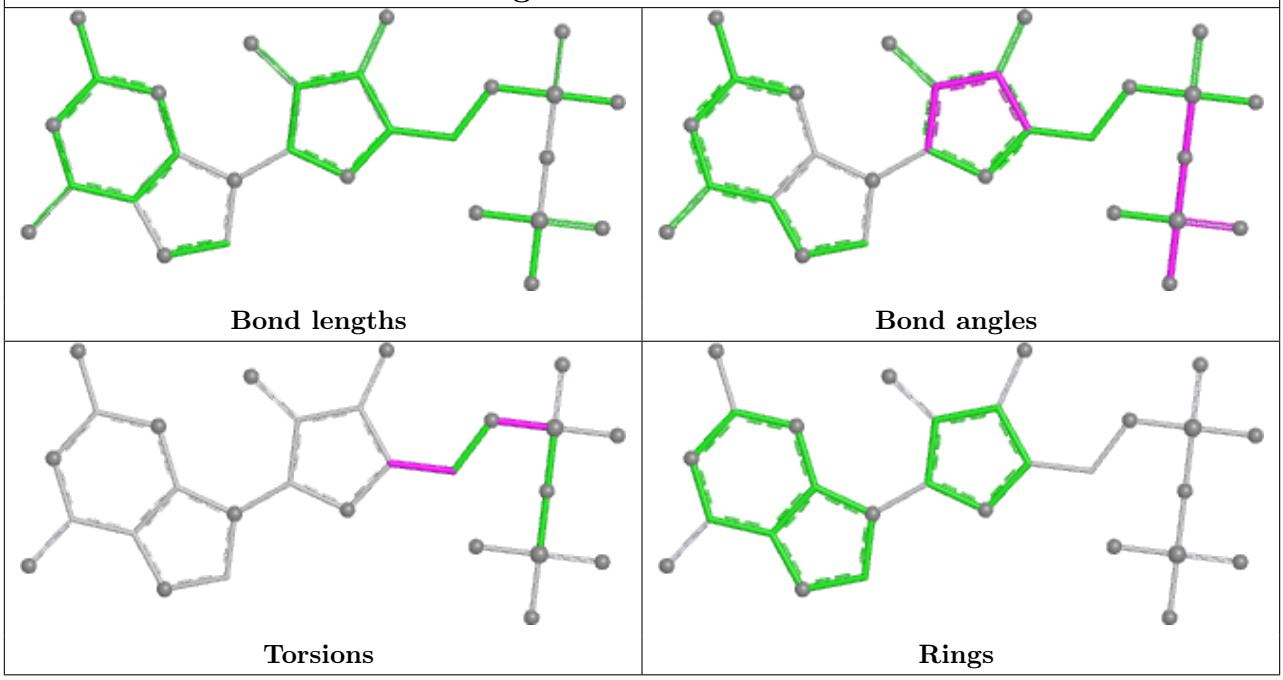
16 monomers are involved in 52 short contacts:

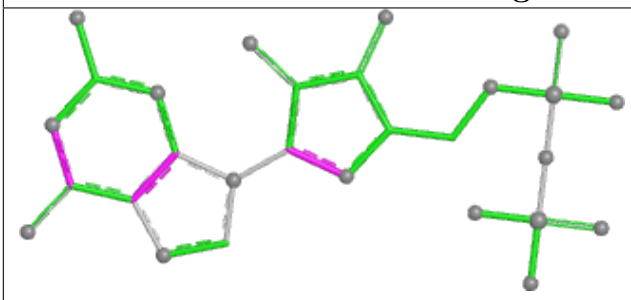
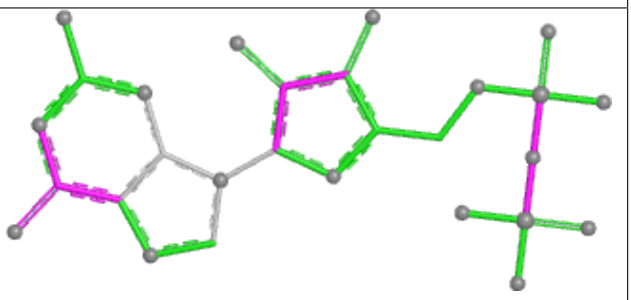
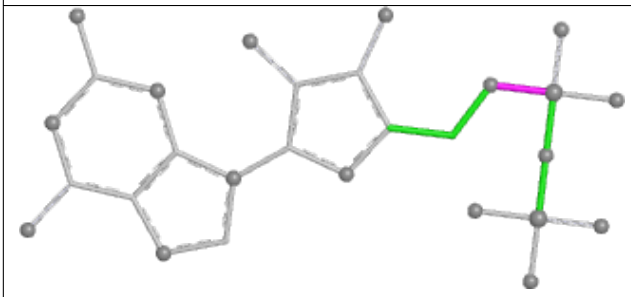
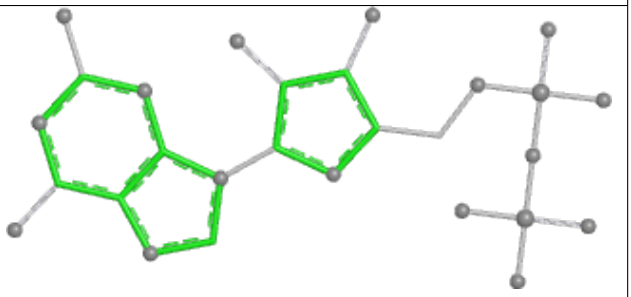
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	1A	501	GDP	2	0
4	1B	501	GDP	3	0
4	2A	501	GDP	2	0
4	3A	501	GDP	2	0
4	3B	501	GDP	3	0
4	5A	501	GDP	2	0
4	6B	501	GDP	3	0
4	6A	501	GDP	5	0
4	7A	501	GDP	7	0
4	8B	501	GDP	3	0
4	4A	501	GDP	2	0
4	7B	501	GDP	3	0
4	5B	501	GDP	3	0
4	4B	501	GDP	3	0
4	2B	501	GDP	3	0
4	8A	501	GDP	6	0

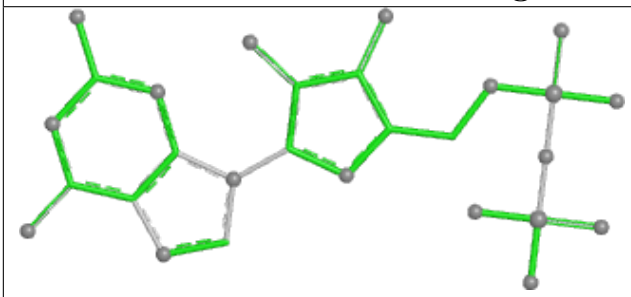
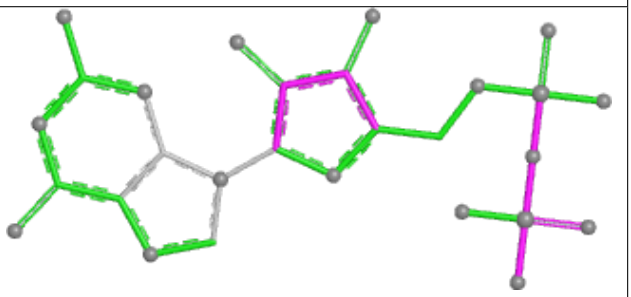
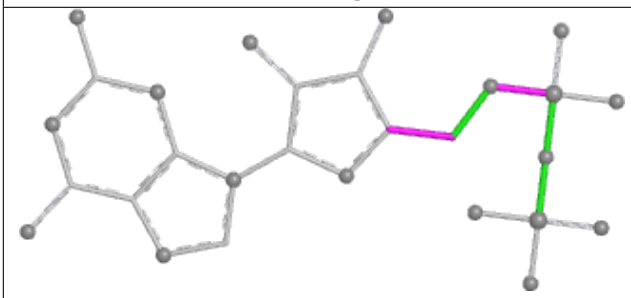
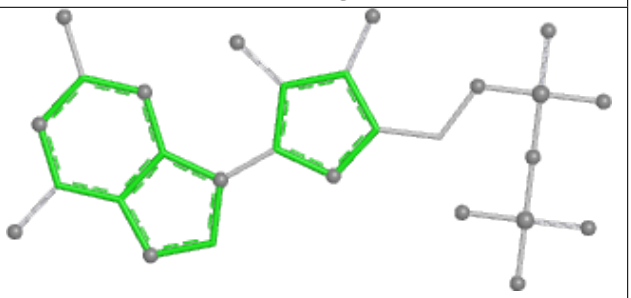
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 GDP 1A 501



Ligand GDP 1B 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP 2A 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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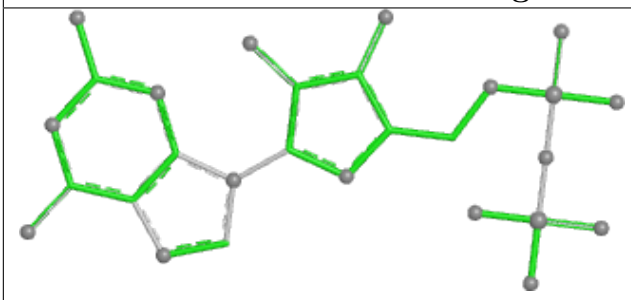
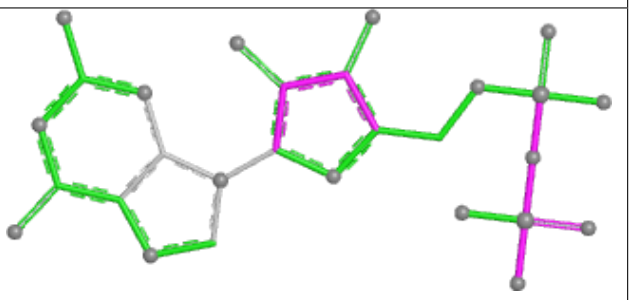
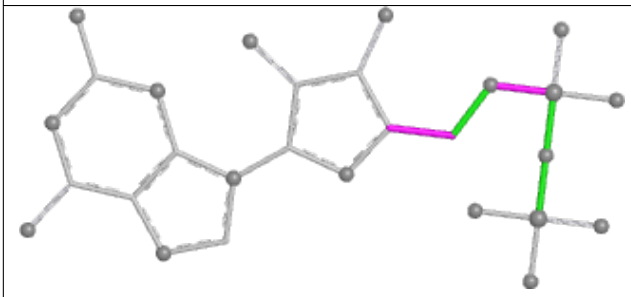
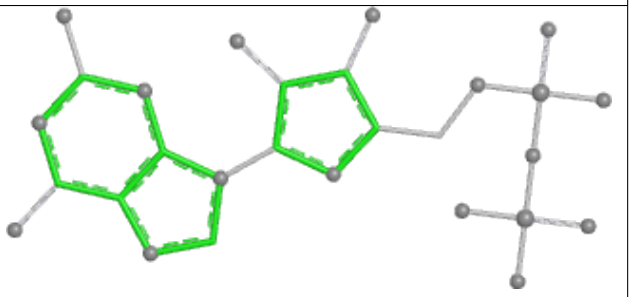
 Bond lengths	 Bond angles
 Torsions	 Rings

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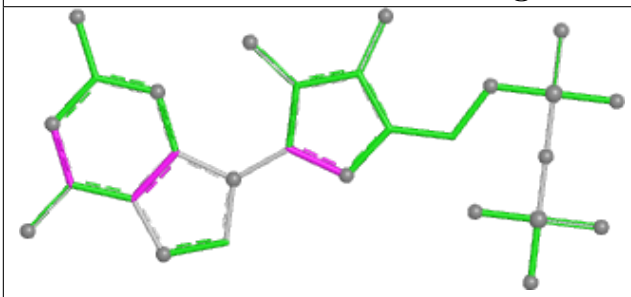
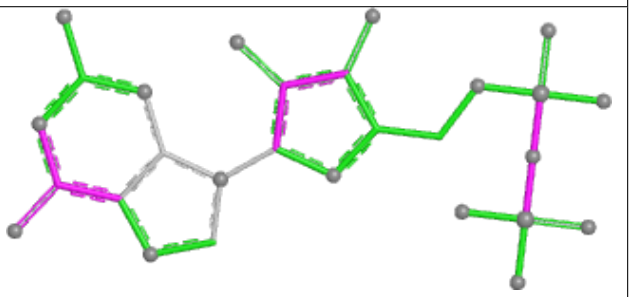
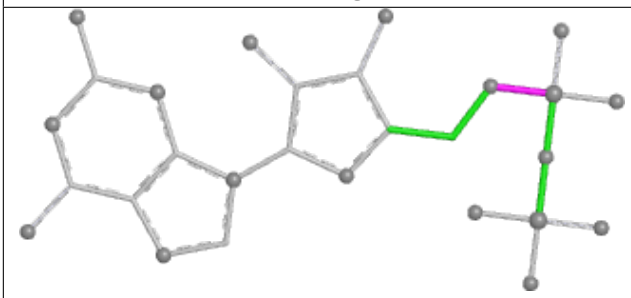
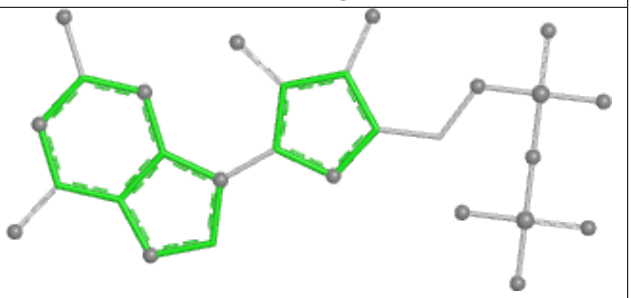
 Bond lengths	 Bond angles
 Torsions	 Rings

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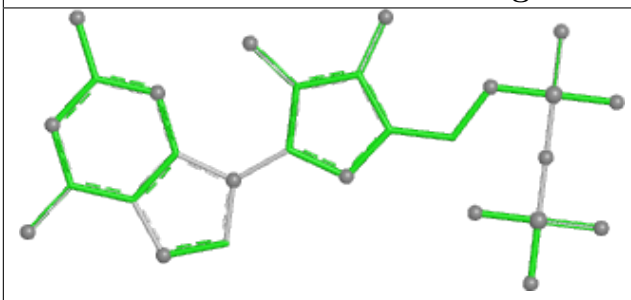
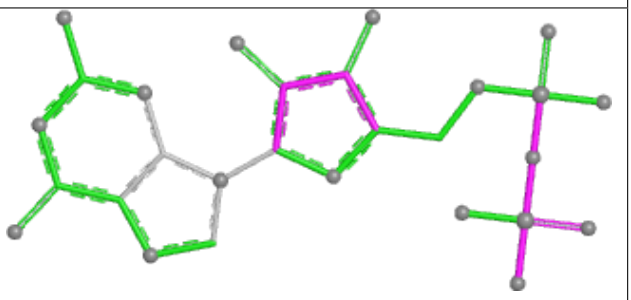
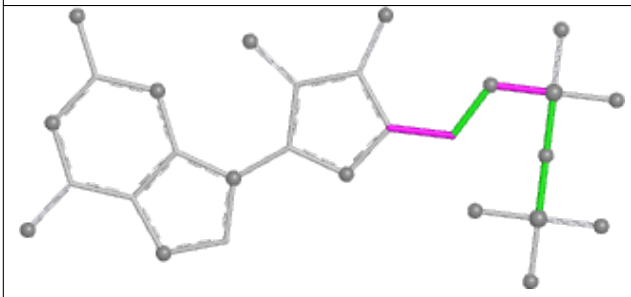
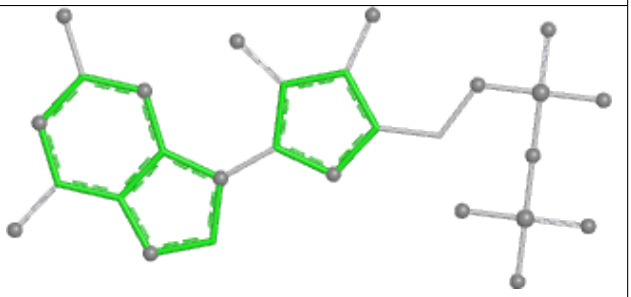
 Bond lengths	 Bond angles
 Torsions	 Rings

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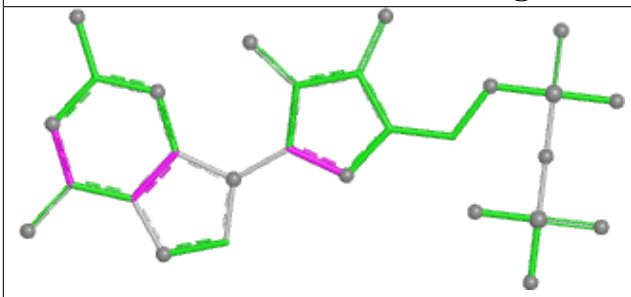
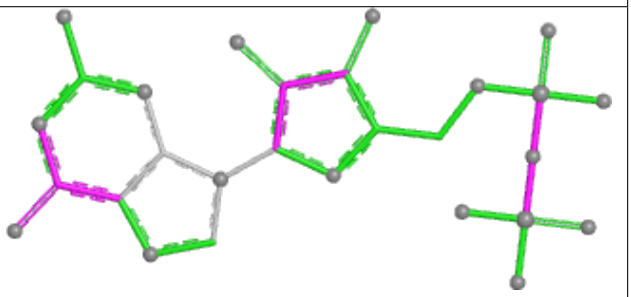
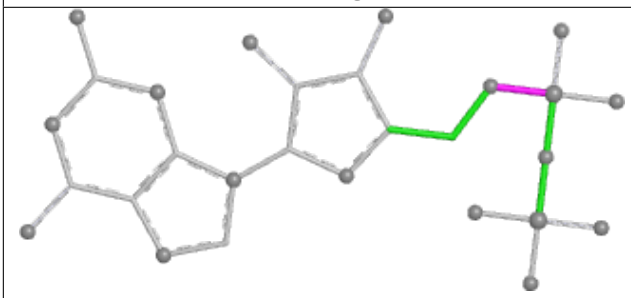
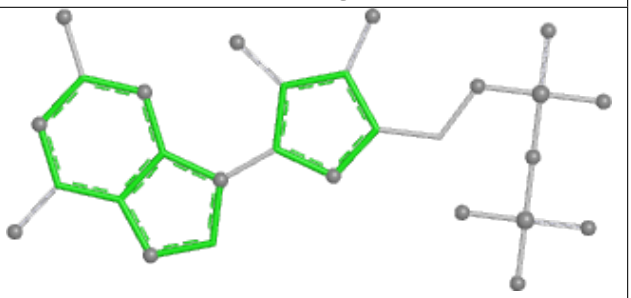
 Bond lengths	 Bond angles
 Torsions	 Rings

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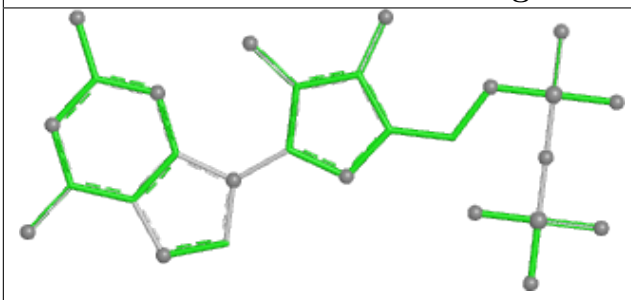
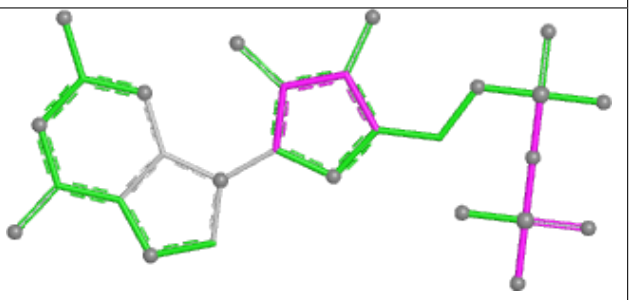
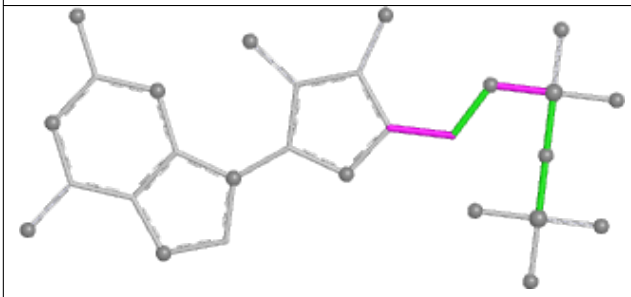
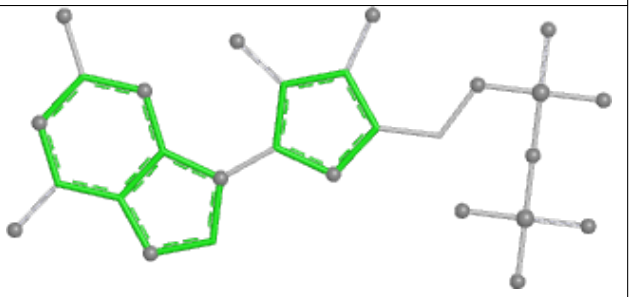
 Bond lengths	 Bond angles
 Torsions	 Rings

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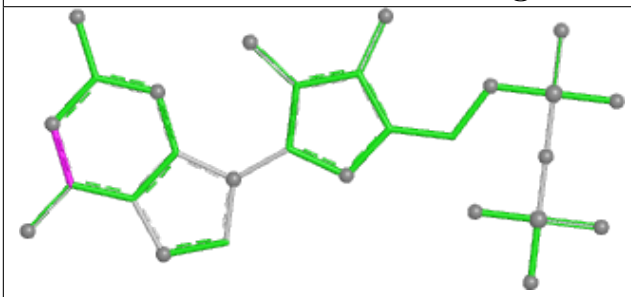
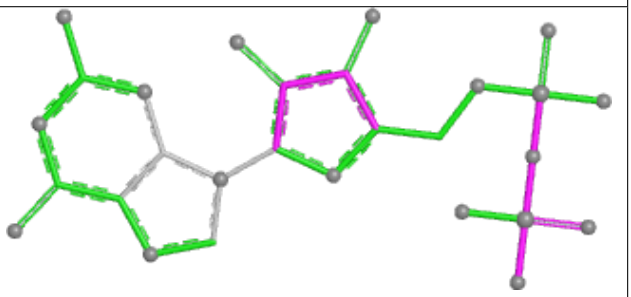
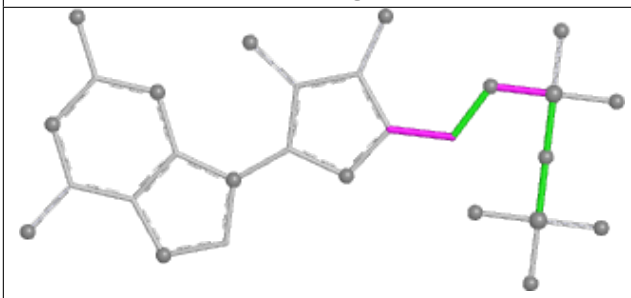
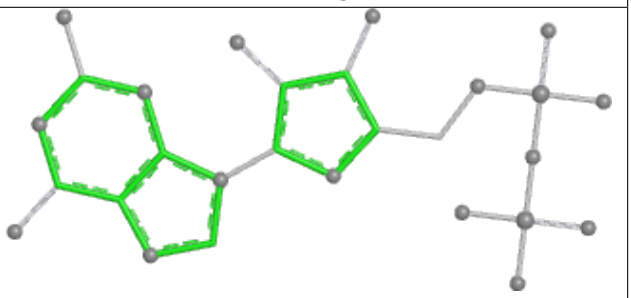
 Bond lengths	 Bond angles
 Torsions	 Rings

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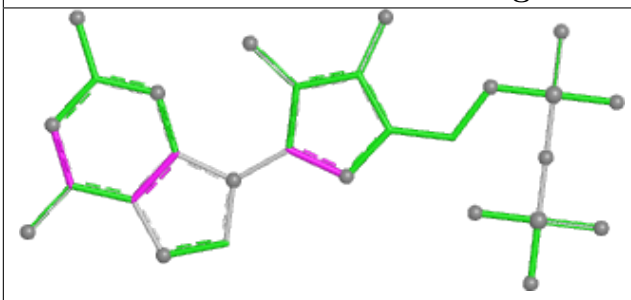

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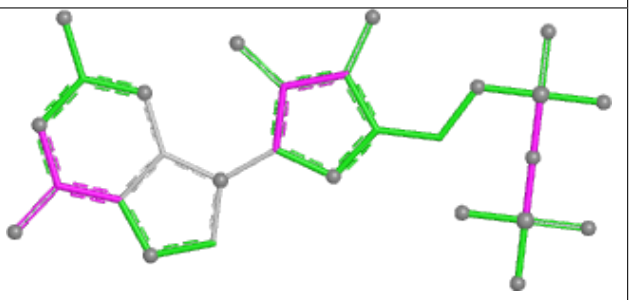

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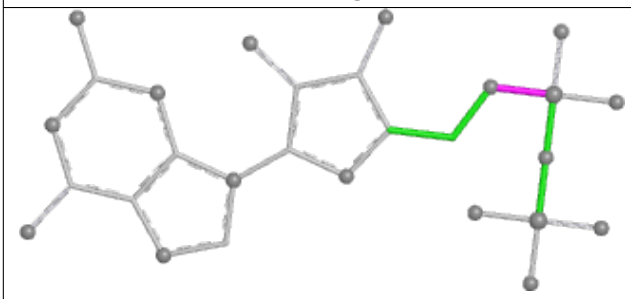

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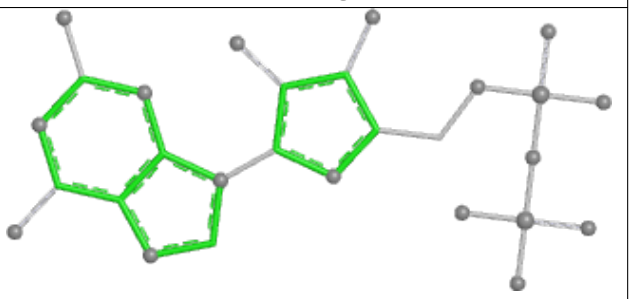

Rings

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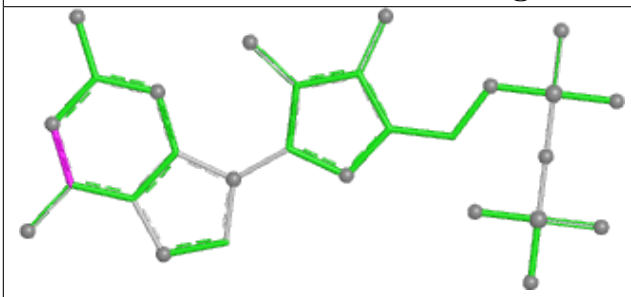

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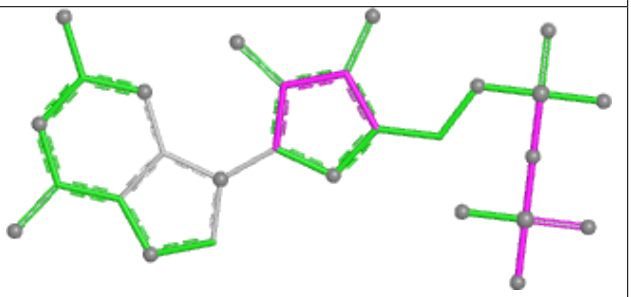

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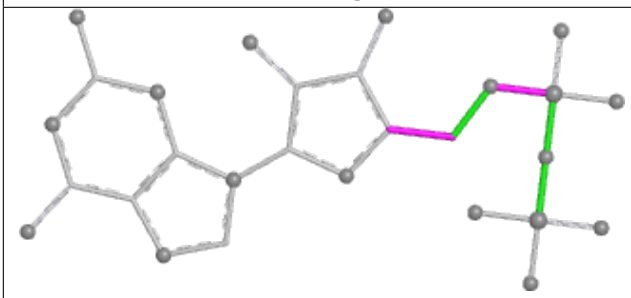

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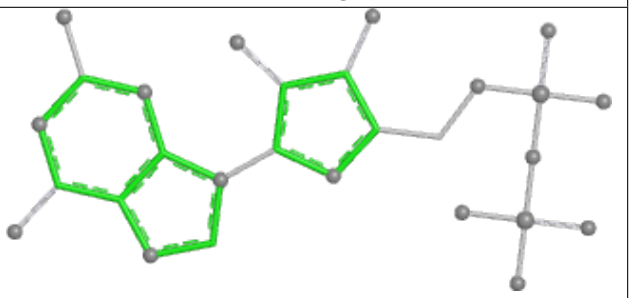

Rings

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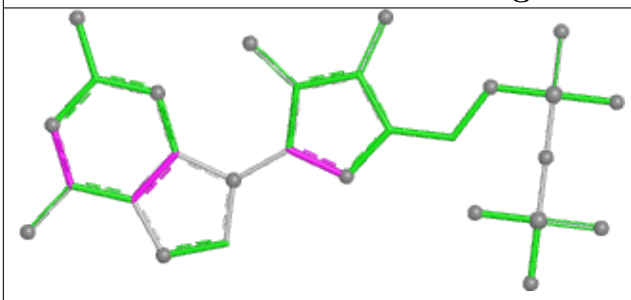
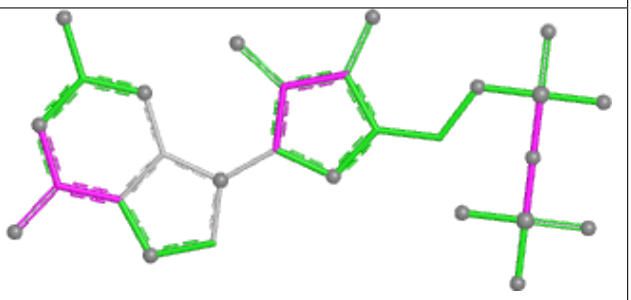
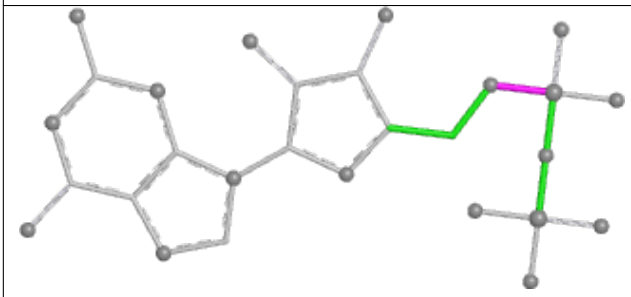
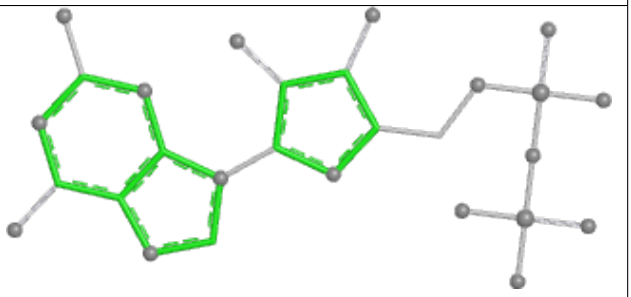
 Bond lengths	 Bond angles
 Torsions	 Rings

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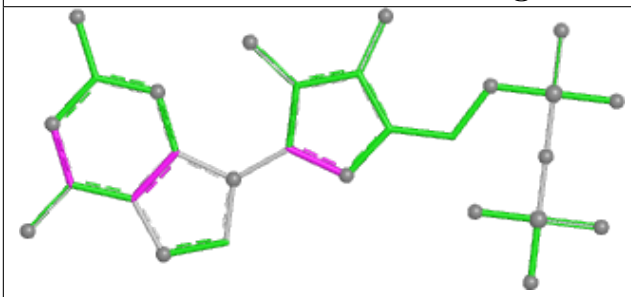
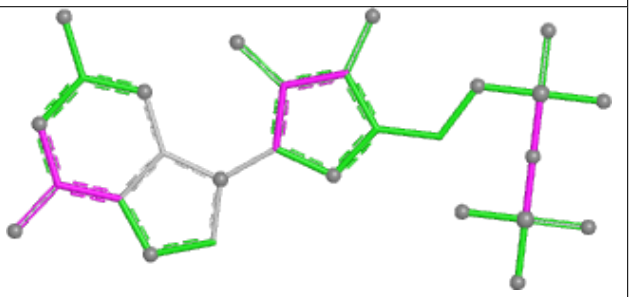
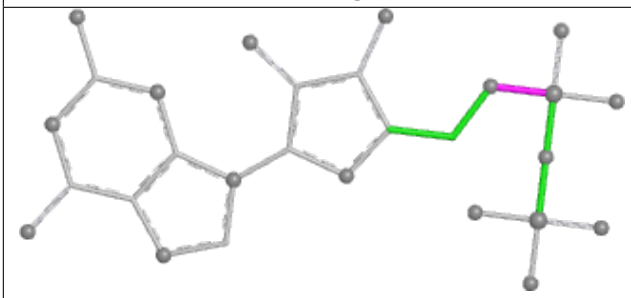
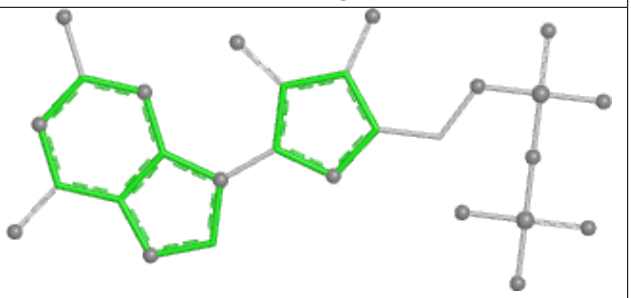
 Bond lengths	 Bond angles
 Torsions	 Rings

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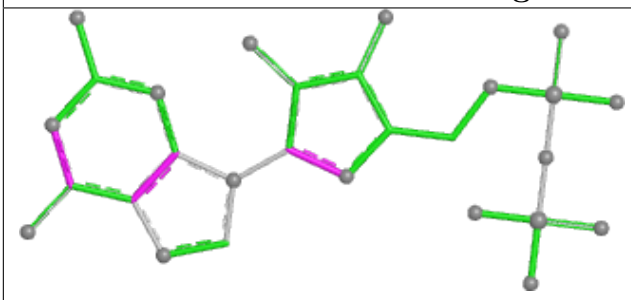
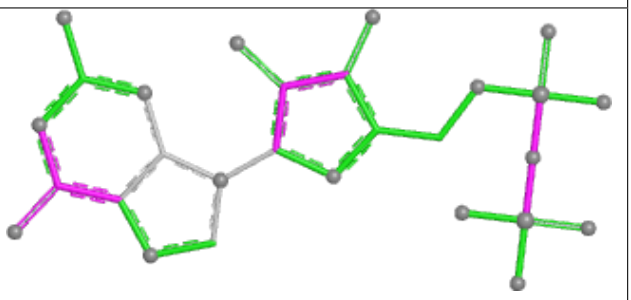
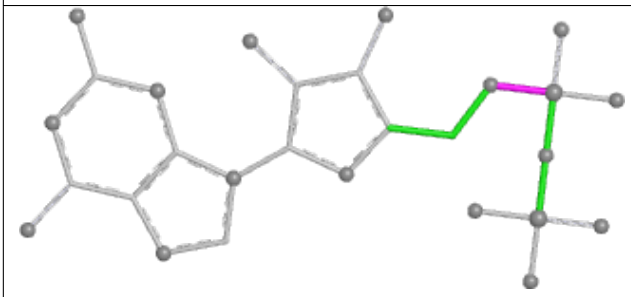
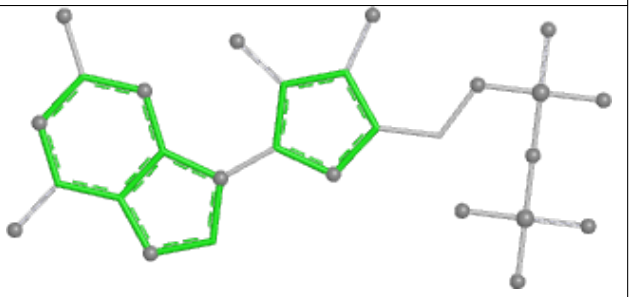
 Bond lengths	 Bond angles
 Torsions	 Rings

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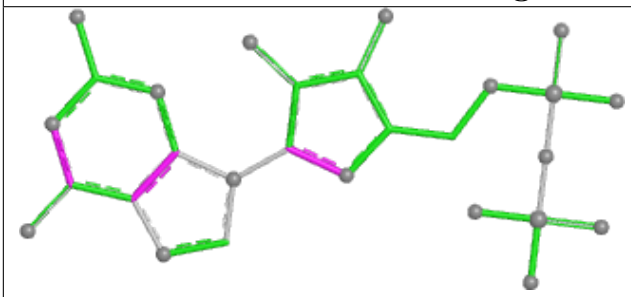
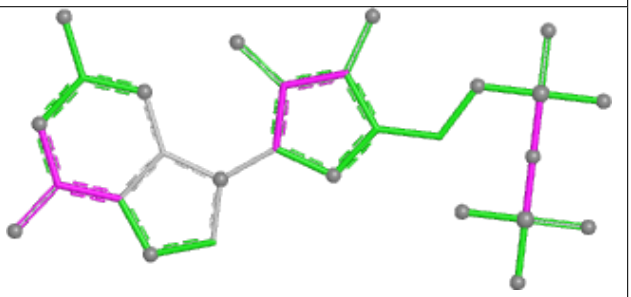
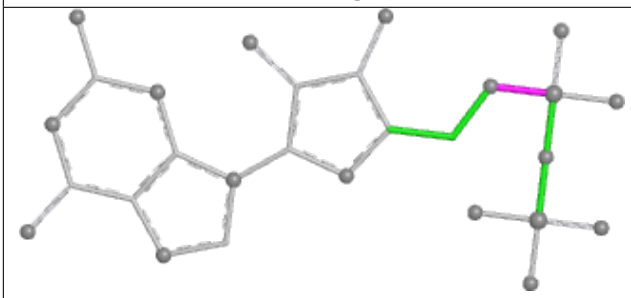
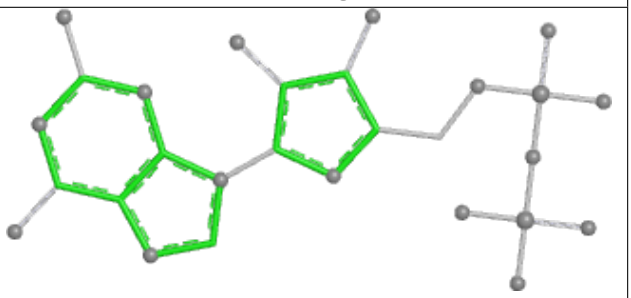
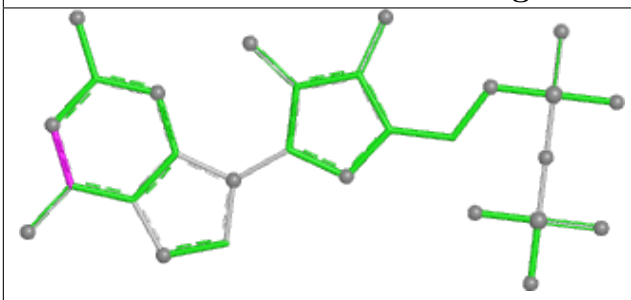
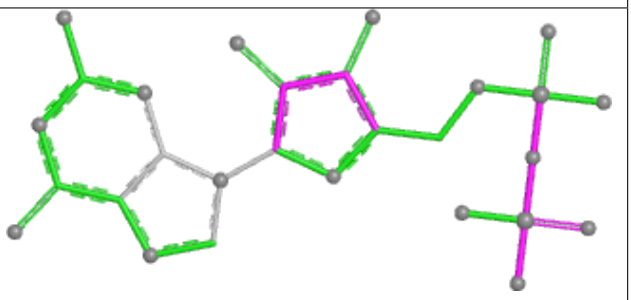
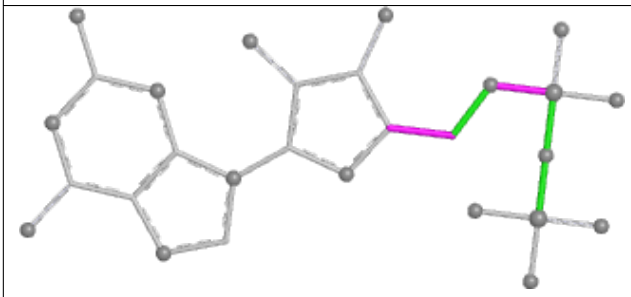
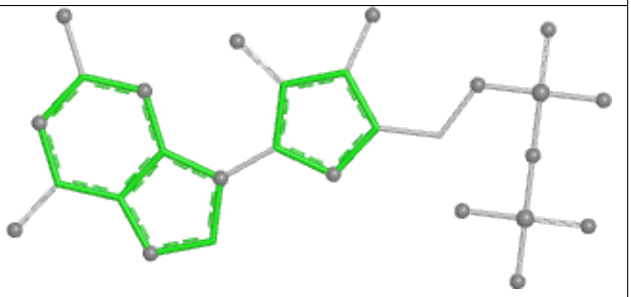
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP 8A 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

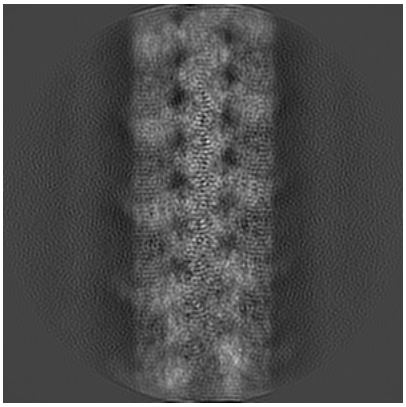
6 Map visualisation (i)

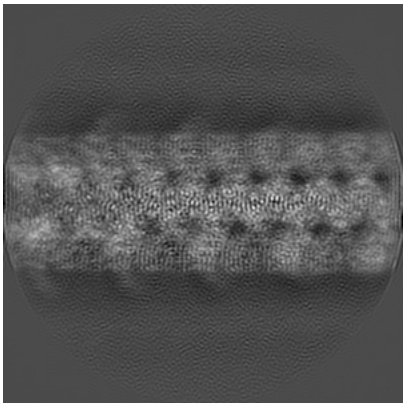
This section contains visualisations of the EMDB entry EMD-3726. These allow visual inspection of the internal detail of the map and identification of artifacts.

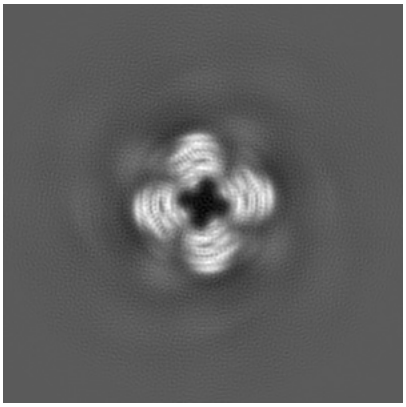
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

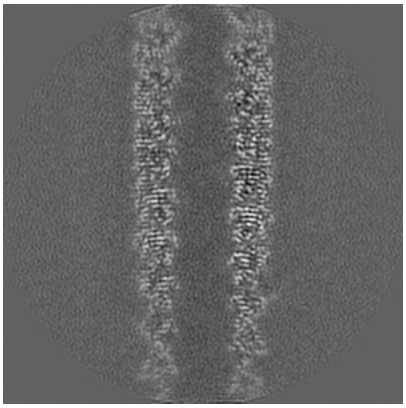

Y

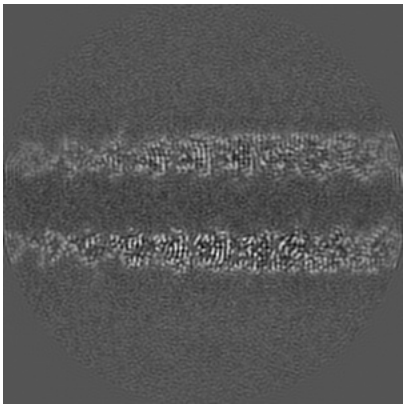

Z

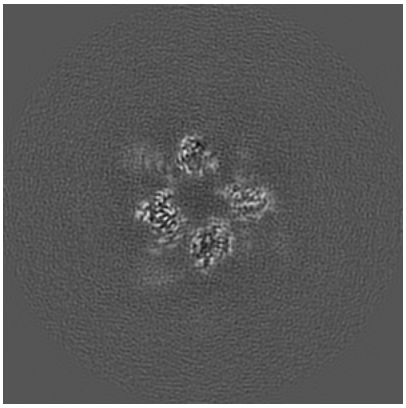
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 140

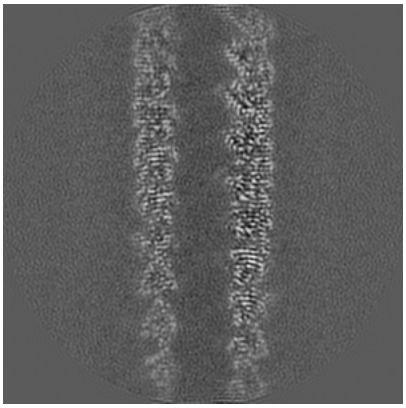

Y Index: 140


Z Index: 140

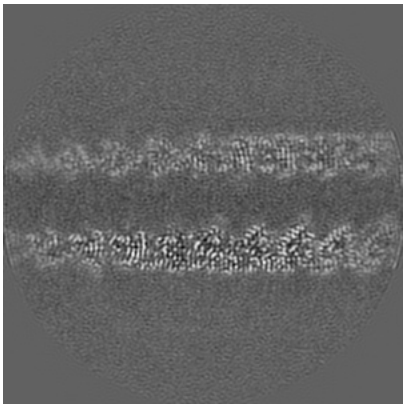
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 138



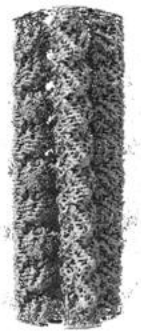
Y Index: 137

Z Index: 146

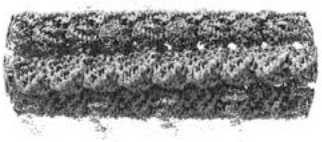
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0967. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

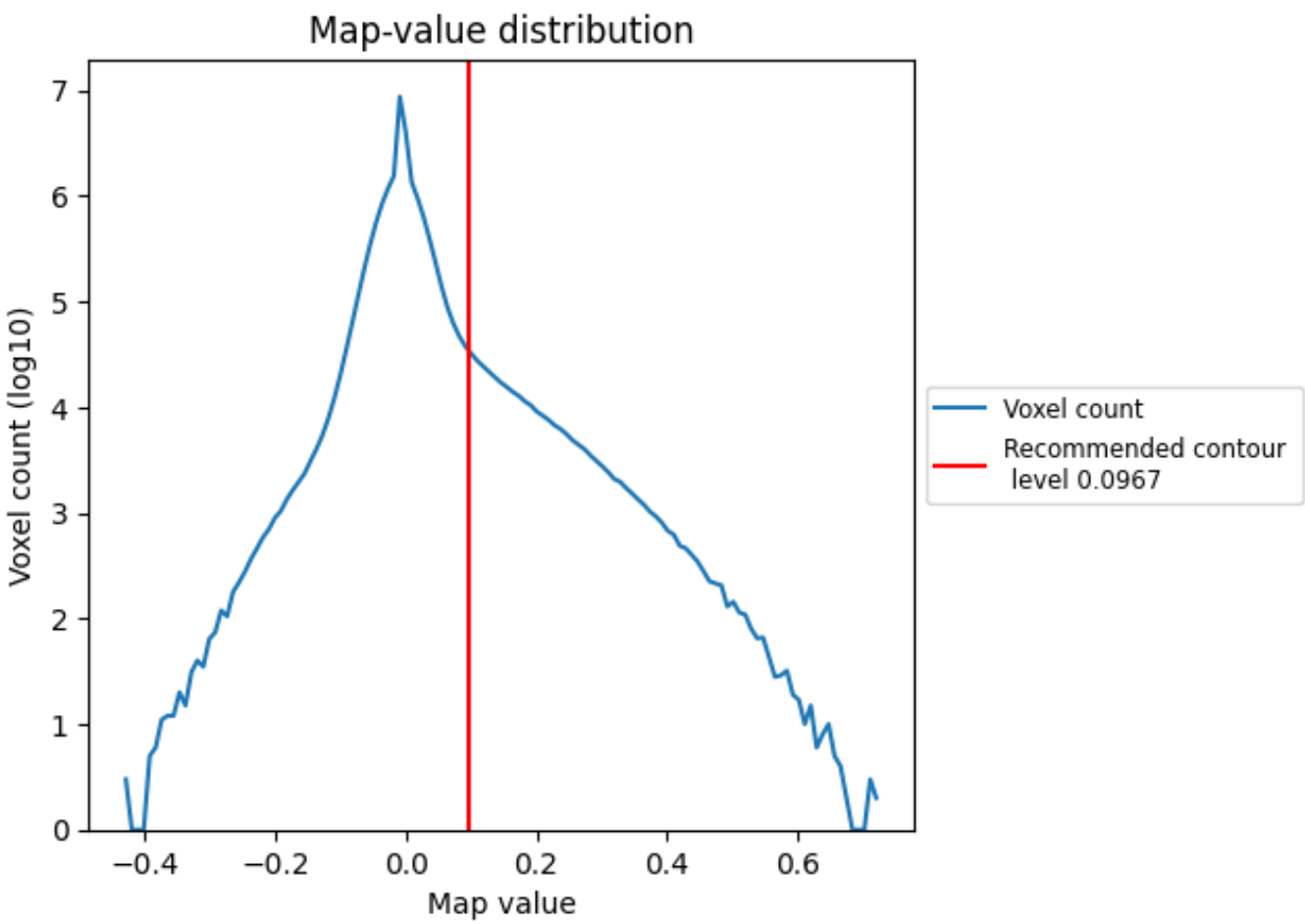
6.5 Mask visualisation (i)

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

7 Map analysis (i)

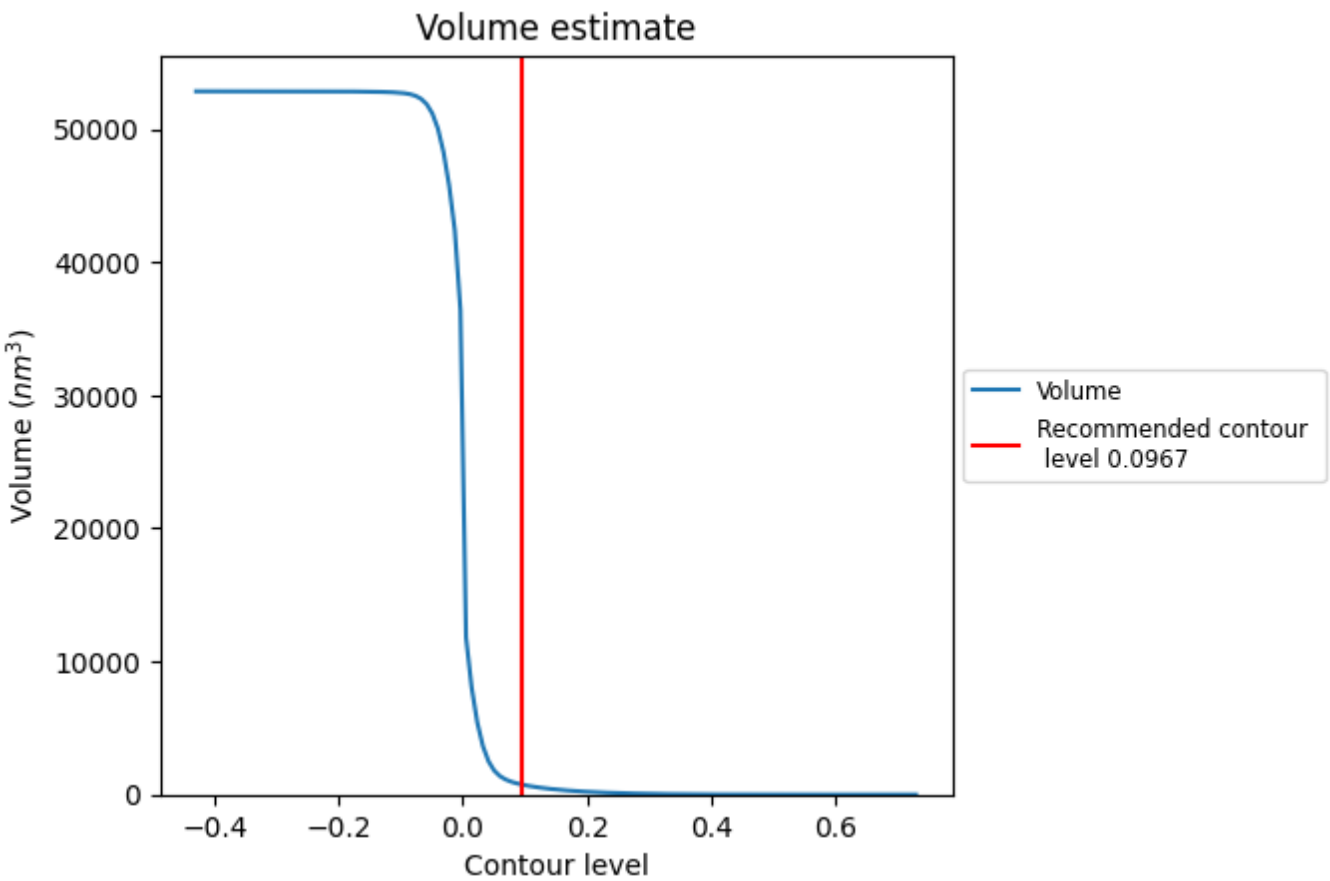
This section contains the results of statistical analysis of the map.

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.

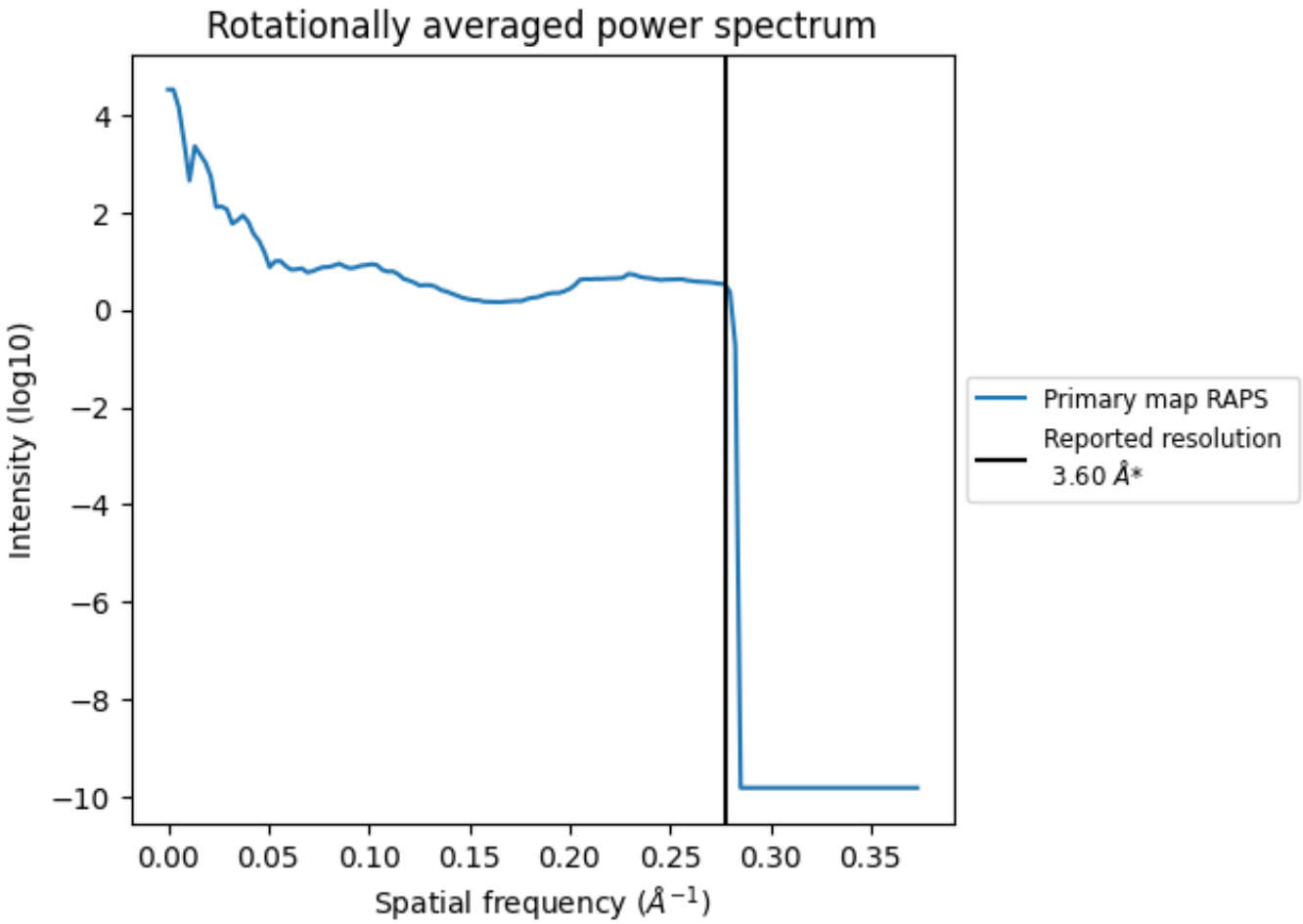
7.2 Volume estimate (i)



The volume at the recommended contour level is 737 nm^3; this corresponds to an approximate mass of 665 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)

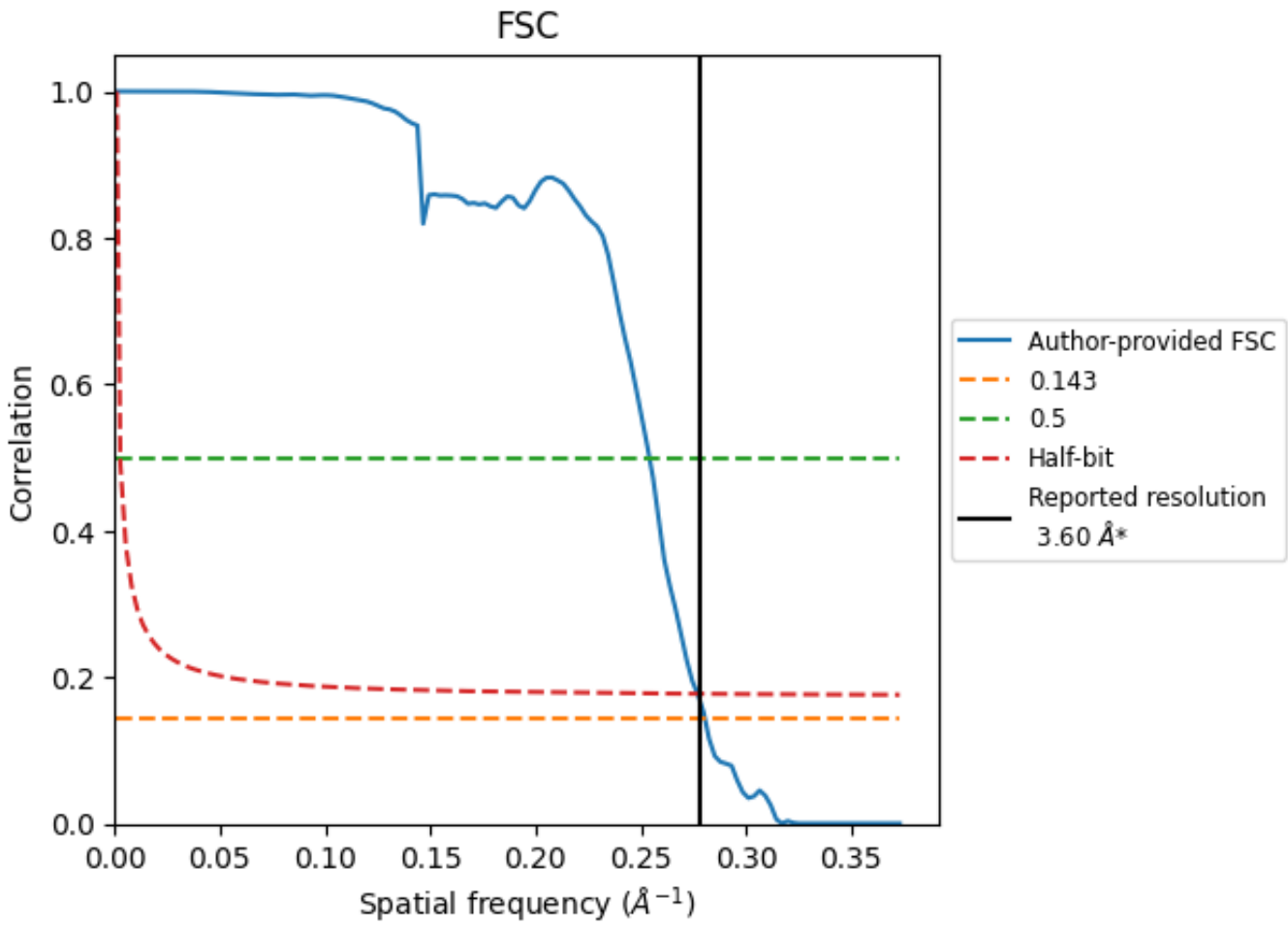


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

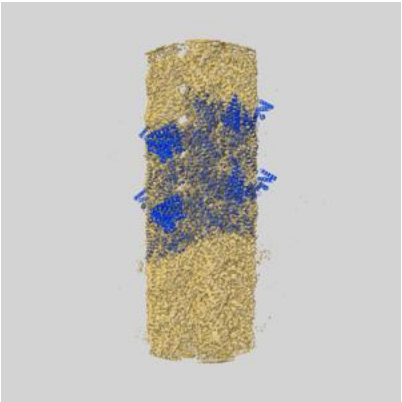
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.57	3.94	3.61
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

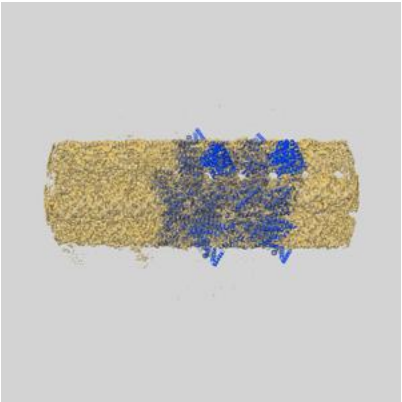
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3726 and PDB model 5O09. Per-residue inclusion information can be found in section 3 on page 7.

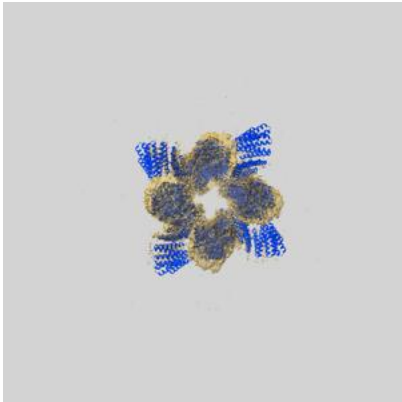
9.1 Map-model overlay (i)



X



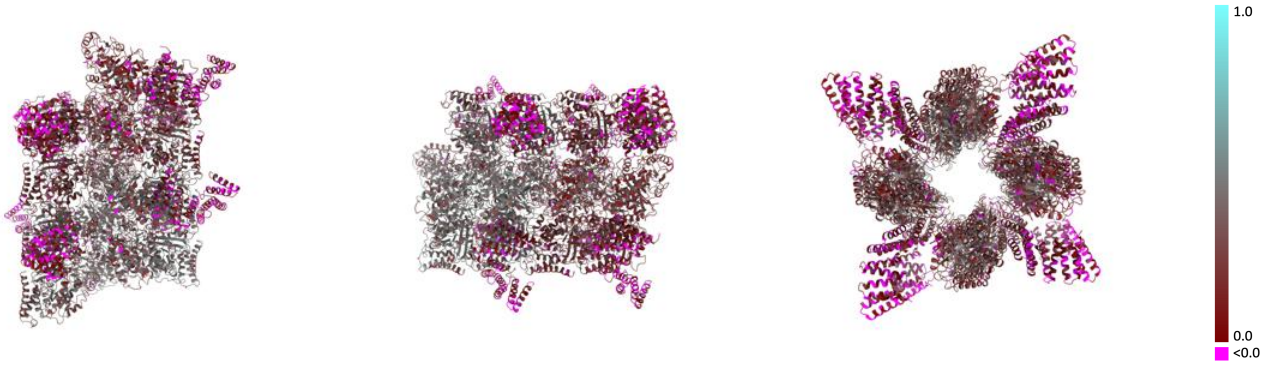
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0967 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.

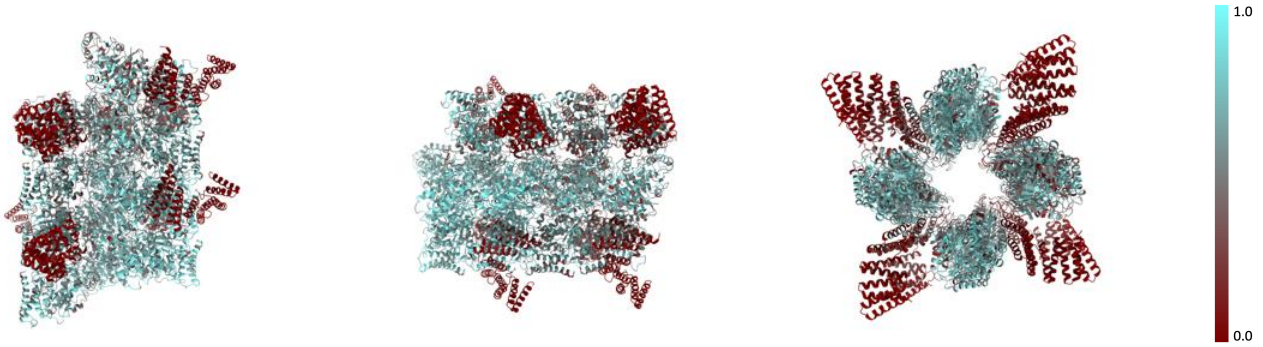
9.2 Q-score mapped to coordinate model (i)



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.

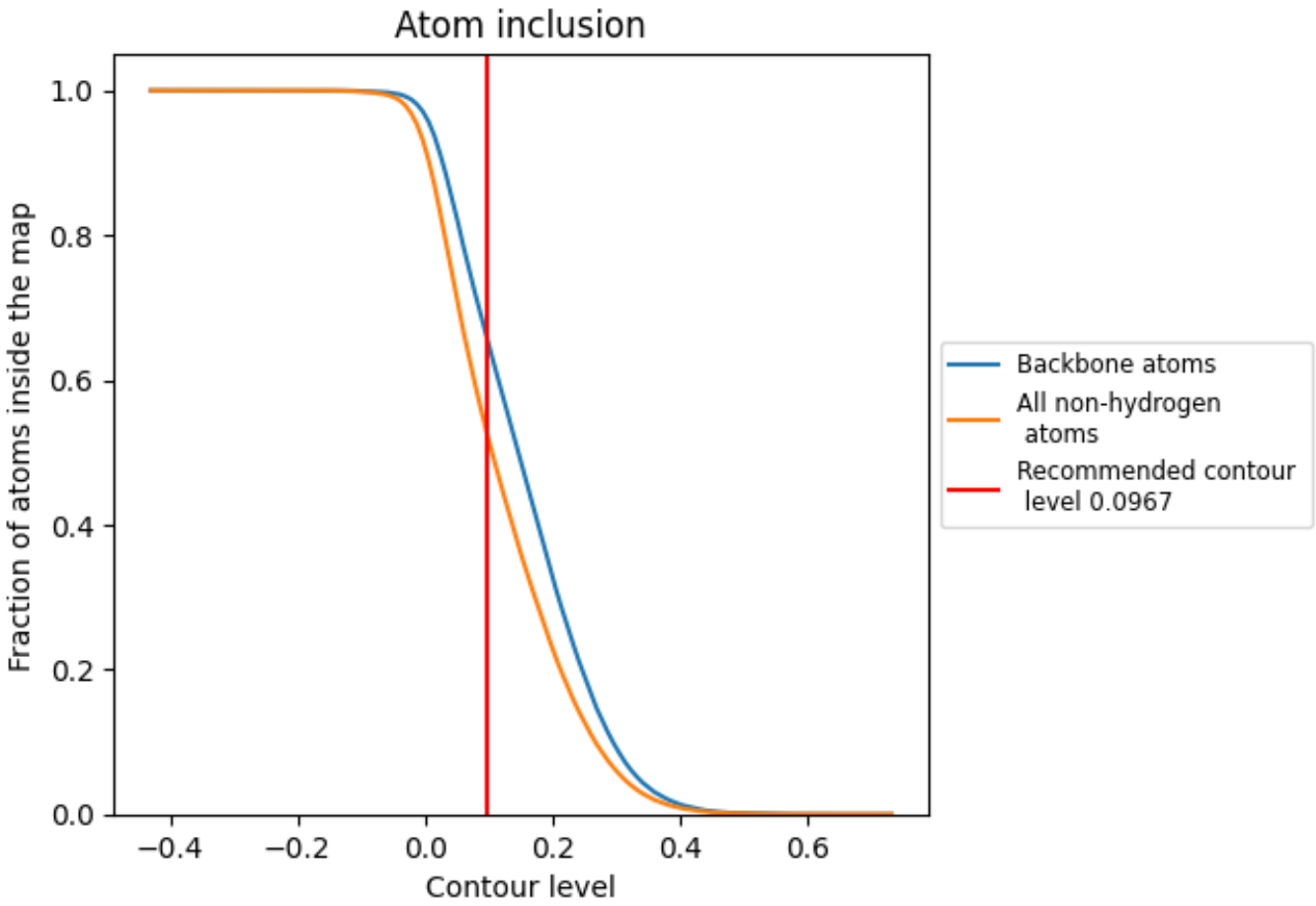
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0967).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 53% 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 (0.0967) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5266	0.2760
1A	0.7537	0.4400
1B	0.7801	0.4400
1C	0.1319	0.0990
2A	0.7284	0.4140
2B	0.7360	0.4190
2C	0.1292	0.0960
3A	0.6678	0.3810
3B	0.7035	0.3920
3C	0.0418	0.0940
4A	0.6626	0.3760
4B	0.6843	0.3820
4C	0.0337	0.0740
5A	0.6492	0.2870
5B	0.6355	0.2790
5C	0.0988	0.0710
6A	0.6306	0.2650
6B	0.6221	0.2560
6C	0.0901	0.0710
7A	0.5840	0.2570
7B	0.6214	0.2750
7C	0.0282	0.0520
8A	0.5386	0.2350
8B	0.5222	0.2360
8C	0.0152	0.0690