



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 02:17 PM UTC

PDB ID : 3FHJ / pdb_00003fhj
Title : Independent saturation of three TrpRS subsites generates a partially-assembled state similar to those observed in molecular simulations
Authors : Laowanapiban, P.; Kapustina, M.; Vonnrhein, C.; Delarue, M.; Koehl, P.; Carter Jr., C.W.
Deposited on : 2008-12-09
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

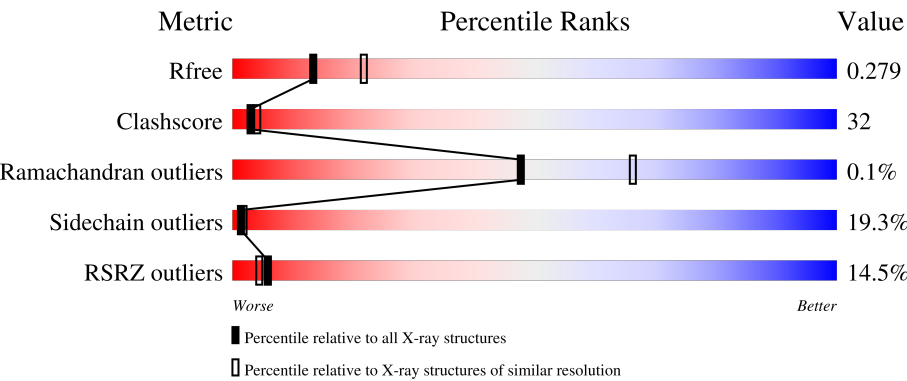
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

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



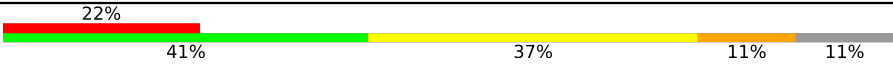
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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

Mol	Chain	Length	Quality of chain
1	A	328	5% 54% 29% 8% 9%
1	B	328	11% 45% 34% 10% 11%
1	C	328	20% 42% 33% 10% 15%
1	D	328	12% 48% 29% 10% 13%

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Mol	Chain	Length	Quality of chain
1	E	328	
1	F	328	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	1002	-	-	X	-
3	PO4	B	1002	-	-	X	-
3	PO4	D	1002	-	-	X	-
4	AMP	A	1003	-	-	-	X
4	AMP	B	1003	-	-	X	-
4	AMP	C	1003	-	-	-	X
4	AMP	D	1003	-	-	-	X
4	AMP	E	1003	-	-	X	-
4	AMP	F	1003	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14203 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

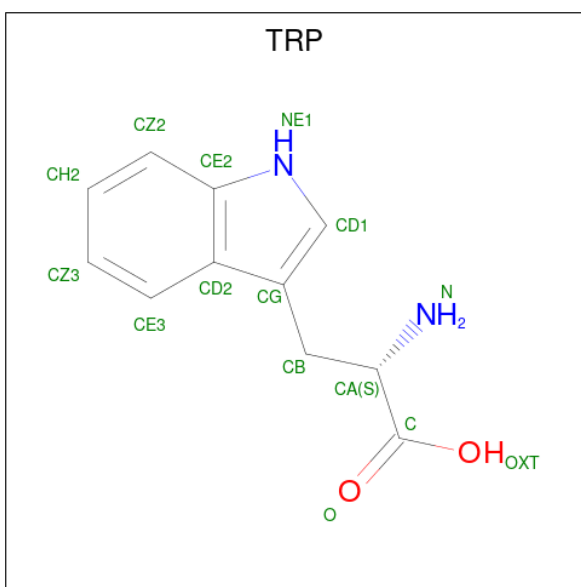
- Molecule 1 is a protein called Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2394	1520	413	448	13			
1	D	286	Total	C	N	O	S	0	0	0
			2281	1451	391	426	13			
1	B	291	Total	C	N	O	S	0	0	0
			2338	1484	401	440	13			
1	C	279	Total	C	N	O	S	0	0	0
			2225	1415	384	413	13			
1	E	292	Total	C	N	O	S	0	0	0
			2337	1485	403	436	13			
1	F	296	Total	C	N	O	S	0	0	0
			2370	1505	408	444	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	LEU	LYS	conflict	UNP P00953
D	64	LEU	LYS	conflict	UNP P00953
B	64	LEU	LYS	conflict	UNP P00953
C	64	LEU	LYS	conflict	UNP P00953
E	64	LEU	LYS	conflict	UNP P00953
F	64	LEU	LYS	conflict	UNP P00953

- Molecule 2 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



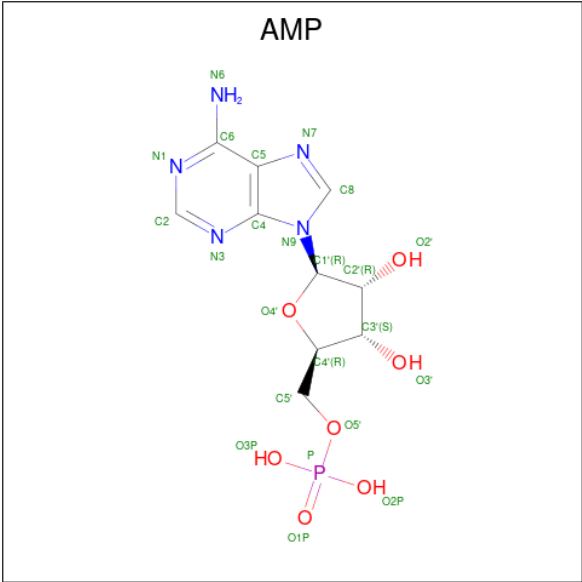
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	D	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		
2	C	1	Total	C	N	O	0	0
			15	11	2	2		
2	E	1	Total	C	N	O	0	0
			15	11	2	2		
2	F	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).

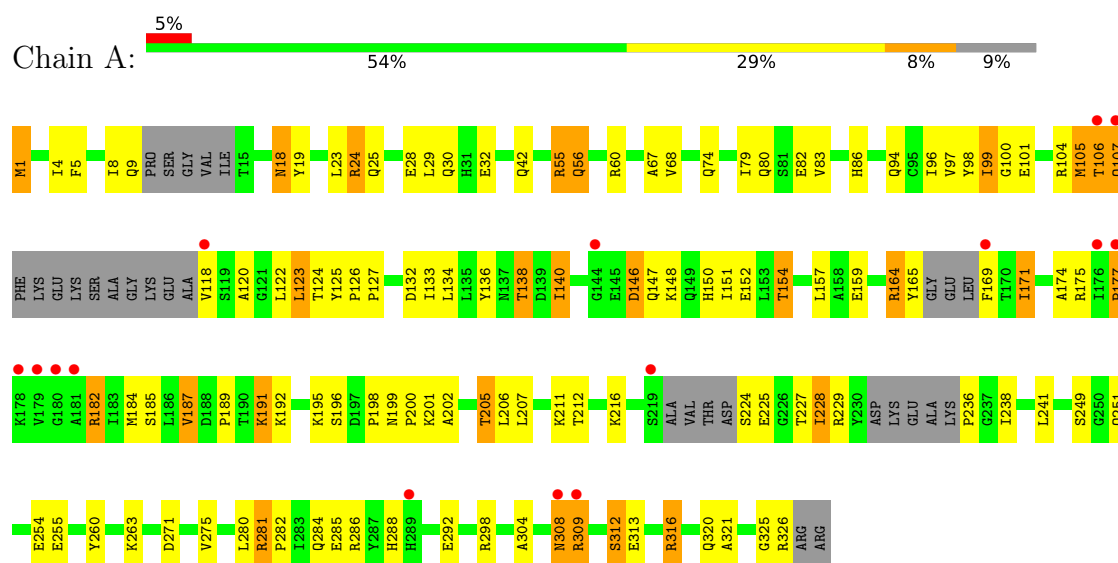


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

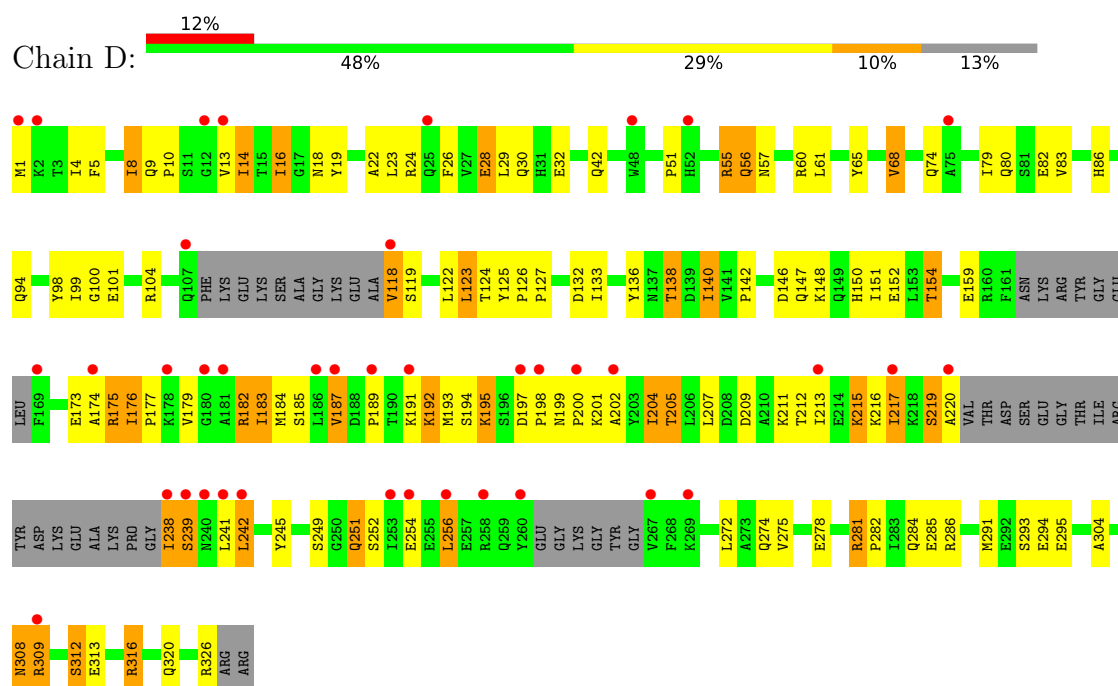
3 Residue-property plots

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 electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tryptophanyl-tRNA synthetase



• Molecule 1: Tryptophanyl-tRNA synthetase



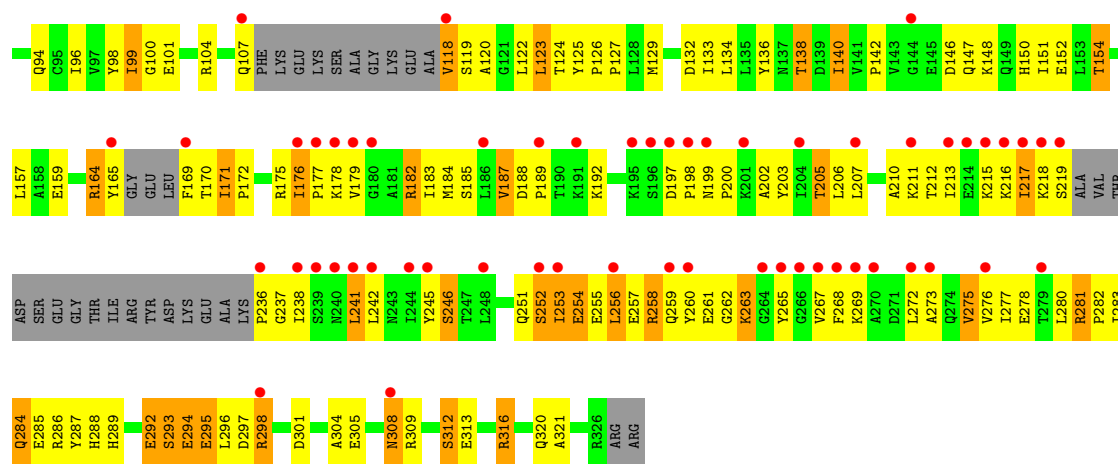
Chain B:

11% 45% 34% 10% 11%

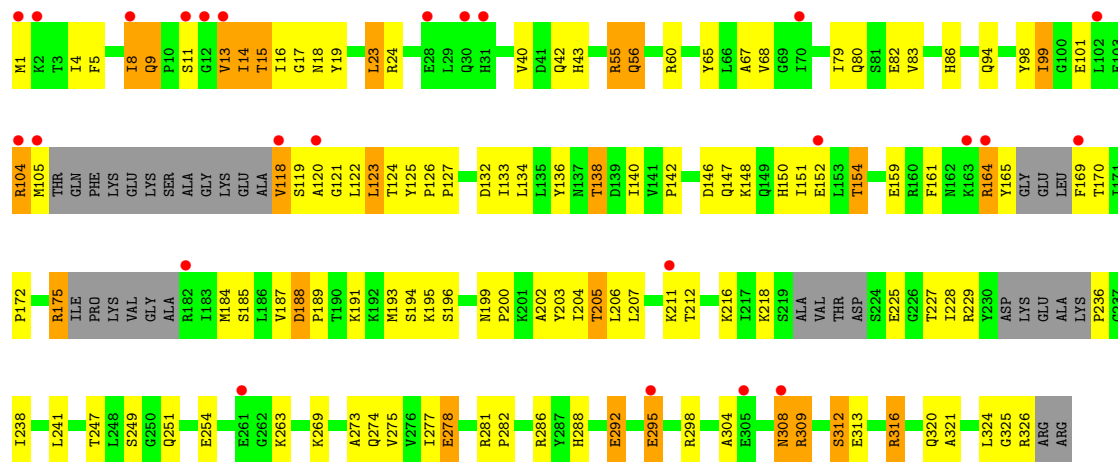
M1 I4 F5 I8 Q9 PR0 SER GLY VAL ILE T15 I16 G17 N18 Y19 I20 G21 A22 L23 R24 Q25 F26 V27 E28 L29 Q30 N34 F37 V40 D41 Q42 R55 Q56 R60 L64 Y65 V68 D71 P72 T73 Q74 I79 Q80 S91 E82 V83 H86 Q94 Y98 I99 G100 E101 R104 Q107 PHE GLY GLU LYS SER ALA GLY LYS GLU ALA V118 S119 A120 G121 L122 L123 T124 Y125 P126 P127 D132 I133 L134 L135 Y136 N137 T138 D139 L140 G144 E145 D146 Q147 K148 G149 H150 I151 E152 L153 T154 E159 R164 Y165 GLY GLU L171 F169 T170 I171 P172 E173 ALA ARG ILE PRO LYS VAL GLY ALA R182 I183 M184 S185 L186 V187 D188 P189 T190 K191 K192 M193 S194 D197 G198 N199 P200 K201 A202 Y203 T204 T205 L206 L207 D208 K211 T212 K215 T216 T217 K218 S219 ALA VAL THR ASP S224 E225 G226 T227 L228 R229 V230 Y231 LYS GLU ALA P236 G237 T238 S239 N240 L241 L242 T247 L248 S249 G250 Q251 Q252 I253 E254 E255 L256 E257 R258 Q259 E261 G262 K263 G264 Y265 G266 V267 F268 K269 A270 D271 L272 A273 Q274 V275 E278 R281 P282 R286 Y287 H288 H289 M290 E291 E292 S293 E294 D297 R298 D301 E302 G303 A304 F305 K306 A307 N308 R309 S312 E313 R316 Q320 A321 G325 R326 ARG ARG

[illegible]

Chain E:



• Molecule 1: Tryptophanyl-tRNA synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.61Å 91.99Å 158.32Å 90.00° 134.01° 90.00°	Depositor
Resolution (Å)	25.00 – 2.65 25.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	92.5 (25.00-2.65) 98.2 (25.00-2.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.32Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.270 0.275 , 0.279	Depositor DCC
R_{free} test set	3990 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h+2*k,-h-l 0.000 for h,-k,-h-l 0.005 for -h-2*k,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14203	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5371e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, AMP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/2435	0.72	1/3285 (0.0%)
1	B	0.33	0/2377	0.71	0/3205
1	C	0.39	0/2262	0.68	0/3053
1	D	0.31	0/2320	0.71	0/3137
1	E	0.30	0/2378	0.68	0/3210
1	F	0.28	0/2411	0.69	0/3253
All	All	0.36	0/14183	0.70	1/19143 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ILE	N-CA-C	6.82	113.51	106.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2394	0	2408	116	0
1	B	2338	0	2341	180	0
1	C	2225	0	2249	177	0
1	D	2281	0	2306	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2337	0	2355	195	0
1	F	2370	0	2380	146	0
2	A	15	0	9	0	0
2	B	15	0	9	0	0
2	C	15	0	9	0	0
2	D	15	0	9	0	0
2	E	15	0	9	2	0
2	F	15	0	9	0	0
3	A	5	0	0	3	0
3	B	5	0	0	2	0
3	C	5	0	0	0	0
3	D	5	0	0	4	0
3	E	5	0	0	0	0
3	F	5	0	0	1	0
4	A	23	0	12	4	0
4	B	23	0	12	7	0
4	C	23	0	12	5	0
4	D	23	0	12	5	0
4	E	23	0	12	7	0
4	F	23	0	12	5	0
All	All	14203	0	14165	909	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 32.

All (909) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:CG1	1:B:99:ILE:HG13	1.58	1.32
1:C:206:LEU:CD1	1:C:280:LEU:HD22	1.70	1.20
1:F:13:VAL:HG21	1:F:205:THR:HG23	1.22	1.20
1:B:23:LEU:HA	1:B:26:PHE:CD2	1.77	1.19
1:E:215:LYS:O	1:E:218:LYS:HG2	1.40	1.19
1:C:213:ILE:HG21	1:C:276:VAL:HG12	1.23	1.18
1:B:230:TYR:CE1	1:B:239:SER:HB3	1.78	1.17
1:D:140:ILE:HD11	1:D:175:ARG:CG	1.77	1.15
1:C:206:LEU:CD1	1:C:280:LEU:CD2	2.26	1.14
1:B:16:ILE:HD13	1:B:204:ILE:HB	1.21	1.12
1:B:230:TYR:CD1	1:B:239:SER:HB3	1.84	1.12
1:C:64:LEU:HD21	1:C:207:LEU:HD21	1.22	1.12
1:C:176:ILE:CG2	1:C:179:VAL:HG13	1.79	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:HG12	1:B:99:ILE:CG1	1.80	1.09
1:D:200:PRO:O	1:D:216:LYS:HE2	1.51	1.09
1:E:187:VAL:HG11	1:E:199:ASN:ND2	1.67	1.08
1:A:205:THR:HG22	1:A:207:LEU:H	1.11	1.08
1:C:206:LEU:HD11	1:C:280:LEU:HD22	1.33	1.07
1:D:140:ILE:HD11	1:D:175:ARG:HG2	1.13	1.07
1:C:272:LEU:HA	1:C:275:VAL:HG13	1.37	1.06
1:C:213:ILE:HG21	1:C:276:VAL:CG1	1.84	1.06
1:E:215:LYS:HG2	1:E:218:LYS:HE2	1.07	1.06
1:F:15:THR:HG22	1:F:18:ASN:H	1.14	1.06
1:C:187:VAL:HG21	1:C:199:ASN:OD1	1.56	1.04
1:D:140:ILE:CD1	1:D:175:ARG:HG2	1.88	1.04
1:E:19:TYR:O	1:E:24:ARG:HB3	1.57	1.04
1:F:104:ARG:HG3	1:F:104:ARG:HH11	1.20	1.03
1:C:182:ARG:HG2	1:C:184:MET:CE	1.88	1.03
1:E:215:LYS:HG2	1:E:218:LYS:CE	1.87	1.02
1:F:205:THR:HG22	1:F:207:LEU:H	1.20	1.02
1:C:206:LEU:HD11	1:C:280:LEU:CD2	1.85	1.01
1:C:176:ILE:HG22	1:C:179:VAL:HG13	1.39	1.01
1:C:295:GLU:HG2	1:C:298:ARG:HH21	1.25	1.00
1:E:215:LYS:CG	1:E:218:LYS:HE2	1.92	1.00
1:E:197:ASP:OD1	1:E:198:PRO:HD2	1.62	0.99
1:F:140:ILE:HD11	1:F:175:ARG:HB3	1.42	0.99
1:D:215:LYS:NZ	1:D:215:LYS:HB3	1.74	0.99
1:B:23:LEU:HA	1:B:26:PHE:HD2	0.85	0.99
1:C:206:LEU:HD12	1:C:280:LEU:HD22	1.45	0.98
1:B:187:VAL:HG11	1:B:199:ASN:ND2	1.79	0.97
1:A:140:ILE:HD11	1:A:175:ARG:HD3	1.47	0.95
1:D:19:TYR:O	1:D:24:ARG:HB2	1.65	0.94
1:C:210:ALA:HB1	1:C:277:ILE:HD13	1.46	0.94
1:B:23:LEU:CA	1:B:26:PHE:HD2	1.78	0.94
1:C:64:LEU:HD21	1:C:207:LEU:CD2	1.98	0.93
1:A:18:ASN:C	1:A:18:ASN:HD22	1.77	0.93
1:D:140:ILE:HD11	1:D:175:ARG:CD	1.99	0.93
1:C:176:ILE:O	1:C:179:VAL:HG22	1.70	0.92
1:E:305:GLU:O	1:E:309:ARG:HG2	1.68	0.92
1:B:282:PRO:HB2	1:B:286:ARG:NH2	1.84	0.92
1:D:205:THR:HG22	1:D:207:LEU:H	1.34	0.91
1:E:107:GLN:H	1:E:107:GLN:NE2	1.69	0.91
1:E:213:ILE:O	1:E:217:ILE:HG13	1.68	0.91
1:C:213:ILE:CG2	1:C:276:VAL:CG1	2.48	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:GLU:C	1:E:263:LYS:HE2	1.96	0.91
1:B:205:THR:HG23	1:B:207:LEU:H	1.34	0.91
1:C:206:LEU:HD12	1:C:280:LEU:CD2	1.97	0.90
1:A:118:VAL:HG12	1:B:99:ILE:HG13	0.91	0.90
1:C:19:TYR:CE2	1:C:24:ARG:HD3	2.07	0.89
1:C:23:LEU:HD12	1:C:23:LEU:O	1.72	0.89
1:D:215:LYS:HB3	1:D:215:LYS:HZ3	1.29	0.89
1:F:15:THR:HG23	1:F:17:GLY:H	1.38	0.89
1:C:218:LYS:CB	1:C:218:LYS:NZ	2.35	0.88
1:E:283:ILE:HG13	1:E:286:ARG:NH2	1.88	0.88
1:C:134:LEU:HB3	1:C:169:PHE:CD1	2.08	0.88
1:C:213:ILE:CG2	1:C:276:VAL:HG11	2.03	0.88
1:A:99:ILE:HG13	1:B:118:VAL:HG23	1.56	0.88
1:D:215:LYS:NZ	1:D:215:LYS:CB	2.36	0.88
1:C:218:LYS:HB3	1:C:218:LYS:HZ3	1.39	0.86
1:C:26:PHE:O	1:C:30:GLN:HB3	1.75	0.86
1:F:13:VAL:CG2	1:F:14:ILE:N	2.38	0.86
1:C:16:ILE:O	1:C:20:ILE:HD12	1.75	0.86
1:C:126:PRO:HB2	1:C:127:PRO:HD3	1.58	0.85
1:C:213:ILE:HG23	1:C:276:VAL:HG11	1.56	0.85
1:B:304:ALA:O	1:B:308:ASN:HB2	1.76	0.85
1:F:126:PRO:HB2	1:F:127:PRO:HD3	1.59	0.85
1:B:126:PRO:HB2	1:B:127:PRO:HD3	1.58	0.84
1:E:29:LEU:HD11	1:E:177:PRO:HB2	1.57	0.84
1:F:105:MET:HE2	1:F:150:HIS:CE1	2.12	0.84
1:E:140:ILE:HD11	1:E:175:ARG:CG	2.08	0.84
1:B:281:ARG:HG3	1:B:281:ARG:HH11	1.43	0.84
1:D:4:ILE:HG12	1:D:140:ILE:HG22	1.59	0.84
1:E:126:PRO:HB2	1:E:127:PRO:HD3	1.58	0.84
1:C:200:PRO:HA	1:C:203:TYR:CE1	2.12	0.83
1:C:206:LEU:CD1	1:C:280:LEU:HD21	2.05	0.83
1:D:217:ILE:O	1:D:220:ALA:HB3	1.78	0.83
1:B:184:MET:HG3	1:B:191:LYS:O	1.78	0.83
1:C:4:ILE:HG12	1:C:140:ILE:HG22	1.60	0.83
1:D:176:ILE:HB	1:D:179:VAL:HG12	1.58	0.83
1:D:126:PRO:HB2	1:D:127:PRO:HD3	1.60	0.82
1:F:205:THR:HG22	1:F:207:LEU:N	1.94	0.82
1:B:205:THR:HG22	1:B:208:ASP:N	1.95	0.82
1:C:64:LEU:CD2	1:C:207:LEU:HD21	2.07	0.82
1:C:281:ARG:N	1:C:282:PRO:HD2	1.94	0.82
1:B:134:LEU:HB3	1:B:169:PHE:CD1	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ALA:O	1:C:26:PHE:CE2	2.33	0.82
1:C:16:ILE:HG23	1:C:204:ILE:O	1.79	0.82
1:E:261:GLU:HG3	1:E:261:GLU:O	1.80	0.82
1:A:126:PRO:HB2	1:A:127:PRO:HD3	1.59	0.81
1:E:134:LEU:HB3	1:E:169:PHE:CD1	2.14	0.81
1:B:22:ALA:O	1:B:26:PHE:CD2	2.34	0.81
1:B:4:ILE:HG12	1:B:140:ILE:HG22	1.62	0.81
1:F:164:ARG:HD2	1:F:165:TYR:CE2	2.16	0.81
1:C:22:ALA:O	1:C:26:PHE:CD2	2.33	0.81
1:C:281:ARG:H	1:C:282:PRO:HD2	1.46	0.81
1:F:15:THR:CG2	1:F:18:ASN:H	1.92	0.81
1:B:230:TYR:CD1	1:B:239:SER:CB	2.63	0.80
1:F:175:ARG:HG2	1:F:175:ARG:HH11	1.46	0.80
1:C:182:ARG:HG2	1:C:184:MET:HE1	1.62	0.80
1:A:205:THR:HG22	1:A:207:LEU:N	1.93	0.80
1:B:205:THR:HG22	1:B:208:ASP:H	1.46	0.80
1:E:4:ILE:HG12	1:E:140:ILE:HG22	1.61	0.80
1:F:188:ASP:HB3	1:F:191:LYS:HB3	1.63	0.80
1:A:4:ILE:HG12	1:A:140:ILE:HG22	1.64	0.80
1:D:140:ILE:HD11	1:D:175:ARG:HD2	1.64	0.80
1:D:205:THR:CG2	1:D:207:LEU:H	1.95	0.79
1:F:13:VAL:HG21	1:F:205:THR:CG2	2.10	0.79
1:F:140:ILE:CD1	1:F:175:ARG:HB3	2.13	0.79
1:F:175:ARG:HG2	1:F:175:ARG:NH1	1.98	0.79
1:B:60:ARG:HG2	1:B:291:MET:CE	2.13	0.79
1:D:320:GLN:HA	1:C:55:ARG:NH2	1.98	0.79
1:E:197:ASP:OD1	1:E:198:PRO:CD	2.30	0.79
1:F:4:ILE:HG12	1:F:140:ILE:HG22	1.63	0.78
1:B:16:ILE:CD1	1:B:204:ILE:HB	2.10	0.78
1:B:187:VAL:HG22	1:B:202:ALA:HB2	1.65	0.78
1:D:13:VAL:HG21	1:D:205:THR:HG23	1.63	0.78
1:E:55:ARG:HH22	1:F:320:GLN:HA	1.48	0.78
1:D:193:MET:HB3	4:D:1003:AMP:N6	1.98	0.77
1:B:200:PRO:HA	1:B:203:TYR:CZ	2.18	0.77
1:E:281:ARG:NE	1:E:281:ARG:HA	2.00	0.77
1:E:205:THR:HG22	1:E:207:LEU:H	1.50	0.77
1:F:13:VAL:HG22	1:F:14:ILE:N	1.98	0.77
1:E:205:THR:CG2	1:E:207:LEU:H	1.98	0.77
1:A:189:PRO:HB2	1:A:236:PRO:HB2	1.67	0.77
1:A:205:THR:CG2	1:A:207:LEU:H	1.94	0.77
1:E:185:SER:OG	1:E:202:ALA:HB1	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ALA:O	1:D:26:PHE:CD2	2.39	0.76
1:B:282:PRO:HB2	1:B:286:ARG:HH21	1.49	0.76
1:F:104:ARG:HG3	1:F:104:ARG:NH1	1.91	0.76
1:C:29:LEU:CD1	1:C:177:PRO:HB2	2.15	0.76
1:E:29:LEU:CD1	1:E:177:PRO:HB2	2.16	0.76
1:A:124:THR:HG21	1:B:124:THR:HG21	1.68	0.76
1:A:24:ARG:HH11	1:A:24:ARG:HB3	1.50	0.76
1:C:176:ILE:HG21	1:C:179:VAL:HG13	1.67	0.75
1:B:189:PRO:HB2	1:B:236:PRO:HB2	1.68	0.75
1:E:218:LYS:HG3	1:E:219:SER:N	1.99	0.75
1:E:288:HIS:O	1:E:292:GLU:HG2	1.85	0.75
1:E:55:ARG:HD2	1:F:325:GLY:O	1.85	0.75
1:E:320:GLN:HA	1:F:55:ARG:HH22	1.51	0.75
1:B:193:MET:HE2	1:B:203:TYR:HA	1.67	0.75
1:C:23:LEU:HD12	1:C:23:LEU:C	2.11	0.75
1:E:273:ALA:O	1:E:277:ILE:HD12	1.85	0.75
1:F:13:VAL:HG23	1:F:14:ILE:H	1.52	0.75
1:D:198:PRO:HA	1:E:198:PRO:HA	1.69	0.75
1:E:140:ILE:HD11	1:E:175:ARG:HH11	1.51	0.75
1:F:205:THR:CG2	1:F:207:LEU:H	1.97	0.75
1:B:170:THR:O	1:B:172:PRO:HD3	1.86	0.74
1:E:140:ILE:CD1	1:E:175:ARG:HH11	1.99	0.74
1:F:121:GLY:O	1:F:125:TYR:HB3	1.87	0.74
1:E:19:TYR:CE2	1:E:24:ARG:HD2	2.22	0.74
1:E:263:LYS:N	1:E:263:LYS:HD3	2.03	0.74
1:F:15:THR:HG23	1:F:17:GLY:N	2.03	0.73
1:B:187:VAL:HG22	1:B:202:ALA:CB	2.18	0.73
1:F:13:VAL:CG2	1:F:205:THR:HG23	2.13	0.73
1:B:252:SER:OG	1:B:254:GLU:HG2	1.88	0.73
1:C:272:LEU:HA	1:C:275:VAL:CG1	2.16	0.73
1:F:140:ILE:HD11	1:F:175:ARG:CB	2.18	0.73
1:D:16:ILE:HD13	1:D:204:ILE:HB	1.69	0.73
1:C:218:LYS:HZ2	1:C:218:LYS:HB2	1.54	0.73
1:E:253:ILE:O	1:E:257:GLU:HG2	1.88	0.73
1:D:187:VAL:HG13	1:D:202:ALA:HA	1.70	0.73
1:D:185:SER:OG	1:D:202:ALA:HB1	1.89	0.73
1:B:200:PRO:O	1:B:216:LYS:HE2	1.88	0.73
1:D:320:GLN:HA	1:C:55:ARG:HH22	1.53	0.72
1:E:265:TYR:O	1:E:269:LYS:HG3	1.88	0.72
1:C:192:LYS:HG2	1:C:193:MET:N	2.05	0.72
1:A:164:ARG:HD2	1:A:165:TYR:CE2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ALA:HB1	1:D:26:PHE:CE2	2.25	0.72
1:D:22:ALA:HB1	1:D:26:PHE:HE2	1.53	0.72
1:E:187:VAL:HG11	1:E:199:ASN:HD21	1.54	0.72
1:C:218:LYS:NZ	1:C:218:LYS:HB2	2.05	0.72
1:F:13:VAL:CG2	1:F:14:ILE:H	2.01	0.71
1:E:295:GLU:HG2	1:E:298:ARG:NH2	2.06	0.71
1:A:134:LEU:HB3	1:A:169:PHE:CD1	2.26	0.71
1:E:189:PRO:HB2	1:E:236:PRO:HB2	1.74	0.70
1:F:125:TYR:N	1:F:126:PRO:HD2	2.06	0.70
1:B:249:SER:OG	1:B:251:GLN:HG3	1.92	0.70
1:C:210:ALA:CB	1:C:277:ILE:HD13	2.21	0.70
1:F:134:LEU:HB3	1:F:169:PHE:CD1	2.26	0.70
1:A:320:GLN:HA	1:B:55:ARG:HH22	1.55	0.70
1:E:215:LYS:HG3	1:E:218:LYS:HZ3	1.55	0.70
1:F:13:VAL:C	1:F:14:ILE:HD13	2.17	0.70
1:F:184:MET:HG3	1:F:189:PRO:O	1.92	0.70
1:A:304:ALA:O	1:A:308:ASN:HB2	1.92	0.70
1:B:60:ARG:HG2	1:B:291:MET:HE1	1.72	0.70
1:C:16:ILE:HD13	1:C:204:ILE:HB	1.72	0.70
1:F:8:ILE:HD12	1:F:65:TYR:OH	1.92	0.70
1:A:140:ILE:HD11	1:A:175:ARG:CD	2.21	0.69
1:A:140:ILE:CD1	1:A:175:ARG:HD3	2.19	0.69
1:C:16:ILE:CG2	1:C:204:ILE:HG22	2.21	0.69
1:F:212:THR:HG22	1:F:216:LYS:HD2	1.73	0.69
1:D:205:THR:HG22	1:D:207:LEU:N	2.04	0.69
1:C:304:ALA:O	1:C:308:ASN:HB2	1.93	0.69
1:F:14:ILE:HG22	1:F:15:THR:N	2.05	0.69
1:A:107:GLN:H	1:A:107:GLN:NE2	1.90	0.69
1:C:100:GLY:O	1:C:104:ARG:HG3	1.93	0.69
1:C:29:LEU:HD13	1:C:177:PRO:HB2	1.75	0.68
1:E:100:GLY:O	1:E:104:ARG:HG3	1.93	0.68
1:F:18:ASN:HD21	4:F:1003:AMP:H5'1	1.57	0.68
1:A:320:GLN:HA	1:B:55:ARG:NH2	2.07	0.68
1:D:304:ALA:O	1:D:308:ASN:HB2	1.93	0.68
1:E:304:ALA:O	1:E:308:ASN:HB2	1.91	0.68
1:A:288:HIS:O	1:A:292:GLU:HG2	1.93	0.68
1:F:105:MET:CE	1:F:150:HIS:CE1	2.76	0.68
1:E:213:ILE:O	1:E:217:ILE:CG1	2.42	0.68
1:A:150:HIS:O	1:A:154:THR:HG22	1.93	0.68
1:F:150:HIS:O	1:F:154:THR:HG22	1.93	0.68
1:B:24:ARG:HH11	1:B:24:ARG:CB	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:LEU:HA	1:D:26:PHE:HD2	1.59	0.68
1:B:150:HIS:O	1:B:154:THR:HG22	1.94	0.68
1:C:150:HIS:O	1:C:154:THR:HG22	1.95	0.67
1:E:150:HIS:O	1:E:154:THR:HG22	1.94	0.67
1:B:189:PRO:HB2	1:B:236:PRO:CB	2.23	0.67
1:E:189:PRO:HB3	1:E:237:GLY:HA2	1.76	0.67
1:F:304:ALA:O	1:F:308:ASN:HB2	1.94	0.67
1:D:100:GLY:O	1:D:104:ARG:HG3	1.93	0.67
1:B:187:VAL:HG11	1:B:199:ASN:HD21	1.57	0.67
1:E:283:ILE:HG13	1:E:286:ARG:HH21	1.60	0.67
1:F:282:PRO:HB2	1:F:286:ARG:HH21	1.58	0.67
1:C:16:ILE:CD1	1:C:204:ILE:HB	2.25	0.67
1:B:259:GLN:HG2	1:B:260:TYR:CD2	2.30	0.67
1:E:19:TYR:CZ	1:E:24:ARG:HB2	2.30	0.67
1:F:15:THR:HG22	1:F:18:ASN:N	1.99	0.67
1:D:150:HIS:O	1:D:154:THR:HG22	1.95	0.66
1:A:281:ARG:NH2	1:A:285:GLU:OE2	2.28	0.66
1:A:55:ARG:HH22	1:B:320:GLN:HA	1.59	0.66
1:C:218:LYS:NZ	1:C:218:LYS:HB3	1.98	0.66
1:A:140:ILE:HD11	1:A:175:ARG:HB3	1.76	0.66
1:D:13:VAL:HG21	1:D:205:THR:CG2	2.25	0.66
1:D:13:VAL:CG2	1:D:205:THR:HG23	2.24	0.66
1:C:4:ILE:HG12	1:C:140:ILE:CG2	2.25	0.66
1:C:182:ARG:HG2	1:C:184:MET:HE3	1.74	0.66
1:E:297:ASP:HA	1:F:326:ARG:NH1	2.10	0.66
1:F:189:PRO:HB2	1:F:236:PRO:HB2	1.77	0.66
1:F:175:ARG:HH11	1:F:175:ARG:CG	2.09	0.66
1:D:193:MET:HB3	4:D:1003:AMP:HN62	1.57	0.66
1:B:100:GLY:O	1:B:104:ARG:HG3	1.96	0.66
1:C:164:ARG:HD2	1:C:165:TYR:CE2	2.31	0.66
1:F:67:ALA:O	1:F:286:ARG:NH1	2.29	0.66
1:D:19:TYR:HA	1:D:23:LEU:HB3	1.78	0.66
1:C:295:GLU:HG2	1:C:298:ARG:NH2	2.04	0.66
1:F:142:PRO:HA	1:F:175:ARG:O	1.95	0.65
1:A:192:LYS:HE2	4:A:1003:AMP:C5	2.31	0.65
1:D:55:ARG:NH2	1:C:320:GLN:HA	2.12	0.65
1:B:182:ARG:CZ	1:B:192:LYS:HD3	2.26	0.65
1:E:182:ARG:HB3	1:E:184:MET:CE	2.26	0.65
1:B:16:ILE:HD13	1:B:204:ILE:CB	2.14	0.65
1:F:125:TYR:N	1:F:126:PRO:CD	2.60	0.65
1:D:173:GLU:CD	1:D:175:ARG:NH1	2.54	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1002:PO4:O2	4:B:1003:AMP:H5'1	1.97	0.65
1:D:282:PRO:HB2	1:D:286:ARG:NH2	2.12	0.65
1:D:4:ILE:HG12	1:D:140:ILE:CG2	2.26	0.65
1:D:140:ILE:HD13	1:D:177:PRO:HG3	1.78	0.65
1:D:198:PRO:O	1:D:200:PRO:HD3	1.97	0.64
1:B:187:VAL:CG2	1:B:202:ALA:HB2	2.26	0.64
1:E:198:PRO:O	1:E:200:PRO:HD3	1.98	0.64
3:D:1002:PO4:O4	4:D:1003:AMP:H5'2	1.98	0.64
1:C:25:GLN:O	1:C:29:LEU:HG	1.97	0.64
1:D:30:GLN:O	1:D:74:GLN:HG3	1.97	0.64
1:C:83:VAL:HG13	1:C:308:ASN:ND2	2.12	0.64
1:C:244:ILE:O	1:C:248:LEU:HB2	1.97	0.64
1:E:320:GLN:HA	1:F:55:ARG:NH2	2.13	0.64
1:F:19:TYR:HA	1:F:23:LEU:HB3	1.78	0.64
1:B:24:ARG:HH11	1:B:24:ARG:HB3	1.63	0.64
1:C:267:VAL:O	1:C:271:ASP:CG	2.41	0.64
1:B:278:GLU:OE1	1:B:281:ARG:NH2	2.29	0.64
1:E:297:ASP:HA	1:F:326:ARG:HH12	1.61	0.64
1:A:280:LEU:O	1:A:284:GLN:HG3	1.96	0.64
1:C:185:SER:OG	1:C:202:ALA:HB1	1.98	0.64
1:E:215:LYS:CG	1:E:218:LYS:CE	2.65	0.64
1:F:185:SER:HB3	1:F:188:ASP:O	1.96	0.64
1:C:281:ARG:N	1:C:282:PRO:CD	2.61	0.64
1:C:16:ILE:CG2	1:C:204:ILE:O	2.47	0.64
1:C:205:THR:HG23	1:C:206:LEU:H	1.63	0.63
1:E:164:ARG:HD2	1:E:165:TYR:CE2	2.32	0.63
1:E:215:LYS:O	1:E:218:LYS:CG	2.32	0.63
1:F:14:ILE:CG2	1:F:15:THR:N	2.61	0.63
1:F:188:ASP:HB3	1:F:191:LYS:CB	2.27	0.63
1:E:215:LYS:CG	1:E:218:LYS:HZ3	2.10	0.63
1:F:83:VAL:HG13	1:F:308:ASN:ND2	2.13	0.63
1:D:142:PRO:HA	1:D:175:ARG:O	1.99	0.63
1:D:215:LYS:CB	1:D:215:LYS:HZ2	2.11	0.63
1:E:171:ILE:N	1:E:171:ILE:HD12	2.14	0.63
1:E:142:PRO:HA	1:E:175:ARG:O	1.99	0.63
1:F:281:ARG:HB3	1:F:282:PRO:CD	2.29	0.63
1:A:55:ARG:NH2	1:B:320:GLN:HA	2.12	0.63
1:A:133:ILE:O	1:A:138:THR:HG23	1.99	0.62
1:D:192:LYS:HE3	1:D:193:MET:O	2.00	0.62
1:B:164:ARG:HD2	1:B:165:TYR:CE2	2.34	0.62
1:B:313:GLU:OE2	1:B:316:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:288:HIS:O	1:F:292:GLU:HG3	2.00	0.62
1:C:182:ARG:NH1	1:C:192:LYS:HD2	2.14	0.62
1:B:8:ILE:HD12	1:B:65:TYR:OH	1.98	0.62
1:D:22:ALA:O	1:D:26:PHE:CE2	2.52	0.62
1:E:218:LYS:CG	1:E:219:SER:H	2.13	0.62
1:C:24:ARG:O	1:C:27:VAL:HB	2.00	0.62
1:A:18:ASN:C	1:A:18:ASN:ND2	2.49	0.62
1:A:100:GLY:O	1:A:104:ARG:HG3	1.98	0.62
1:A:281:ARG:HG3	1:A:282:PRO:HD3	1.81	0.62
1:A:86:HIS:HD2	1:A:132:ASP:OD1	1.83	0.62
1:F:281:ARG:HG3	1:F:281:ARG:HH11	1.64	0.62
1:A:212:THR:HG22	1:A:216:LYS:HD2	1.80	0.61
1:D:19:TYR:O	1:D:24:ARG:CB	2.45	0.61
1:C:204:ILE:O	1:C:204:ILE:HG22	1.98	0.61
1:E:187:VAL:HG11	1:E:199:ASN:HD22	1.57	0.61
1:A:199:ASN:ND2	1:A:201:LYS:H	1.99	0.61
1:E:83:VAL:HG13	1:E:308:ASN:ND2	2.15	0.61
1:B:281:ARG:HB3	1:B:282:PRO:CD	2.31	0.61
1:C:29:LEU:HD13	1:C:177:PRO:CB	2.30	0.61
1:F:200:PRO:O	1:F:216:LYS:HE2	2.01	0.61
1:C:192:LYS:HE2	4:C:1003:AMP:C5	2.35	0.61
1:E:205:THR:HG22	1:E:207:LEU:N	2.15	0.61
1:D:22:ALA:C	1:D:26:PHE:CE2	2.78	0.61
1:E:55:ARG:NH2	1:F:320:GLN:HA	2.14	0.61
1:A:105:MET:CA	1:A:105:MET:HE2	2.31	0.61
1:D:124:THR:HG21	1:C:124:THR:HG21	1.82	0.61
1:D:200:PRO:O	1:D:216:LYS:CE	2.40	0.61
1:E:218:LYS:CG	1:E:219:SER:N	2.62	0.61
1:F:16:ILE:HG23	1:F:204:ILE:O	2.01	0.61
1:D:199:ASN:ND2	1:D:201:LYS:HG3	2.16	0.61
1:F:133:ILE:O	1:F:138:THR:HG23	2.01	0.61
1:B:16:ILE:CG2	1:B:204:ILE:HG22	2.31	0.60
1:D:10:PRO:HA	1:D:61:LEU:HD22	1.82	0.60
1:D:83:VAL:HG13	1:D:308:ASN:ND2	2.15	0.60
1:B:189:PRO:CB	1:B:236:PRO:HB2	2.30	0.60
1:E:218:LYS:HG3	1:E:219:SER:H	1.64	0.60
1:F:4:ILE:HG12	1:F:140:ILE:CG2	2.29	0.60
1:A:199:ASN:HD22	1:A:201:LYS:H	1.48	0.60
1:D:133:ILE:O	1:D:138:THR:HG23	2.01	0.60
1:C:86:HIS:HD2	1:C:132:ASP:OD1	1.84	0.60
1:D:55:ARG:HH22	1:C:320:GLN:HA	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:PRO:HA	1:B:203:TYR:CE2	2.36	0.60
1:E:86:HIS:HD2	1:E:132:ASP:OD1	1.84	0.60
1:D:28:GLU:HG3	1:D:29:LEU:N	2.17	0.60
1:E:200:PRO:HA	1:E:203:TYR:CE2	2.36	0.60
1:D:313:GLU:OE2	1:D:316:ARG:NH2	2.35	0.60
1:C:16:ILE:HG21	1:C:204:ILE:CG2	2.31	0.60
1:C:197:ASP:OD1	1:C:198:PRO:HD2	2.00	0.60
1:E:4:ILE:HG12	1:E:140:ILE:CG2	2.31	0.60
1:A:107:GLN:H	1:A:107:GLN:CD	2.07	0.60
1:D:183:ILE:HG22	1:D:193:MET:HE3	1.82	0.60
1:B:133:ILE:O	1:B:138:THR:HG23	2.02	0.60
1:E:215:LYS:C	1:E:218:LYS:HG2	2.23	0.60
1:E:245:TYR:CB	1:E:272:LEU:HD13	2.32	0.59
1:B:125:TYR:CG	1:B:126:PRO:HD3	2.37	0.59
1:A:24:ARG:HH11	1:A:24:ARG:CB	2.14	0.59
1:A:29:LEU:CD1	1:A:177:PRO:HG2	2.32	0.59
1:E:133:ILE:O	1:E:138:THR:HG23	2.02	0.59
1:E:212:THR:CG2	1:E:216:LYS:HE3	2.32	0.59
1:B:24:ARG:NH1	1:B:25:GLN:HE22	2.00	0.59
1:A:325:GLY:O	1:B:55:ARG:HD2	2.03	0.59
1:D:238:ILE:O	1:D:242:LEU:HD12	2.02	0.59
1:B:16:ILE:HG23	1:B:204:ILE:HG22	1.82	0.59
1:E:254:GLU:O	1:E:258:ARG:HG3	2.02	0.59
1:B:18:ASN:HD21	4:B:1003:AMP:C1'	2.15	0.59
1:E:24:ARG:HG2	1:E:25:GLN:NE2	2.17	0.59
1:F:14:ILE:CG2	1:F:15:THR:H	2.16	0.59
1:E:125:TYR:CG	1:E:126:PRO:HD3	2.38	0.59
1:F:282:PRO:HB2	1:F:286:ARG:NH2	2.17	0.59
1:D:19:TYR:O	1:D:24:ARG:N	2.36	0.59
1:D:199:ASN:HD21	1:D:201:LYS:HG3	1.67	0.59
1:B:212:THR:HG22	1:B:216:LYS:HD2	1.84	0.59
1:E:313:GLU:OE2	1:E:316:ARG:NH2	2.35	0.59
1:F:14:ILE:N	1:F:14:ILE:HD13	2.18	0.59
1:E:124:THR:HG21	1:F:124:THR:CG2	2.33	0.59
1:F:124:THR:O	1:F:127:PRO:HD2	2.02	0.59
1:F:313:GLU:OE2	1:F:316:ARG:NH2	2.36	0.59
1:C:205:THR:CG2	1:C:206:LEU:N	2.66	0.59
1:C:206:LEU:HD12	1:C:280:LEU:CD1	2.32	0.59
1:A:313:GLU:OE2	1:A:316:ARG:NH2	2.35	0.58
1:D:86:HIS:HD2	1:D:132:ASP:OD1	1.86	0.58
1:D:183:ILE:N	1:D:183:ILE:HD13	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ASN:ND2	4:B:1003:AMP:C1'	2.65	0.58
1:A:83:VAL:HG13	1:A:308:ASN:ND2	2.18	0.58
1:D:13:VAL:O	1:D:195:LYS:HE2	2.02	0.58
1:C:133:ILE:O	1:C:138:THR:HG23	2.02	0.58
1:C:205:THR:HG23	1:C:206:LEU:N	2.16	0.58
1:E:301:ASP:OD1	1:F:326:ARG:NH2	2.37	0.58
1:A:4:ILE:HG12	1:A:140:ILE:CG2	2.32	0.58
1:A:281:ARG:HG3	1:A:282:PRO:CD	2.34	0.58
1:D:23:LEU:HD21	1:D:68:VAL:HG21	1.84	0.58
1:F:193:MET:HB3	4:F:1003:AMP:N6	2.19	0.58
1:A:19:TYR:HA	1:A:23:LEU:HB3	1.86	0.58
1:B:187:VAL:HG11	1:B:199:ASN:HD22	1.62	0.58
1:C:280:LEU:O	1:C:284:GLN:HB2	2.03	0.58
1:C:313:GLU:OE2	1:C:316:ARG:NH2	2.34	0.58
1:A:29:LEU:HD11	1:A:177:PRO:HG2	1.86	0.58
1:C:125:TYR:CG	1:C:126:PRO:HD3	2.39	0.58
1:A:199:ASN:HD22	1:A:199:ASN:C	2.11	0.58
1:B:281:ARG:HG3	1:B:281:ARG:NH1	2.11	0.58
1:C:134:LEU:HB3	1:C:169:PHE:HD1	1.63	0.58
1:A:125:TYR:CG	1:A:126:PRO:HD3	2.37	0.58
1:B:86:HIS:HD2	1:B:132:ASP:OD1	1.85	0.58
1:E:262:GLY:N	1:E:263:LYS:HE2	2.19	0.58
1:B:271:ASP:O	1:B:275:VAL:HG13	2.04	0.57
1:F:86:HIS:HD2	1:F:132:ASP:OD1	1.85	0.57
1:D:193:MET:O	4:D:1003:AMP:N6	2.36	0.57
1:B:4:ILE:HG12	1:B:140:ILE:CG2	2.31	0.57
1:B:83:VAL:HG13	1:B:308:ASN:ND2	2.19	0.57
1:C:19:TYR:CZ	1:C:24:ARG:HD3	2.39	0.57
1:E:280:LEU:HB3	1:E:284:GLN:OE1	2.04	0.57
1:B:118:VAL:HG23	1:B:118:VAL:O	2.03	0.57
1:E:18:ASN:ND2	4:E:1003:AMP:H8	2.02	0.57
1:F:16:ILE:CG2	1:F:204:ILE:HG22	2.34	0.57
1:F:308:ASN:O	1:F:312:SER:HB2	2.05	0.57
1:A:182:ARG:HE	1:A:184:MET:HE1	1.69	0.57
1:B:218:LYS:HA	1:B:269:LYS:HD3	1.85	0.57
1:F:18:ASN:ND2	4:F:1003:AMP:H5'1	2.19	0.57
1:B:24:ARG:HH12	1:B:25:GLN:HE22	1.52	0.57
1:B:230:TYR:HD2	1:B:253:ILE:HG21	1.70	0.57
1:C:155:ARG:NH1	1:C:171:ILE:HG22	2.19	0.57
1:C:217:ILE:O	1:C:269:LYS:HG2	2.04	0.57
1:C:308:ASN:O	1:C:312:SER:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:ALA:HB2	1:E:287:TYR:HA	1.86	0.57
1:E:140:ILE:HD11	1:E:175:ARG:HG3	1.86	0.57
1:B:184:MET:HG2	1:B:189:PRO:O	2.04	0.57
1:D:125:TYR:CG	1:D:126:PRO:HD3	2.40	0.56
1:B:287:TYR:OH	1:B:291:MET:HE2	2.05	0.56
1:C:67:ALA:O	1:C:286:ARG:NH1	2.39	0.56
1:C:210:ALA:HA	1:C:277:ILE:HG12	1.87	0.56
1:C:218:LYS:CB	1:C:218:LYS:HZ3	2.04	0.56
1:C:218:LYS:CG	1:C:219:SER:N	2.69	0.56
1:E:245:TYR:HB2	1:E:272:LEU:HD13	1.85	0.56
1:C:282:PRO:HB2	1:C:286:ARG:HH21	1.69	0.56
1:E:213:ILE:HD13	1:E:276:VAL:HG12	1.87	0.56
1:F:125:TYR:CG	1:F:126:PRO:HD3	2.41	0.56
1:D:187:VAL:HG13	1:D:202:ALA:CA	2.34	0.56
1:B:22:ALA:C	1:B:26:PHE:CD2	2.83	0.56
1:B:205:THR:CG2	1:B:207:LEU:H	2.13	0.56
1:C:19:TYR:O	1:C:24:ARG:HB2	2.05	0.56
1:A:281:ARG:CG	1:A:282:PRO:HD3	2.35	0.56
1:B:254:GLU:O	1:B:258:ARG:HG2	2.05	0.56
1:D:176:ILE:O	1:D:179:VAL:HG13	2.05	0.56
1:B:23:LEU:O	1:B:26:PHE:HB2	2.06	0.56
1:D:252:SER:OG	1:D:254:GLU:HG2	2.06	0.56
1:A:308:ASN:O	1:A:312:SER:HB2	2.05	0.56
1:F:105:MET:HE2	1:F:150:HIS:HE1	1.67	0.56
1:B:229:ARG:HB2	1:B:257:GLU:OE2	2.05	0.55
1:C:212:THR:CG2	1:C:216:LYS:HE3	2.36	0.55
1:E:297:ASP:CA	1:F:326:ARG:HH12	2.19	0.55
1:F:125:TYR:H	1:F:126:PRO:HD2	1.69	0.55
1:E:189:PRO:CG	1:E:236:PRO:HB2	2.37	0.55
1:A:171:ILE:N	1:A:171:ILE:HD13	2.21	0.55
1:B:24:ARG:NH1	1:B:25:GLN:NE2	2.54	0.55
1:C:240:ASN:O	1:C:244:ILE:HG13	2.06	0.55
1:F:14:ILE:HG23	1:F:18:ASN:CB	2.37	0.55
1:D:187:VAL:HG22	1:D:202:ALA:HB2	1.87	0.55
1:B:22:ALA:HB1	1:B:26:PHE:CE2	2.41	0.55
1:D:147:GLN:OE1	1:D:150:HIS:HD2	1.90	0.55
1:E:252:SER:O	1:E:256:LEU:HD12	2.07	0.55
1:F:278:GLU:OE2	1:F:281:ARG:NE	2.35	0.55
1:B:22:ALA:C	1:B:26:PHE:CE2	2.85	0.55
1:B:22:ALA:O	1:B:26:PHE:CE2	2.59	0.55
1:A:30:GLN:O	1:A:74:GLN:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:LYS:CG	1:C:193:MET:N	2.70	0.54
1:E:147:GLN:OE1	1:E:150:HIS:HD2	1.90	0.54
1:E:189:PRO:CB	1:E:236:PRO:HB2	2.36	0.54
1:E:281:ARG:N	1:E:282:PRO:HD2	2.22	0.54
1:D:308:ASN:O	1:D:312:SER:HB2	2.06	0.54
1:E:107:GLN:H	1:E:107:GLN:HE21	1.50	0.54
1:F:13:VAL:HG22	1:F:14:ILE:O	2.08	0.54
1:A:147:GLN:OE1	1:A:150:HIS:HD2	1.90	0.54
1:B:147:GLN:OE1	1:B:150:HIS:HD2	1.89	0.54
1:B:60:ARG:HG2	1:B:291:MET:HE2	1.88	0.54
1:C:165:TYR:HB3	1:C:321:ALA:HB1	1.90	0.54
1:C:245:TYR:CD2	1:C:272:LEU:HD13	2.43	0.54
1:E:189:PRO:HB2	1:E:236:PRO:CB	2.37	0.54
1:E:252:SER:O	1:E:255:GLU:HB2	2.08	0.54
1:B:200:PRO:O	1:B:216:LYS:CE	2.54	0.54
1:C:16:ILE:CG2	1:C:204:ILE:CG2	2.85	0.54
1:F:147:GLN:OE1	1:F:150:HIS:HD2	1.90	0.54
1:E:182:ARG:HB3	1:E:184:MET:HE1	1.90	0.54
1:B:255:GLU:O	1:B:259:GLN:HB3	2.08	0.54
1:C:8:ILE:HD12	1:C:65:TYR:OH	2.08	0.54
1:E:215:LYS:CG	1:E:218:LYS:NZ	2.71	0.54
1:D:23:LEU:HA	1:D:26:PHE:CD2	2.42	0.53
1:D:192:LYS:HG2	1:D:193:MET:N	2.23	0.53
1:E:308:ASN:O	1:E:312:SER:HB2	2.08	0.53
1:E:42:GLN:HB2	1:E:80:GLN:OE1	2.08	0.53
1:D:326:ARG:NH1	1:C:297:ASP:HA	2.23	0.53
1:B:8:ILE:HD12	1:B:65:TYR:CZ	2.43	0.53
1:E:192:LYS:HE2	4:E:1003:AMP:C5	2.42	0.53
1:F:18:ASN:HD21	4:F:1003:AMP:C5'	2.20	0.53
1:A:281:ARG:HG3	1:A:282:PRO:N	2.23	0.53
1:D:8:ILE:HD12	1:D:65:TYR:OH	2.08	0.53
1:D:19:TYR:HD1	1:D:23:LEU:HD23	1.73	0.53
1:C:147:GLN:OE1	1:C:150:HIS:HD2	1.91	0.53
1:C:245:TYR:CG	1:C:272:LEU:HD13	2.43	0.53
1:F:165:TYR:HB3	1:F:321:ALA:HB1	1.91	0.53
1:F:200:PRO:HA	1:F:203:TYR:CE2	2.44	0.53
1:A:126:PRO:CB	1:A:127:PRO:HD3	2.36	0.53
1:C:238:ILE:HG22	1:C:238:ILE:O	2.08	0.53
1:E:18:ASN:ND2	4:E:1003:AMP:H5'2	2.22	0.53
1:E:19:TYR:CE2	1:E:24:ARG:HB2	2.44	0.53
1:E:19:TYR:HA	1:E:23:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:VAL:HB	1:F:99:ILE:HG13	1.90	0.53
1:C:185:SER:HB3	1:C:188:ASP:O	2.09	0.53
1:E:59:ARG:NH2	1:E:296:LEU:HD23	2.23	0.53
1:B:254:GLU:HA	1:B:257:GLU:HB2	1.89	0.53
1:F:281:ARG:HB3	1:F:282:PRO:HD3	1.89	0.53
1:A:260:TYR:O	1:A:263:LYS:HB2	2.09	0.53
1:E:18:ASN:ND2	4:E:1003:AMP:C8	2.77	0.53
1:E:187:VAL:HG13	1:E:202:ALA:HA	1.90	0.53
1:D:19:TYR:HE1	1:D:68:VAL:HG13	1.74	0.53
1:B:165:TYR:HB3	1:B:321:ALA:HB1	1.91	0.53
1:F:13:VAL:O	1:F:195:LYS:CE	2.57	0.53
1:D:151:ILE:HG13	1:D:174:ALA:HB2	1.90	0.53
1:A:24:ARG:HH11	1:A:24:ARG:CG	2.22	0.52
1:E:140:ILE:HD11	1:E:175:ARG:HG2	1.87	0.52
1:A:326:ARG:NH2	1:B:301:ASP:OD1	2.37	0.52
1:F:187:VAL:CG2	1:F:202:ALA:HB2	2.39	0.52
1:E:140:ILE:HD11	1:E:175:ARG:CD	2.39	0.52
1:E:237:GLY:O	1:E:241:LEU:HD22	2.10	0.52
1:B:281:ARG:HB3	1:B:282:PRO:HD3	1.90	0.52
1:A:125:TYR:CD2	1:A:126:PRO:HD3	2.45	0.52
1:E:263:LYS:N	1:E:263:LYS:CD	2.67	0.52
1:B:23:LEU:CA	1:B:26:PHE:CD2	2.68	0.52
1:B:27:VAL:CG2	1:B:68:VAL:HG12	2.40	0.52
1:B:42:GLN:HB2	1:B:80:GLN:OE1	2.09	0.52
1:B:125:TYR:CD2	1:B:126:PRO:HD3	2.45	0.52
1:B:288:HIS:O	1:B:292:GLU:HG2	2.09	0.52
1:C:42:GLN:HB2	1:C:80:GLN:OE1	2.09	0.52
1:C:281:ARG:HB3	1:C:282:PRO:CD	2.39	0.52
1:C:192:LYS:NZ	4:C:1003:AMP:H2'	2.25	0.52
1:C:134:LEU:HB3	1:C:169:PHE:CE1	2.45	0.52
1:E:281:ARG:N	1:E:281:ARG:HD2	2.24	0.52
1:F:249:SER:OG	1:F:251:GLN:HG3	2.09	0.52
1:B:24:ARG:HH12	1:B:25:GLN:NE2	2.08	0.52
1:A:165:TYR:HB3	1:A:321:ALA:HB1	1.92	0.51
1:C:23:LEU:HA	1:C:26:PHE:HD2	1.74	0.51
1:C:192:LYS:HE2	4:C:1003:AMP:C6	2.44	0.51
1:E:183:ILE:HB	4:E:1003:AMP:HN62	1.74	0.51
1:A:106:THR:HB	1:A:107:GLN:NE2	2.25	0.51
1:B:188:ASP:OD1	1:B:190:THR:OG1	2.28	0.51
1:B:254:GLU:HA	1:B:257:GLU:OE1	2.10	0.51
1:E:8:ILE:HD12	1:E:65:TYR:OH	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:VAL:HG22	1:D:14:ILE:N	2.24	0.51
1:E:125:TYR:CD2	1:E:126:PRO:HD3	2.45	0.51
1:E:289:HIS:HA	1:E:292:GLU:OE2	2.10	0.51
1:A:249:SER:OG	1:A:251:GLN:HG3	2.10	0.51
1:D:293:SER:OG	1:D:295:GLU:HB2	2.10	0.51
1:C:125:TYR:CD2	1:C:126:PRO:HD3	2.45	0.51
1:C:277:ILE:O	1:C:281:ARG:HB2	2.10	0.51
1:C:281:ARG:HB3	1:C:282:PRO:HD3	1.91	0.51
1:E:19:TYR:CE1	1:E:24:ARG:HB2	2.46	0.51
1:D:245:TYR:CD2	1:D:272:LEU:HD13	2.45	0.51
1:B:197:ASP:OD1	1:B:198:PRO:HD2	2.11	0.51
1:B:272:LEU:O	1:B:275:VAL:HG22	2.10	0.51
1:E:165:TYR:HB3	1:E:321:ALA:HB1	1.92	0.51
1:E:293:SER:OG	1:E:295:GLU:HB2	2.11	0.51
1:F:124:THR:C	1:F:127:PRO:HD2	2.35	0.51
1:B:201:LYS:HA	1:B:216:LYS:HE2	1.91	0.51
1:B:229:ARG:CG	1:B:230:TYR:N	2.71	0.51
1:C:96:ILE:HG13	1:C:157:LEU:HD22	1.93	0.51
1:D:125:TYR:CD2	1:D:126:PRO:HD3	2.45	0.51
1:C:16:ILE:O	1:C:20:ILE:CD1	2.55	0.51
1:C:206:LEU:HD12	1:C:280:LEU:HD13	1.93	0.51
1:B:126:PRO:CB	1:B:127:PRO:HD3	2.36	0.50
1:E:124:THR:HG21	1:F:124:THR:HG21	1.93	0.50
1:F:193:MET:HE2	1:F:203:TYR:HA	1.93	0.50
1:D:13:VAL:CG2	1:D:14:ILE:N	2.74	0.50
1:C:182:ARG:NH1	1:C:192:LYS:HB2	2.25	0.50
1:D:249:SER:OG	1:D:251:GLN:HG3	2.12	0.50
1:C:125:TYR:N	1:C:126:PRO:CD	2.75	0.50
1:E:182:ARG:HG2	1:E:192:LYS:HG3	1.93	0.50
1:E:107:GLN:NE2	1:E:107:GLN:N	2.50	0.50
3:F:1002:PO4:O3	4:F:1003:AMP:O1P	2.30	0.50
1:A:326:ARG:NH1	1:B:297:ASP:HA	2.26	0.50
1:D:197:ASP:OD1	1:D:198:PRO:HD2	2.11	0.50
1:C:126:PRO:HB2	1:C:127:PRO:CD	2.38	0.50
1:E:295:GLU:HG2	1:E:298:ARG:CZ	2.42	0.50
1:F:42:GLN:HB2	1:F:80:GLN:OE1	2.12	0.50
1:C:271:ASP:O	1:C:275:VAL:HG12	2.12	0.50
1:E:261:GLU:O	1:E:263:LYS:HE2	2.11	0.50
1:F:187:VAL:HG22	1:F:202:ALA:CB	2.41	0.50
1:E:18:ASN:HD22	4:E:1003:AMP:H5'2	1.78	0.49
1:C:182:ARG:HH12	1:C:192:LYS:HD2	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ALA:CB	1:D:26:PHE:HE2	2.21	0.49
1:D:42:GLN:HB2	1:D:80:GLN:OE1	2.12	0.49
1:F:125:TYR:CD1	1:F:125:TYR:C	2.89	0.49
1:F:187:VAL:HG22	1:F:202:ALA:HB2	1.94	0.49
1:D:125:TYR:N	1:D:126:PRO:CD	2.74	0.49
1:A:140:ILE:CG1	1:A:175:ARG:HB3	2.42	0.49
1:C:192:LYS:HZ3	4:C:1003:AMP:H2'	1.78	0.49
1:E:125:TYR:N	1:E:126:PRO:HD2	2.28	0.49
1:E:134:LEU:HB3	1:E:169:PHE:HD1	1.72	0.49
1:D:173:GLU:OE2	1:D:175:ARG:NH1	2.46	0.49
3:D:1002:PO4:O4	4:D:1003:AMP:H8	1.96	0.49
1:B:304:ALA:O	1:B:308:ASN:N	2.45	0.49
1:E:126:PRO:CB	1:E:127:PRO:HD3	2.36	0.49
1:E:217:ILE:HD12	1:E:273:ALA:HA	1.95	0.49
1:A:97:VAL:O	1:B:119:SER:HA	2.13	0.48
1:D:9:GLN:HE21	1:D:10:PRO:HD2	1.77	0.48
1:B:30:GLN:O	1:B:74:GLN:HG3	2.13	0.48
1:B:125:TYR:N	1:B:126:PRO:CD	2.76	0.48
1:C:148:LYS:O	1:C:152:GLU:HG3	2.14	0.48
1:E:125:TYR:N	1:E:126:PRO:CD	2.75	0.48
1:D:256:LEU:H	1:D:256:LEU:HG	1.47	0.48
1:B:18:ASN:CG	4:B:1003:AMP:C8	2.92	0.48
1:B:98:TYR:HB2	1:B:101:GLU:HG3	1.96	0.48
1:C:188:ASP:HB3	1:C:191:LYS:HB2	1.95	0.48
1:E:124:THR:HG21	1:F:124:THR:HG22	1.94	0.48
1:F:126:PRO:CB	1:F:127:PRO:HD3	2.37	0.48
1:D:60:ARG:HG2	1:D:291:MET:CE	2.43	0.48
1:D:192:LYS:NZ	3:D:1002:PO4:O3	2.42	0.48
1:D:217:ILE:HA	1:D:220:ALA:HB2	1.95	0.48
1:A:99:ILE:HG13	1:B:118:VAL:CG2	2.38	0.48
1:B:230:TYR:CD1	1:B:230:TYR:C	2.90	0.48
1:F:140:ILE:CG1	1:F:175:ARG:HB3	2.43	0.48
1:A:125:TYR:N	1:A:126:PRO:CD	2.76	0.48
1:A:126:PRO:HB2	1:A:127:PRO:CD	2.39	0.48
1:C:16:ILE:HG21	1:C:204:ILE:HG22	1.90	0.48
1:E:148:LYS:O	1:E:152:GLU:HG3	2.14	0.48
1:F:309:ARG:HE	1:F:309:ARG:HB3	1.50	0.48
1:A:148:LYS:O	1:A:152:GLU:HG3	2.12	0.48
1:D:60:ARG:HG2	1:D:291:MET:HE2	1.94	0.48
1:B:125:TYR:N	1:B:126:PRO:HD2	2.29	0.48
1:D:16:ILE:CD1	1:D:204:ILE:HB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:MET:CG	1:B:191:LYS:O	2.57	0.48
1:F:148:LYS:O	1:F:152:GLU:HG3	2.14	0.48
1:D:215:LYS:O	1:D:219:SER:OG	2.31	0.48
1:C:125:TYR:N	1:C:126:PRO:HD2	2.28	0.48
1:C:186:LEU:HB2	1:C:201:LYS:O	2.14	0.48
1:F:98:TYR:HB2	1:F:101:GLU:HG3	1.96	0.48
1:B:198:PRO:HA	1:C:198:PRO:HA	1.95	0.47
1:F:218:LYS:HA	1:F:269:LYS:HD3	1.96	0.47
1:A:42:GLN:HB2	1:A:80:GLN:OE1	2.14	0.47
1:D:125:TYR:N	1:D:126:PRO:HD2	2.29	0.47
1:D:281:ARG:N	1:D:282:PRO:HD2	2.30	0.47
1:B:148:LYS:O	1:B:152:GLU:HG3	2.14	0.47
1:E:86:HIS:HE1	1:E:136:TYR:OH	1.97	0.47
1:A:118:VAL:O	1:B:98:TYR:HA	2.14	0.47
1:D:251:GLN:HG3	1:D:256:LEU:CD2	2.45	0.47
1:B:9:GLN:OE1	1:B:40:VAL:HG23	2.14	0.47
1:B:254:GLU:O	1:B:257:GLU:N	2.44	0.47
1:C:86:HIS:HE1	1:C:136:TYR:OH	1.98	0.47
1:E:98:TYR:HB2	1:E:101:GLU:HG3	1.96	0.47
1:F:126:PRO:HB2	1:F:127:PRO:CD	2.39	0.47
1:A:125:TYR:N	1:A:126:PRO:HD2	2.29	0.47
1:D:55:ARG:HD2	1:C:325:GLY:O	2.13	0.47
1:C:210:ALA:HB1	1:C:277:ILE:CD1	2.32	0.47
1:E:197:ASP:OD1	1:E:198:PRO:N	2.47	0.47
1:A:140:ILE:HD11	1:A:175:ARG:CB	2.43	0.47
1:B:5:PHE:HB2	1:B:138:THR:HG21	1.95	0.47
1:B:21:GLY:HA3	4:B:1003:AMP:C2	2.48	0.47
1:C:126:PRO:CB	1:C:127:PRO:HD3	2.36	0.47
1:F:5:PHE:HB2	1:F:138:THR:HG21	1.97	0.47
1:A:140:ILE:CD1	1:A:175:ARG:HB3	2.42	0.47
1:A:281:ARG:N	1:A:282:PRO:HD2	2.29	0.47
1:B:134:LEU:HB3	1:B:169:PHE:CE1	2.48	0.47
1:E:212:THR:HG22	1:E:216:LYS:HE3	1.97	0.47
1:A:98:TYR:HB2	1:A:101:GLU:HG3	1.97	0.47
1:A:105:MET:HE2	1:A:105:MET:HA	1.97	0.47
1:B:215:LYS:O	1:B:219:SER:OG	2.29	0.47
1:C:59:ARG:NH2	1:C:296:LEU:HD23	2.29	0.47
1:C:213:ILE:O	1:C:217:ILE:HG13	2.14	0.47
1:F:188:ASP:CB	1:F:191:LYS:HB3	2.39	0.47
1:B:27:VAL:CG2	1:B:68:VAL:CG1	2.93	0.47
1:B:228:ILE:CD1	1:B:268:PHE:HB2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:ASN:HD22	1:F:200:PRO:CD	2.28	0.47
1:A:86:HIS:HE1	1:A:136:TYR:OH	1.97	0.47
1:D:86:HIS:HE1	1:D:136:TYR:OH	1.98	0.47
1:B:86:HIS:HE1	1:B:136:TYR:OH	1.97	0.47
1:B:189:PRO:CG	1:B:236:PRO:HB2	2.45	0.47
1:E:245:TYR:CD2	1:E:272:LEU:HB2	2.50	0.47
1:D:118:VAL:HB	1:C:99:ILE:HG13	1.97	0.47
1:B:19:TYR:CE2	1:B:24:ARG:CD	2.98	0.47
1:A:5:PHE:HB2	1:A:138:THR:HG21	1.97	0.46
1:D:148:LYS:O	1:D:152:GLU:HG3	2.15	0.46
1:D:182:ARG:NE	1:D:184:MET:HE1	2.30	0.46
1:C:272:LEU:HD12	1:C:275:VAL:CG2	2.45	0.46
1:E:238:ILE:HA	1:E:241:LEU:HD22	1.96	0.46
1:A:118:VAL:HG12	1:A:118:VAL:O	2.15	0.46
1:C:26:PHE:HB3	1:C:37:PHE:HZ	1.80	0.46
1:F:123:LEU:O	1:F:126:PRO:HD2	2.15	0.46
1:A:187:VAL:HG13	1:A:202:ALA:HA	1.98	0.46
1:D:19:TYR:CZ	1:D:24:ARG:HG3	2.49	0.46
1:D:140:ILE:CD1	1:D:175:ARG:HD2	2.37	0.46
1:B:182:ARG:NE	1:B:192:LYS:HD3	2.30	0.46
1:E:281:ARG:HA	1:E:281:ARG:HE	1.75	0.46
1:F:14:ILE:CG2	1:F:18:ASN:CB	2.94	0.46
1:A:118:VAL:HG11	1:B:99:ILE:HG13	1.78	0.46
1:D:126:PRO:CB	1:D:127:PRO:HD3	2.37	0.46
1:B:119:SER:C	1:B:121:GLY:N	2.72	0.46
1:B:126:PRO:HB2	1:B:127:PRO:CD	2.38	0.46
1:C:277:ILE:O	1:C:277:ILE:HG22	2.15	0.46
1:D:123:LEU:O	1:D:123:LEU:HG	2.16	0.46
1:D:239:SER:HA	1:D:242:LEU:HB2	1.98	0.46
1:B:230:TYR:HB2	1:B:242:LEU:HD13	1.98	0.46
1:E:5:PHE:HB2	1:E:138:THR:HG21	1.98	0.46
1:E:27:VAL:HG12	1:E:27:VAL:O	2.14	0.46
1:F:19:TYR:CE2	1:F:24:ARG:HB2	2.51	0.46
1:F:125:TYR:CD2	1:F:126:PRO:HD3	2.50	0.46
1:F:281:ARG:HG3	1:F:281:ARG:NH1	2.29	0.46
1:B:18:ASN:ND2	4:B:1003:AMP:O4'	2.33	0.46
1:F:295:GLU:HG2	1:F:298:ARG:HE	1.81	0.46
1:C:271:ASP:O	1:C:275:VAL:CG1	2.64	0.46
1:E:258:ARG:CZ	1:E:258:ARG:CB	2.94	0.46
1:F:9:GLN:HG2	1:F:40:VAL:CG2	2.46	0.46
1:F:203:TYR:O	1:F:216:LYS:NZ	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:ILE:HG23	1:E:281:ARG:HD3	1.96	0.46
1:A:55:ARG:HD2	1:B:325:GLY:O	2.16	0.46
1:A:192:LYS:HE2	4:A:1003:AMP:C6	2.51	0.46
1:D:5:PHE:HB2	1:D:138:THR:HG21	1.98	0.46
1:C:176:ILE:HG21	1:C:179:VAL:CG1	2.43	0.46
1:D:98:TYR:HB2	1:D:101:GLU:HG3	1.97	0.45
1:D:215:LYS:HZ2	1:D:215:LYS:HB2	1.81	0.45
3:B:1002:PO4:P	4:B:1003:AMP:H5'1	2.56	0.45
1:C:98:TYR:HB2	1:C:101:GLU:HG3	1.97	0.45
1:C:141:VAL:O	1:C:174:ALA:HA	2.15	0.45
1:B:25:GLN:CD	1:B:25:GLN:H	2.25	0.45
1:D:10:PRO:O	1:D:57:ASN:HB3	2.17	0.45
1:C:195:LYS:HB3	1:C:195:LYS:HE3	1.76	0.45
1:E:171:ILE:HD12	1:E:171:ILE:H	1.81	0.45
1:A:29:LEU:HD13	1:A:177:PRO:CG	2.46	0.45
1:D:182:ARG:NH2	1:D:184:MET:HE1	2.31	0.45
1:E:129:MET:HE3	2:E:1001:TRP:CE3	2.51	0.45
1:F:164:ARG:HD2	1:F:165:TYR:CZ	2.50	0.45
1:A:107:GLN:CD	1:A:107:GLN:N	2.74	0.45
1:D:19:TYR:CE2	1:D:24:ARG:HG3	2.52	0.45
1:D:56:GLN:O	1:D:60:ARG:HG3	2.16	0.45
1:B:24:ARG:HH11	1:B:24:ARG:CG	2.30	0.45
1:E:242:LEU:O	1:E:246:SER:HB3	2.16	0.45
1:F:16:ILE:HG21	1:F:204:ILE:CG2	2.47	0.45
1:F:86:HIS:HE1	1:F:136:TYR:OH	1.99	0.45
1:A:120:ALA:HA	1:B:99:ILE:CD1	2.47	0.45
1:D:182:ARG:HE	1:D:184:MET:HE1	1.82	0.45
1:B:27:VAL:HG21	1:B:68:VAL:CG1	2.47	0.45
1:B:198:PRO:HB3	1:C:196:SER:O	2.16	0.45
1:C:206:LEU:HD11	1:C:280:LEU:HD21	1.79	0.45
1:E:254:GLU:H	1:E:254:GLU:HG2	1.45	0.45
1:A:24:ARG:CG	1:A:24:ARG:NH1	2.79	0.45
1:A:198:PRO:O	1:A:200:PRO:HD3	2.17	0.45
1:D:173:GLU:OE1	1:D:175:ARG:NH1	2.44	0.45
1:D:209:ASP:O	1:D:213:ILE:HG13	2.16	0.45
1:E:219:SER:O	1:E:219:SER:OG	2.32	0.45
1:D:126:PRO:HB2	1:D:127:PRO:CD	2.40	0.45
1:E:56:GLN:O	1:E:60:ARG:HG3	2.17	0.44
1:B:229:ARG:HG3	1:B:230:TYR:H	1.82	0.44
1:C:272:LEU:HD12	1:C:275:VAL:HG22	1.99	0.44
1:D:23:LEU:HG	1:D:68:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:PHE:HB2	1:C:138:THR:HG21	1.98	0.44
1:C:56:GLN:O	1:C:60:ARG:HG3	2.17	0.44
1:E:305:GLU:O	1:E:309:ARG:CG	2.54	0.44
1:F:56:GLN:O	1:F:60:ARG:HG3	2.18	0.44
1:F:199:ASN:HD22	1:F:200:PRO:HD2	1.82	0.44
1:A:192:LYS:CE	4:A:1003:AMP:C5	2.99	0.44
1:C:182:ARG:NH1	1:C:192:LYS:CB	2.81	0.44
1:C:183:ILE:HG22	1:C:193:MET:HE3	1.99	0.44
1:E:20:ILE:HG22	1:E:20:ILE:O	2.16	0.44
1:E:262:GLY:C	1:E:263:LYS:HD3	2.43	0.44
1:F:13:VAL:O	1:F:195:LYS:HE3	2.17	0.44
1:C:210:ALA:HB2	1:C:277:ILE:HG21	1.99	0.44
1:F:19:TYR:HA	1:F:23:LEU:CB	2.46	0.44
1:A:56:GLN:O	1:A:60:ARG:HG3	2.17	0.44
1:E:171:ILE:N	1:E:171:ILE:CD1	2.80	0.44
1:E:175:ARG:C	1:E:176:ILE:HG13	2.42	0.44
1:B:56:GLN:O	1:B:60:ARG:HG3	2.18	0.44
1:B:281:ARG:NH1	1:B:281:ARG:CG	2.79	0.44
1:C:289:HIS:ND1	1:C:289:HIS:C	2.76	0.44
1:C:309:ARG:HE	1:C:309:ARG:HB3	1.27	0.44
1:E:241:LEU:N	1:E:241:LEU:HD13	2.33	0.44
1:B:19:TYR:HA	1:B:23:LEU:HB3	2.00	0.43
1:E:98:TYR:HA	1:F:118:VAL:O	2.18	0.43
1:E:120:ALA:HA	1:F:99:ILE:CD1	2.48	0.43
1:E:185:SER:HB3	1:E:188:ASP:O	2.18	0.43
1:E:215:LYS:HG2	1:E:218:LYS:NZ	2.31	0.43
1:E:277:ILE:O	1:E:281:ARG:HD2	2.18	0.43
1:B:64:LEU:HD21	1:B:207:LEU:HD21	1.99	0.43
1:B:294:GLU:HB2	1:B:298:ARG:NH2	2.33	0.43
1:E:213:ILE:HD12	1:E:277:ILE:HG13	2.00	0.43
1:F:14:ILE:HG22	1:F:15:THR:H	1.76	0.43
1:A:29:LEU:CD1	1:A:177:PRO:CG	2.95	0.43
1:E:260:TYR:CE2	1:E:268:PHE:HA	2.54	0.43
1:F:170:THR:O	1:F:172:PRO:HD3	2.18	0.43
1:B:241:LEU:HB3	1:B:268:PHE:HE2	1.83	0.43
1:C:155:ARG:HG2	1:C:172:PRO:HD2	2.00	0.43
1:F:9:GLN:OE1	1:F:43:HIS:HB3	2.18	0.43
1:A:124:THR:HG21	1:B:124:THR:CG2	2.45	0.43
1:B:22:ALA:HB1	1:B:26:PHE:HE2	1.82	0.43
1:A:182:ARG:O	1:A:184:MET:HE2	2.18	0.43
1:B:258:ARG:HG3	1:B:258:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:295:GLU:HG2	1:E:298:ARG:HH21	1.83	0.43
1:A:124:THR:CG2	1:B:124:THR:HG21	2.45	0.43
1:D:187:VAL:CG2	1:D:202:ALA:HB2	2.49	0.43
1:E:170:THR:O	1:E:172:PRO:HD3	2.18	0.43
1:E:189:PRO:HG2	1:E:236:PRO:HB2	2.01	0.43
1:E:197:ASP:OD1	1:E:197:ASP:C	2.62	0.43
1:A:195:LYS:N	3:A:1002:PO4:O1	2.32	0.43
1:A:309:ARG:HE	1:A:309:ARG:HB3	1.27	0.43
1:D:309:ARG:HE	1:D:309:ARG:HB3	1.27	0.43
1:C:188:ASP:HB3	1:C:191:LYS:CB	2.49	0.43
1:E:134:LEU:HB3	1:E:169:PHE:CE1	2.54	0.43
1:A:140:ILE:HD11	1:A:175:ARG:CG	2.48	0.42
1:D:215:LYS:HB3	1:D:215:LYS:HZ2	1.66	0.42
1:E:123:LEU:O	1:E:123:LEU:HG	2.19	0.42
1:F:273:ALA:O	1:F:277:ILE:HD12	2.19	0.42
3:A:1002:PO4:O4	4:A:1003:AMP:O1P	2.37	0.42
1:D:79:ILE:HB	1:D:82:GLU:HG3	2.01	0.42
1:D:189:PRO:HG2	1:E:48:TRP:CE2	2.54	0.42
1:D:194:SER:HA	3:D:1002:PO4:O1	2.19	0.42
1:B:302:GLU:O	1:B:306:LYS:HG3	2.18	0.42
1:C:200:PRO:C	1:C:202:ALA:H	2.27	0.42
1:C:218:LYS:HG2	1:C:219:SER:H	1.84	0.42
1:E:99:ILE:CD1	1:F:120:ALA:HA	2.50	0.42
1:A:18:ASN:ND2	1:A:18:ASN:O	2.42	0.42
1:F:16:ILE:HG13	1:F:17:GLY:N	2.34	0.42
1:B:19:TYR:CE2	1:B:24:ARG:HD2	2.55	0.42
1:E:55:ARG:NH1	1:F:324:LEU:O	2.52	0.42
1:E:265:TYR:O	1:E:269:LYS:CG	2.64	0.42
1:F:24:ARG:NH1	1:F:247:THR:O	2.53	0.42
1:C:293:SER:OG	1:C:295:GLU:HB2	2.19	0.42
1:F:11:SER:HB2	1:F:195:LYS:HD2	2.01	0.42
1:C:23:LEU:HA	1:C:26:PHE:CD2	2.53	0.42
1:C:30:GLN:O	1:C:74:GLN:HG3	2.20	0.42
1:E:245:TYR:CG	1:E:272:LEU:HD13	2.55	0.42
1:A:191:LYS:HZ2	1:A:191:LYS:HG2	1.75	0.42
1:D:10:PRO:HA	1:D:61:LEU:CD2	2.49	0.42
1:D:51:PRO:HA	1:C:323:GLY:HA3	2.02	0.42
1:D:151:ILE:HG21	1:D:174:ALA:HB2	2.02	0.42
1:B:205:THR:HG23	1:B:207:LEU:N	2.16	0.42
1:E:126:PRO:HB2	1:E:127:PRO:CD	2.38	0.42
1:E:183:ILE:HB	4:E:1003:AMP:N6	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:HG23	1:A:140:ILE:CG2	2.50	0.42
1:A:123:LEU:O	1:A:123:LEU:HG	2.20	0.41
1:A:313:GLU:CD	1:A:316:ARG:HH21	2.28	0.41
1:B:25:GLN:O	1:B:29:LEU:HG	2.19	0.41
1:B:119:SER:C	1:B:121:GLY:H	2.27	0.41
1:E:210:ALA:HA	1:E:277:ILE:HG12	2.01	0.41
1:F:14:ILE:CG2	1:F:18:ASN:HB3	2.49	0.41
1:A:96:ILE:HG13	1:A:157:LEU:HD22	2.02	0.41
1:A:281:ARG:CG	1:A:282:PRO:CD	2.97	0.41
1:B:192:LYS:HE2	1:B:192:LYS:HB3	1.48	0.41
1:C:211:LYS:HB3	1:C:211:LYS:HE3	1.82	0.41
1:A:146:ASP:OD1	1:A:146:ASP:N	2.50	0.41
1:B:238:ILE:HD13	1:B:238:ILE:HA	1.79	0.41
1:B:278:GLU:OE1	1:B:278:GLU:HA	2.18	0.41
1:B:308:ASN:HD22	1:B:308:ASN:HA	1.66	0.41
1:C:17:GLY:HA3	4:C:1003:AMP:N6	2.35	0.41
1:E:64:LEU:HG	1:E:287:TYR:CE1	2.55	0.41
1:E:189:PRO:HB3	1:E:237:GLY:CA	2.46	0.41
1:E:294:GLU:C	1:E:296:LEU:H	2.28	0.41
1:F:151:ILE:O	1:F:154:THR:HG23	2.20	0.41
1:A:67:ALA:O	1:A:286:ARG:NH1	2.51	0.41
1:D:212:THR:O	1:D:215:LYS:HG2	2.20	0.41
1:C:26:PHE:HB3	1:C:37:PHE:CZ	2.55	0.41
1:C:178:LYS:O	1:C:179:VAL:C	2.63	0.41
1:C:267:VAL:O	1:C:271:ASP:OD2	2.37	0.41
1:E:129:MET:HE3	2:E:1001:TRP:CZ3	2.55	0.41
1:E:258:ARG:NH2	1:E:258:ARG:HB2	2.35	0.41
1:A:151:ILE:HG21	1:A:174:ALA:HB2	2.03	0.41
1:D:176:ILE:HB	1:D:179:VAL:CG1	2.40	0.41
1:C:29:LEU:HD11	1:C:177:PRO:HB2	1.96	0.41
1:E:308:ASN:HD22	1:E:308:ASN:HA	1.62	0.41
1:F:4:ILE:HG23	1:F:140:ILE:HG23	2.02	0.41
1:B:313:GLU:CD	1:B:316:ARG:HH21	2.25	0.41
1:E:289:HIS:O	1:E:292:GLU:HG3	2.20	0.41
1:F:14:ILE:N	1:F:14:ILE:CD1	2.83	0.41
1:A:79:ILE:HB	1:A:82:GLU:HG3	2.02	0.41
1:D:22:ALA:C	1:D:26:PHE:HE2	2.28	0.41
1:B:71:ASP:HA	1:B:72:PRO:HD2	1.91	0.41
1:B:118:VAL:O	1:B:118:VAL:CG2	2.68	0.41
1:B:187:VAL:HG21	1:B:199:ASN:HD22	1.85	0.41
1:E:21:GLY:O	1:E:179:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:ASP:HA	1:E:72:PRO:HD2	1.91	0.41
1:E:140:ILE:HD11	1:E:175:ARG:HD3	2.03	0.41
1:F:104:ARG:NH1	1:F:104:ARG:CG	2.65	0.41
1:F:205:THR:CG2	1:F:206:LEU:N	2.83	0.41
1:A:195:LYS:HG2	3:A:1002:PO4:O1	2.21	0.41
1:A:254:GLU:H	1:A:254:GLU:CD	2.28	0.41
1:B:79:ILE:HB	1:B:82:GLU:HG3	2.01	0.41
1:C:187:VAL:CG2	1:C:199:ASN:OD1	2.46	0.41
1:E:79:ILE:HB	1:E:82:GLU:HG3	2.02	0.41
1:E:187:VAL:HG13	1:E:202:ALA:CA	2.51	0.41
1:E:205:THR:HG23	1:E:207:LEU:H	1.79	0.41
1:F:184:MET:CG	1:F:189:PRO:O	2.66	0.41
1:D:182:ARG:HH21	1:D:184:MET:HE1	1.85	0.41
1:B:19:TYR:CE2	1:B:24:ARG:HD3	2.56	0.41
1:B:200:PRO:O	1:B:216:LYS:NZ	2.54	0.41
1:B:229:ARG:CG	1:B:230:TYR:H	2.33	0.41
1:E:151:ILE:O	1:E:154:THR:HG23	2.20	0.41
1:F:79:ILE:HB	1:F:82:GLU:HG3	2.03	0.41
1:D:313:GLU:CD	1:D:316:ARG:HH21	2.26	0.40
1:B:19:TYR:O	1:B:24:ARG:HB2	2.21	0.40
1:B:258:ARG:HG2	1:B:258:ARG:H	1.37	0.40
1:C:183:ILE:N	1:C:183:ILE:HD13	2.37	0.40
1:C:313:GLU:CD	1:C:316:ARG:HH21	2.28	0.40
1:A:1:MET:SD	1:A:32:GLU:O	2.79	0.40
1:B:308:ASN:O	1:B:312:SER:HB2	2.21	0.40
1:E:118:VAL:O	1:F:99:ILE:CG1	2.69	0.40
1:B:134:LEU:HB3	1:B:169:PHE:HD1	1.72	0.40
1:E:213:ILE:CD1	1:E:277:ILE:HG13	2.51	0.40
1:F:161:PHE:CD2	1:F:169:PHE:HE2	2.39	0.40
1:D:14:ILE:HG22	1:D:18:ASN:HB3	2.04	0.40
1:B:225:GLU:OE1	1:B:227:THR:HG23	2.21	0.40
1:C:151:ILE:O	1:C:154:THR:HG23	2.21	0.40
1:E:96:ILE:HG13	1:E:157:LEU:HD22	2.03	0.40
1:E:272:LEU:HA	1:E:275:VAL:HG13	2.04	0.40
1:E:283:ILE:N	1:E:286:ARG:HH21	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	287/328 (88%)	279 (97%)	7 (2%)	1 (0%)	36	52
1	B	277/328 (84%)	269 (97%)	8 (3%)	0	100	100
1	C	265/328 (81%)	250 (94%)	15 (6%)	0	100	100
1	D	276/328 (84%)	263 (95%)	13 (5%)	0	100	100
1	E	282/328 (86%)	263 (93%)	19 (7%)	0	100	100
1	F	284/328 (87%)	273 (96%)	11 (4%)	0	100	100
All	All	1671/1968 (85%)	1597 (96%)	73 (4%)	1 (0%)	48	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/280 (92%)	210 (81%)	48 (19%)	1	2
1	B	253/280 (90%)	207 (82%)	46 (18%)	2	2
1	C	241/280 (86%)	192 (80%)	49 (20%)	1	1
1	D	248/280 (89%)	197 (79%)	51 (21%)	1	1
1	E	252/280 (90%)	199 (79%)	53 (21%)	1	1
1	F	256/280 (91%)	211 (82%)	45 (18%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1508/1680 (90%)	1216 (81%)	292 (19%)	1 2

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	ILE
1	A	9	GLN
1	A	18	ASN
1	A	24	ARG
1	A	25	GLN
1	A	28	GLU
1	A	55	ARG
1	A	56	GLN
1	A	68	VAL
1	A	94	GLN
1	A	99	ILE
1	A	105	MET
1	A	106	THR
1	A	107	GLN
1	A	122	LEU
1	A	123	LEU
1	A	138	THR
1	A	140	ILE
1	A	146	ASP
1	A	154	THR
1	A	159	GLU
1	A	164	ARG
1	A	171	ILE
1	A	182	ARG
1	A	185	SER
1	A	187	VAL
1	A	191	LYS
1	A	196	SER
1	A	205	THR
1	A	206	LEU
1	A	211	LYS
1	A	224	SER
1	A	225	GLU
1	A	227	THR
1	A	228	ILE
1	A	229	ARG

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Mol	Chain	Res	Type
1	A	238	ILE
1	A	241	LEU
1	A	255	GLU
1	A	271	ASP
1	A	275	VAL
1	A	281	ARG
1	A	298	ARG
1	A	308	ASN
1	A	309	ARG
1	A	312	SER
1	A	316	ARG
1	D	1	MET
1	D	8	ILE
1	D	14	ILE
1	D	16	ILE
1	D	28	GLU
1	D	32	GLU
1	D	55	ARG
1	D	56	GLN
1	D	68	VAL
1	D	94	GLN
1	D	99	ILE
1	D	118	VAL
1	D	119	SER
1	D	122	LEU
1	D	123	LEU
1	D	138	THR
1	D	140	ILE
1	D	146	ASP
1	D	154	THR
1	D	159	GLU
1	D	175	ARG
1	D	176	ILE
1	D	182	ARG
1	D	183	ILE
1	D	187	VAL
1	D	191	LYS
1	D	192	LYS
1	D	195	LYS
1	D	204	ILE
1	D	205	THR
1	D	211	LYS

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Mol	Chain	Res	Type
1	D	215	LYS
1	D	217	ILE
1	D	219	SER
1	D	238	ILE
1	D	239	SER
1	D	241	LEU
1	D	242	LEU
1	D	251	GLN
1	D	256	LEU
1	D	274	GLN
1	D	275	VAL
1	D	278	GLU
1	D	281	ARG
1	D	284	GLN
1	D	285	GLU
1	D	294	GLU
1	D	308	ASN
1	D	309	ARG
1	D	312	SER
1	D	316	ARG
1	B	8	ILE
1	B	16	ILE
1	B	18	ASN
1	B	24	ARG
1	B	55	ARG
1	B	56	GLN
1	B	68	VAL
1	B	94	GLN
1	B	99	ILE
1	B	107	GLN
1	B	122	LEU
1	B	123	LEU
1	B	138	THR
1	B	140	ILE
1	B	146	ASP
1	B	154	THR
1	B	159	GLU
1	B	164	ARG
1	B	182	ARG
1	B	185	SER
1	B	191	LYS
1	B	192	LYS

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Mol	Chain	Res	Type
1	B	194	SER
1	B	205	THR
1	B	211	LYS
1	B	217	ILE
1	B	227	THR
1	B	229	ARG
1	B	238	ILE
1	B	241	LEU
1	B	251	GLN
1	B	252	SER
1	B	254	GLU
1	B	257	GLU
1	B	258	ARG
1	B	259	GLN
1	B	263	LYS
1	B	274	GLN
1	B	275	VAL
1	B	278	GLU
1	B	293	SER
1	B	294	GLU
1	B	298	ARG
1	B	308	ASN
1	B	312	SER
1	B	316	ARG
1	C	1	MET
1	C	8	ILE
1	C	16	ILE
1	C	23	LEU
1	C	55	ARG
1	C	56	GLN
1	C	68	VAL
1	C	94	GLN
1	C	99	ILE
1	C	106	THR
1	C	107	GLN
1	C	119	SER
1	C	122	LEU
1	C	123	LEU
1	C	138	THR
1	C	140	ILE
1	C	146	ASP
1	C	154	THR

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Mol	Chain	Res	Type
1	C	159	GLU
1	C	164	ARG
1	C	179	VAL
1	C	182	ARG
1	C	183	ILE
1	C	192	LYS
1	C	195	LYS
1	C	196	SER
1	C	204	ILE
1	C	205	THR
1	C	207	LEU
1	C	211	LYS
1	C	217	ILE
1	C	218	LYS
1	C	219	SER
1	C	225	GLU
1	C	227	THR
1	C	241	LEU
1	C	248	LEU
1	C	267	VAL
1	C	275	VAL
1	C	276	VAL
1	C	278	GLU
1	C	285	GLU
1	C	289	HIS
1	C	293	SER
1	C	298	ARG
1	C	308	ASN
1	C	309	ARG
1	C	312	SER
1	C	316	ARG
1	E	8	ILE
1	E	9	GLN
1	E	15	THR
1	E	24	ARG
1	E	25	GLN
1	E	55	ARG
1	E	56	GLN
1	E	68	VAL
1	E	94	GLN
1	E	99	ILE
1	E	118	VAL

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Mol	Chain	Res	Type
1	E	119	SER
1	E	122	LEU
1	E	123	LEU
1	E	138	THR
1	E	140	ILE
1	E	146	ASP
1	E	154	THR
1	E	159	GLU
1	E	164	ARG
1	E	171	ILE
1	E	176	ILE
1	E	178	LYS
1	E	182	ARG
1	E	187	VAL
1	E	205	THR
1	E	206	LEU
1	E	211	LYS
1	E	217	ILE
1	E	241	LEU
1	E	246	SER
1	E	251	GLN
1	E	252	SER
1	E	253	ILE
1	E	254	GLU
1	E	256	LEU
1	E	258	ARG
1	E	259	GLN
1	E	263	LYS
1	E	267	VAL
1	E	275	VAL
1	E	278	GLU
1	E	281	ARG
1	E	284	GLN
1	E	285	GLU
1	E	292	GLU
1	E	293	SER
1	E	294	GLU
1	E	295	GLU
1	E	298	ARG
1	E	308	ASN
1	E	312	SER
1	E	316	ARG

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Mol	Chain	Res	Type
1	F	1	MET
1	F	8	ILE
1	F	9	GLN
1	F	13	VAL
1	F	14	ILE
1	F	15	THR
1	F	23	LEU
1	F	55	ARG
1	F	56	GLN
1	F	68	VAL
1	F	94	GLN
1	F	99	ILE
1	F	104	ARG
1	F	118	VAL
1	F	119	SER
1	F	122	LEU
1	F	123	LEU
1	F	138	THR
1	F	146	ASP
1	F	154	THR
1	F	159	GLU
1	F	164	ARG
1	F	175	ARG
1	F	188	ASP
1	F	194	SER
1	F	196	SER
1	F	205	THR
1	F	211	LYS
1	F	225	GLU
1	F	227	THR
1	F	228	ILE
1	F	229	ARG
1	F	238	ILE
1	F	241	LEU
1	F	254	GLU
1	F	263	LYS
1	F	274	GLN
1	F	275	VAL
1	F	278	GLU
1	F	292	GLU
1	F	295	GLU
1	F	308	ASN

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Mol	Chain	Res	Type
1	F	309	ARG
1	F	312	SER
1	F	316	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	18	ASN
1	A	34	ASN
1	A	86	HIS
1	A	94	GLN
1	A	107	GLN
1	A	137	ASN
1	A	150	HIS
1	A	199	ASN
1	A	259	GLN
1	A	284	GLN
1	A	289	HIS
1	A	308	ASN
1	A	320	GLN
1	D	9	GLN
1	D	34	ASN
1	D	43	HIS
1	D	74	GLN
1	D	86	HIS
1	D	94	GLN
1	D	150	HIS
1	D	199	ASN
1	D	284	GLN
1	D	308	ASN
1	D	320	GLN
1	B	25	GLN
1	B	34	ASN
1	B	43	HIS
1	B	86	HIS
1	B	94	GLN
1	B	107	GLN
1	B	150	HIS
1	B	284	GLN
1	B	308	ASN
1	B	320	GLN

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Mol	Chain	Res	Type
1	C	9	GLN
1	C	34	ASN
1	C	43	HIS
1	C	86	HIS
1	C	137	ASN
1	C	150	HIS
1	C	284	GLN
1	C	308	ASN
1	C	320	GLN
1	E	9	GLN
1	E	18	ASN
1	E	25	GLN
1	E	34	ASN
1	E	86	HIS
1	E	107	GLN
1	E	150	HIS
1	E	199	ASN
1	E	308	ASN
1	E	320	GLN
1	F	9	GLN
1	F	18	ASN
1	F	31	HIS
1	F	34	ASN
1	F	43	HIS
1	F	86	HIS
1	F	94	GLN
1	F	150	HIS
1	F	199	ASN
1	F	251	GLN
1	F	259	GLN
1	F	289	HIS
1	F	308	ASN
1	F	320	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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$
2	TRP	B	1001	-	15,16,16	0.68	0	18,22,22	0.40	0
2	TRP	E	1001	-	15,16,16	0.66	0	18,22,22	0.40	0
3	PO4	B	1002	-	4,4,4	2.16	1 (25%)	6,6,6	0.37	0
2	TRP	A	1001	-	15,16,16	0.66	0	18,22,22	0.40	0
3	PO4	D	1002	-	4,4,4	2.01	1 (25%)	6,6,6	0.50	0
2	TRP	D	1001	-	15,16,16	0.66	0	18,22,22	0.38	0
4	AMP	F	1003	-	25,25,25	0.63	0	37,38,38	0.69	0
4	AMP	A	1003	-	25,25,25	0.68	0	37,38,38	0.78	1 (2%)
4	AMP	E	1003	-	25,25,25	0.64	0	37,38,38	0.68	0
3	PO4	A	1002	-	4,4,4	2.16	1 (25%)	6,6,6	0.41	0
3	PO4	C	1002	-	4,4,4	1.99	1 (25%)	6,6,6	0.43	0
3	PO4	E	1002	-	4,4,4	1.96	1 (25%)	6,6,6	0.40	0
2	TRP	C	1001	-	15,16,16	0.67	0	18,22,22	0.40	0
3	PO4	F	1002	-	4,4,4	2.03	1 (25%)	6,6,6	0.48	0
4	AMP	D	1003	-	25,25,25	0.64	0	37,38,38	0.76	0
4	AMP	B	1003	-	25,25,25	0.64	0	37,38,38	0.67	0
4	AMP	C	1003	-	25,25,25	0.66	0	37,38,38	0.75	1 (2%)
2	TRP	F	1001	-	15,16,16	0.68	0	18,22,22	0.40	0

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
2	TRP	B	1001	-	-	0/8/8/8	0/2/2/2
2	TRP	E	1001	-	-	0/8/8/8	0/2/2/2
2	TRP	A	1001	-	-	0/8/8/8	0/2/2/2
2	TRP	D	1001	-	-	0/8/8/8	0/2/2/2
4	AMP	F	1003	-	-	3/10/26/26	0/3/3/3
4	AMP	A	1003	-	-	3/10/26/26	0/3/3/3
4	AMP	E	1003	-	-	1/10/26/26	0/3/3/3
2	TRP	C	1001	-	-	0/8/8/8	0/2/2/2
4	AMP	D	1003	-	-	3/10/26/26	0/3/3/3
4	AMP	B	1003	-	-	5/10/26/26	0/3/3/3
4	AMP	C	1003	-	-	2/10/26/26	0/3/3/3
2	TRP	F	1001	-	-	0/8/8/8	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	PO4	P-O1	3.61	1.59	1.50
3	A	1002	PO4	P-O1	3.61	1.59	1.50
3	D	1002	PO4	P-O1	3.40	1.58	1.50
3	F	1002	PO4	P-O1	3.32	1.58	1.50
3	C	1002	PO4	P-O1	3.27	1.58	1.50
3	E	1002	PO4	P-O1	3.27	1.58	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	AMP	C2'-C3'-C4'	-2.21	98.33	102.61
4	C	1003	AMP	C3'-C2'-C1'	2.13	105.49	101.46

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	AMP	C5'-O5'-P-O1P
4	A	1003	AMP	C5'-O5'-P-O2P
4	A	1003	AMP	C5'-O5'-P-O3P
4	B	1003	AMP	C5'-O5'-P-O1P
4	B	1003	AMP	C5'-O5'-P-O2P
4	B	1003	AMP	C5'-O5'-P-O3P
4	F	1003	AMP	C5'-O5'-P-O1P
4	C	1003	AMP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	B	1003	AMP	O4'-C4'-C5'-O5'
4	C	1003	AMP	O4'-C4'-C5'-O5'
4	D	1003	AMP	C5'-O5'-P-O1P
4	D	1003	AMP	C3'-C4'-C5'-O5'
4	D	1003	AMP	O4'-C4'-C5'-O5'
4	F	1003	AMP	C5'-O5'-P-O2P
4	B	1003	AMP	C3'-C4'-C5'-O5'
4	F	1003	AMP	O4'-C4'-C5'-O5'
4	E	1003	AMP	C5'-O5'-P-O3P

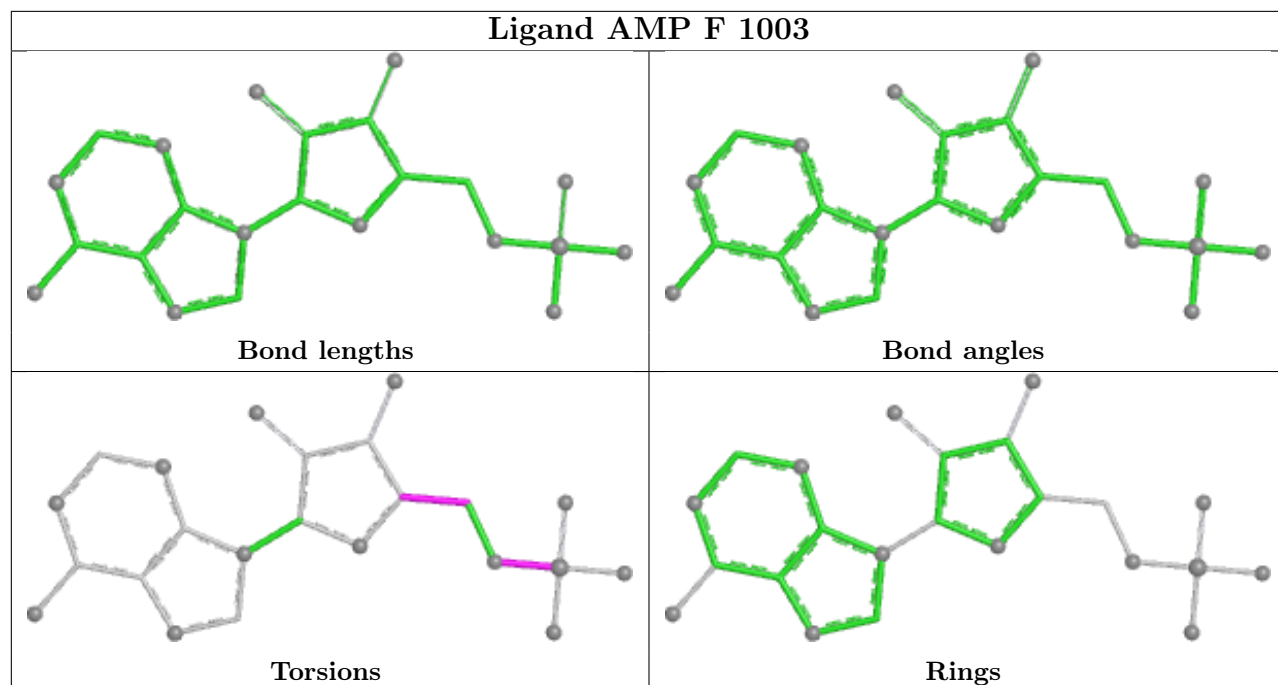
There are no ring outliers.

11 monomers are involved in 39 short contacts:

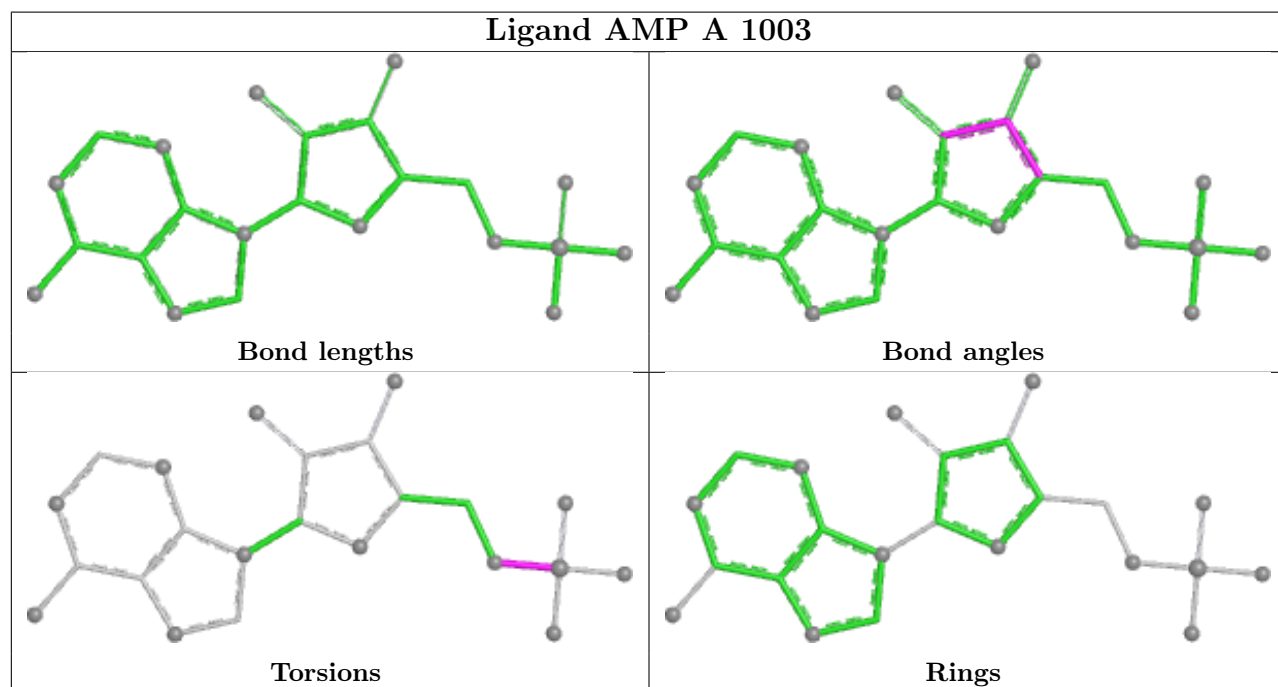
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1001	TRP	2	0
3	B	1002	PO4	2	0
3	D	1002	PO4	4	0
4	F	1003	AMP	5	0
4	A	1003	AMP	4	0
4	E	1003	AMP	7	0
3	A	1002	PO4	3	0
3	F	1002	PO4	1	0
4	D	1003	AMP	5	0
4	B	1003	AMP	7	0
4	C	1003	AMP	5	0

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

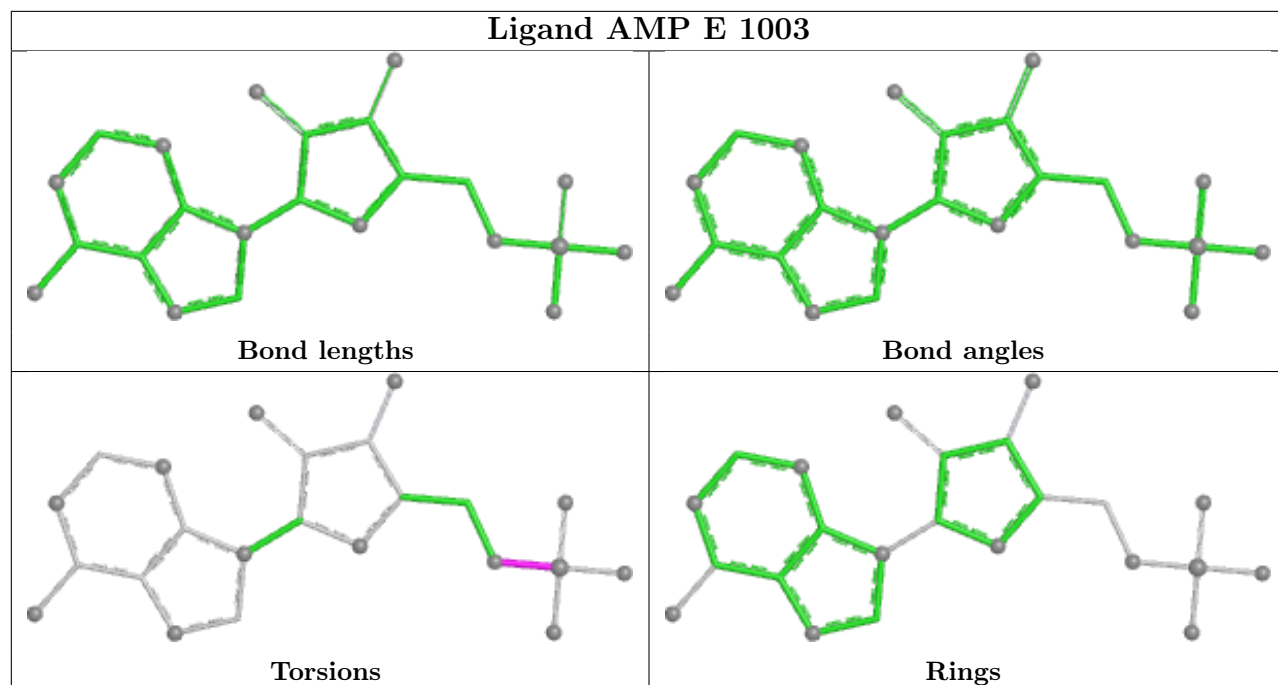
Ligand AMP F 1003



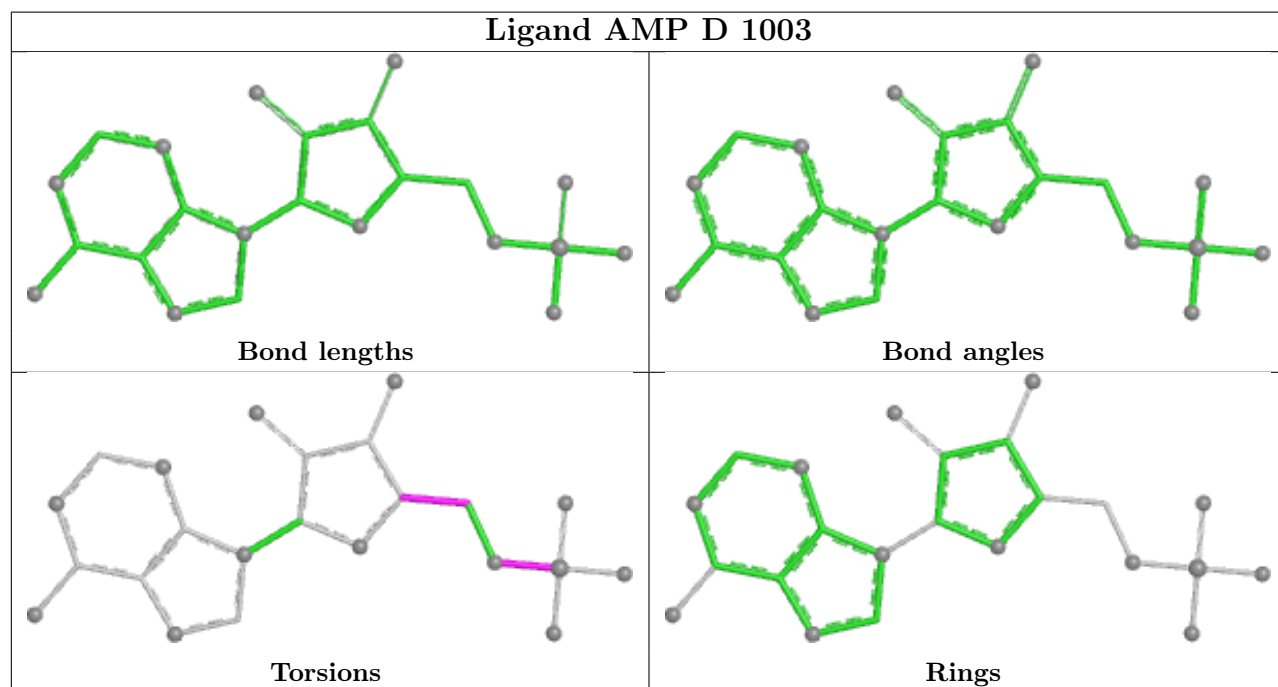
Ligand AMP A 1003

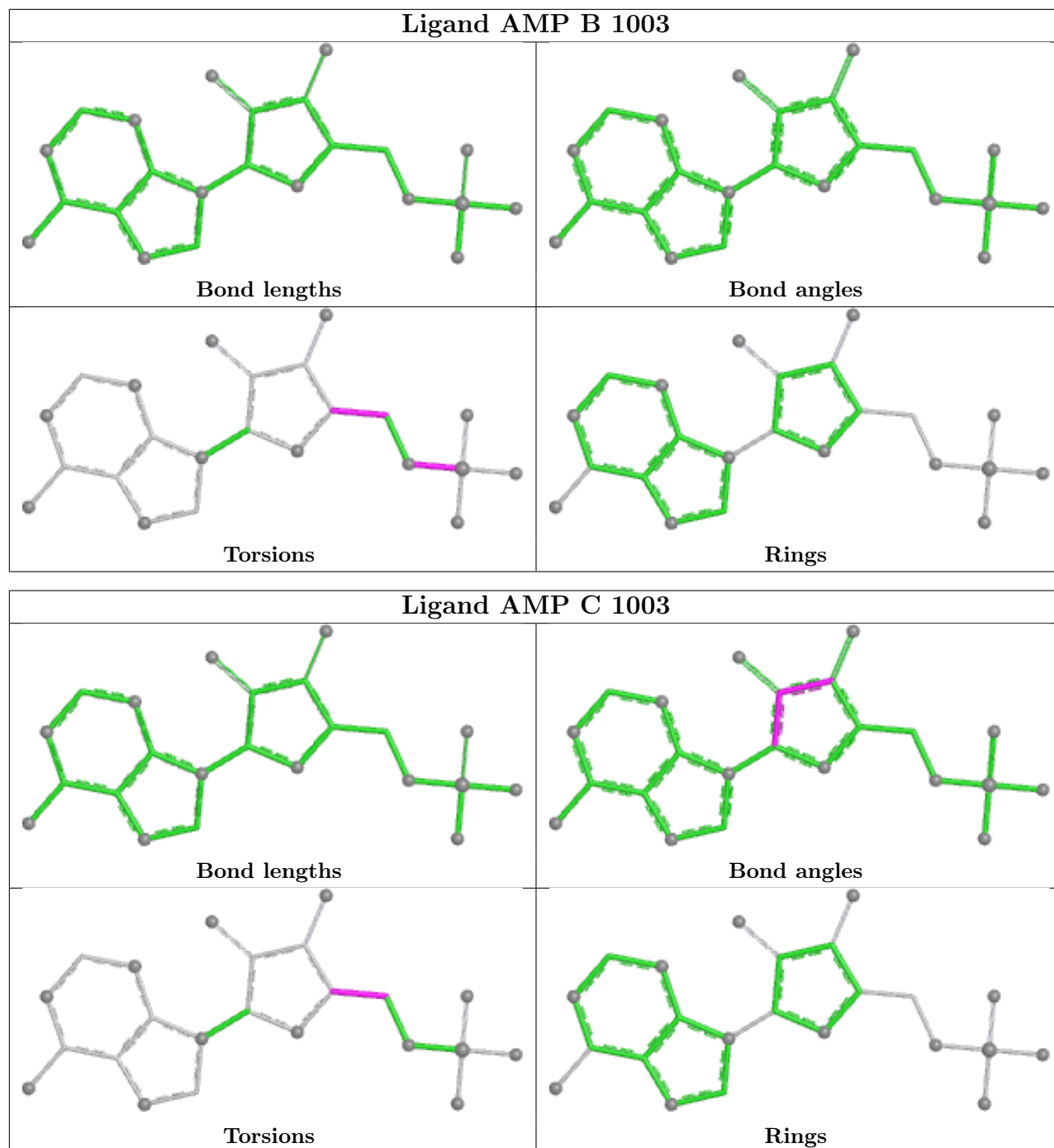


Ligand AMP E 1003



Ligand AMP D 1003





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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	299/328 (91%)	0.52	15 (5%) 34 26	36, 53, 75, 101	0
1	B	291/328 (88%)	0.94	35 (12%) 9 7	38, 66, 91, 103	0
1	C	279/328 (85%)	1.27	67 (24%) 2 1	41, 66, 99, 116	0
1	D	286/328 (87%)	0.97	39 (13%) 7 5	39, 64, 96, 109	0
1	E	292/328 (89%)	1.40	71 (24%) 2 1	54, 85, 114, 124	0
1	F	296/328 (90%)	0.85	25 (8%) 17 12	27, 62, 81, 98	0
All	All	1743/1968 (88%)	0.99	252 (14%) 6 4	27, 64, 101, 124	0

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	26	PHE	7.2
1	F	11	SER	7.0
1	A	180	GLY	6.9
1	C	22	ALA	6.0
1	D	238	ILE	5.6
1	C	236	PRO	5.5
1	C	238	ILE	5.5
1	E	22	ALA	4.8
1	D	260	TYR	4.8
1	C	177	PRO	4.8
1	C	219	SER	4.7
1	E	198	PRO	4.5
1	C	268	PHE	4.4
1	A	179	VAL	4.4
1	D	181	ALA	4.3
1	C	239	SER	4.2
1	B	26	PHE	4.1
1	E	118	VAL	4.1
1	C	227	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	198	PRO	4.0
1	B	230	TYR	4.0
1	D	12	GLY	4.0
1	E	267	VAL	4.0
1	E	219	SER	4.0
1	C	269	LYS	4.0
1	C	266	GLY	4.0
1	E	177	PRO	4.0
1	C	267	VAL	4.0
1	C	181	ALA	3.9
1	E	253	ILE	3.9
1	D	253	ILE	3.8
1	E	236	PRO	3.8
1	D	220	ALA	3.8
1	E	186	LEU	3.7
1	D	217	ILE	3.7
1	A	181	ALA	3.7
1	C	224	SER	3.7
1	C	272	LEU	3.7
1	E	199	ASN	3.7
1	F	105	MET	3.7
1	C	241	LEU	3.6
1	D	180	GLY	3.6
1	A	106	THR	3.6
1	B	118	VAL	3.6
1	B	236	PRO	3.5
1	E	201	LYS	3.5
1	B	187	VAL	3.5
1	E	176	ILE	3.4
1	B	219	SER	3.4
1	D	169	PHE	3.4
1	C	178	LYS	3.4
1	C	169	PHE	3.4
1	B	261	GLU	3.4
1	F	12	GLY	3.4
1	E	269	LYS	3.4
1	C	237	GLY	3.4
1	E	238	ILE	3.3
1	E	239	SER	3.3
1	C	244	ILE	3.3
1	A	177	PRO	3.3
1	E	1	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	9	GLN	3.3
1	A	118	VAL	3.3
1	E	252	SER	3.2
1	E	217	ILE	3.2
1	D	197	ASP	3.2
1	A	176	ILE	3.2
1	D	213	ILE	3.2
1	C	242	LEU	3.1
1	C	274	GLN	3.1
1	C	270	ALA	3.1
1	E	204	ILE	3.1
1	C	187	VAL	3.1
1	F	211	LYS	3.1
1	F	169	PHE	3.1
1	E	241	LEU	3.1
1	E	191	LYS	3.1
1	B	309	ARG	3.1
1	E	207	LEU	3.0
1	E	265	TYR	3.0
1	F	118	VAL	3.0
1	C	210	ALA	3.0
1	C	191	LYS	3.0
1	E	218	LYS	3.0
1	C	205	THR	3.0
1	B	289	HIS	3.0
1	C	225	GLU	2.9
1	E	268	PHE	2.9
1	C	198	PRO	2.9
1	E	240	ASN	2.9
1	D	242	LEU	2.9
1	E	48	TRP	2.8
1	A	144	GLY	2.8
1	D	269	LYS	2.8
1	E	178	LYS	2.8
1	E	180	GLY	2.8
1	E	242	LEU	2.8
1	A	289	HIS	2.8
1	C	204	ILE	2.8
1	C	226	GLY	2.8
1	C	186	LEU	2.8
1	E	260	TYR	2.8
1	D	187	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	118	VAL	2.8
1	E	179	VAL	2.8
1	B	228	ILE	2.8
1	B	224	SER	2.8
1	D	256	LEU	2.8
1	D	13	VAL	2.7
1	E	214	GLU	2.7
1	F	13	VAL	2.7
1	E	165	TYR	2.7
1	E	264	GLY	2.7
1	B	267	VAL	2.7
1	A	178	LYS	2.7
1	E	259	GLN	2.7
1	D	267	VAL	2.7
1	B	218	LYS	2.7
1	F	8	ILE	2.7
1	E	69	GLY	2.7
1	C	308	ASN	2.7
1	C	190	THR	2.7
1	C	216	LYS	2.7
1	B	265	TYR	2.6
1	E	244	ILE	2.6
1	D	258	ARG	2.6
1	C	309	ARG	2.6
1	E	273	ALA	2.6
1	A	107	GLN	2.6
1	C	248	LEU	2.6
1	E	29	LEU	2.6
1	D	309	ARG	2.6
1	E	107	GLN	2.6
1	C	175	ARG	2.6
1	F	31	HIS	2.6
1	B	173	GLU	2.6
1	F	120	ALA	2.6
1	C	218	LYS	2.6
1	B	199	ASN	2.6
1	E	215	LYS	2.5
1	D	254	GLU	2.5
1	D	239	SER	2.5
1	D	48	TRP	2.5
1	C	182	ARG	2.5
1	E	195	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	182	ARG	2.5
1	D	25	GLN	2.5
1	E	197	ASP	2.5
1	C	17	GLY	2.5
1	C	52	HIS	2.4
1	E	248	LEU	2.4
1	F	308	ASN	2.4
1	C	245	TYR	2.4
1	D	75	ALA	2.4
1	E	213	ILE	2.4
1	C	163	LYS	2.4
1	B	264	GLY	2.4
1	D	174	ALA	2.4
1	E	256	LEU	2.4
1	B	247	THR	2.4
1	C	214	GLU	2.4
1	D	198	PRO	2.4
1	B	107	GLN	2.4
1	D	118	VAL	2.4
1	E	169	PHE	2.4
1	D	189	PRO	2.3
1	C	217	ILE	2.3
1	F	70	ILE	2.3
1	D	200	PRO	2.3
1	E	211	LYS	2.3
1	B	188	ASP	2.3
1	B	258	ARG	2.3
1	E	35	CYS	2.3
1	D	178	LYS	2.3
1	E	15	THR	2.3
1	E	216	LYS	2.3
1	F	28	GLU	2.3
1	A	308	ASN	2.3
1	B	274	GLN	2.3
1	B	256	LEU	2.3
1	C	201	LYS	2.2
1	C	28	GLU	2.2
1	E	17	GLY	2.2
1	E	144	GLY	2.2
1	C	206	LEU	2.2
1	B	22	ALA	2.2
1	F	2	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	1	MET	2.2
1	D	107	GLN	2.2
1	C	271	ASP	2.2
1	D	191	LYS	2.2
1	E	245	TYR	2.2
1	D	241	LEU	2.2
1	B	144	GLY	2.2
1	C	23	LEU	2.2
1	E	276	VAL	2.2
1	B	169	PHE	2.2
1	E	67	ALA	2.2
1	E	298	ARG	2.2
1	D	240	ASN	2.2
1	C	243	ASN	2.2
1	E	36	TYR	2.2
1	C	25	GLN	2.2
1	C	192	LYS	2.2
1	B	37	PHE	2.2
1	F	295	GLU	2.1
1	B	104	ARG	2.1
1	C	189	PRO	2.1
1	E	189	PRO	2.1
1	F	163	LYS	2.1
1	E	66	LEU	2.1
1	D	52	HIS	2.1
1	C	183	ILE	2.1
1	C	213	ILE	2.1
1	E	50	ASP	2.1
1	E	196	SER	2.1
1	A	169	PHE	2.1
1	F	152	GLU	2.1
1	F	164	ARG	2.1
1	C	240	ASN	2.1
1	F	102	LEU	2.1
1	C	312	SER	2.1
1	C	273	ALA	2.1
1	C	32	GLU	2.1
1	D	186	LEU	2.1
1	B	165	TYR	2.1
1	B	217	ILE	2.1
1	C	179	VAL	2.1
1	E	27	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	202	ALA	2.1
1	D	2	LYS	2.1
1	C	106	THR	2.1
1	B	197	ASP	2.0
1	F	104	ARG	2.0
1	F	305	GLU	2.0
1	A	219	SER	2.0
1	D	1	MET	2.0
1	C	30	GLN	2.0
1	F	30	GLN	2.0
1	B	34	ASN	2.0
1	B	271	ASP	2.0
1	F	261	GLU	2.0
1	E	270	ALA	2.0
1	C	15	THR	2.0
1	E	279	THR	2.0
1	E	272	LEU	2.0
1	C	199	ASN	2.0
1	E	70	ILE	2.0
1	E	266	GLY	2.0
1	E	308	ASN	2.0
1	A	309	ARG	2.0
1	E	19	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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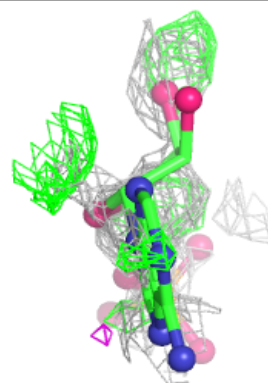
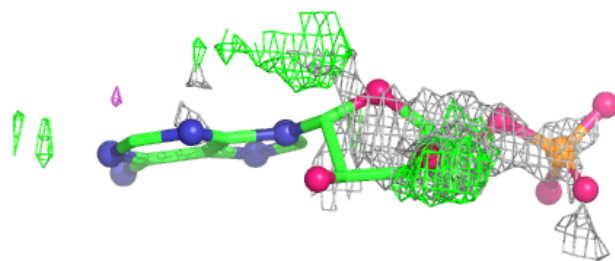
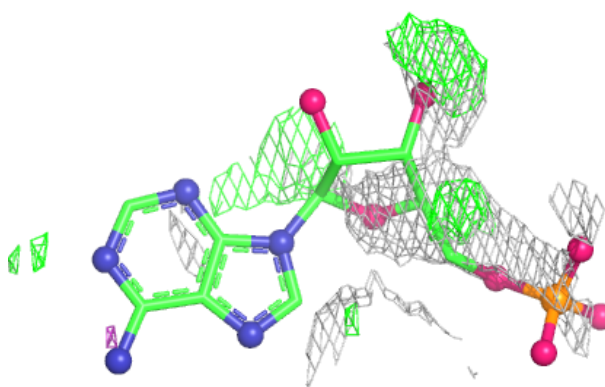
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AMP	C	1003	23/23	0.59	0.47	64,67,72,73	23
4	AMP	D	1003	23/23	0.68	0.47	62,66,70,71	23
4	AMP	A	1003	23/23	0.69	0.44	41,47,54,56	23
4	AMP	F	1003	23/23	0.69	0.43	55,61,66,67	23
4	AMP	E	1003	23/23	0.71	0.32	72,76,81,82	23
3	PO4	F	1002	5/5	0.72	0.14	89,92,95,95	0
4	AMP	B	1003	23/23	0.74	0.32	42,50,57,59	23
3	PO4	E	1002	5/5	0.78	0.15	73,76,79,80	5
3	PO4	C	1002	5/5	0.78	0.14	83,86,89,90	0
3	PO4	B	1002	5/5	0.80	0.14	74,77,80,81	0
3	PO4	A	1002	5/5	0.80	0.12	55,58,61,62	5
2	TRP	E	1001	15/15	0.85	0.19	63,70,94,94	15
3	PO4	D	1002	5/5	0.86	0.15	73,76,79,80	5
2	TRP	B	1001	15/15	0.88	0.12	36,42,67,67	15
2	TRP	A	1001	15/15	0.90	0.11	30,36,61,61	15
2	TRP	F	1001	15/15	0.90	0.13	36,42,67,67	15
2	TRP	D	1001	15/15	0.91	0.13	44,50,74,75	15
2	TRP	C	1001	15/15	0.93	0.11	34,40,65,65	15

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

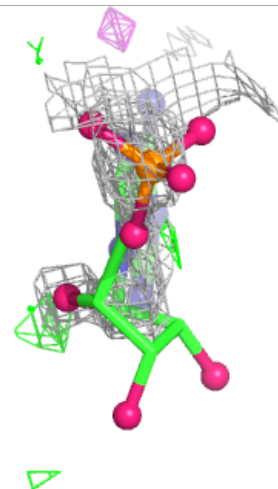
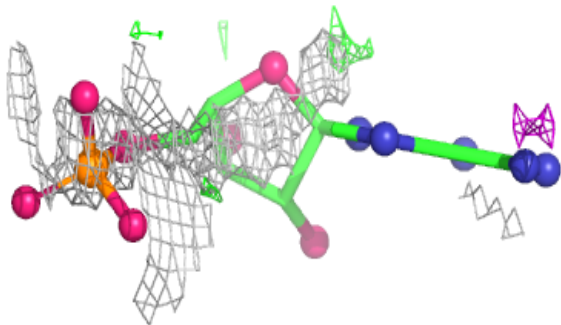
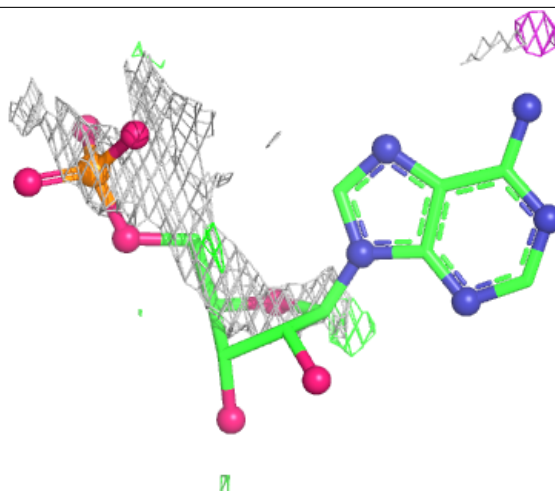
Electron density around AMP C 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



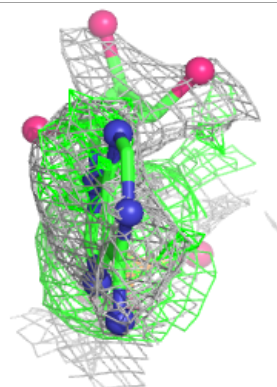
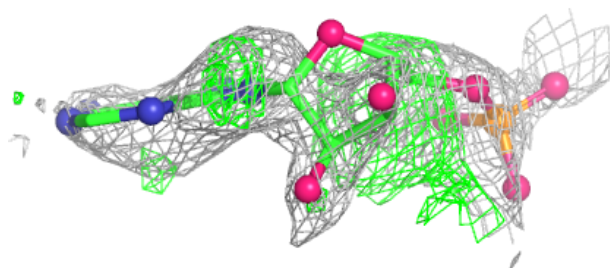
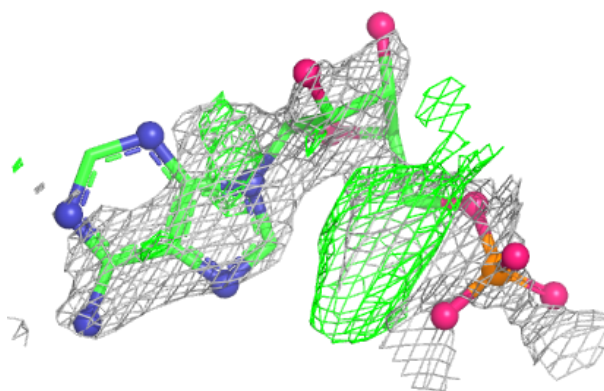
Electron density around AMP D 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

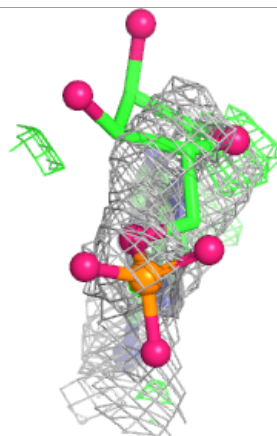
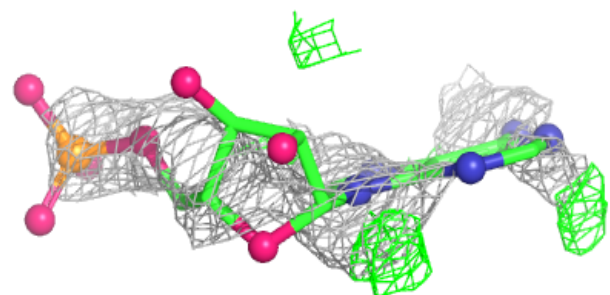
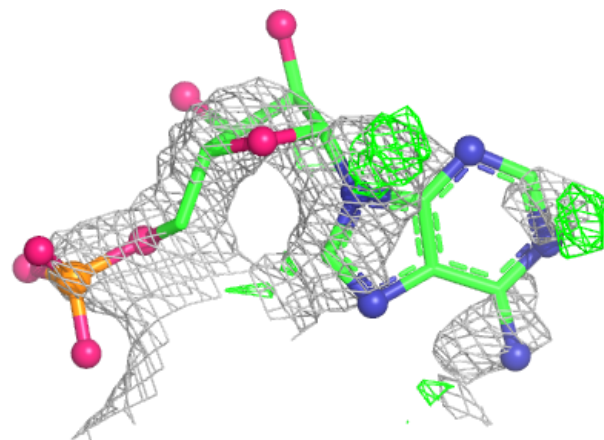


Electron density around AMP A 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

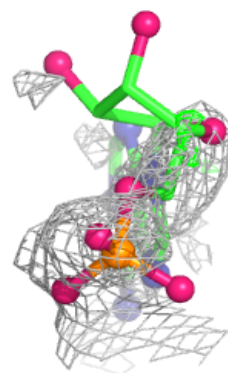
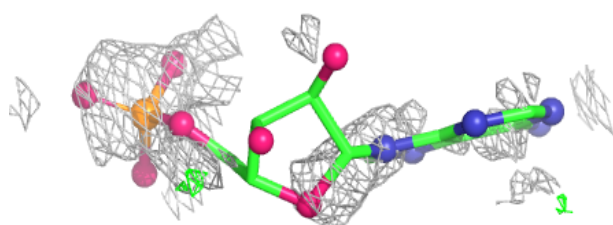
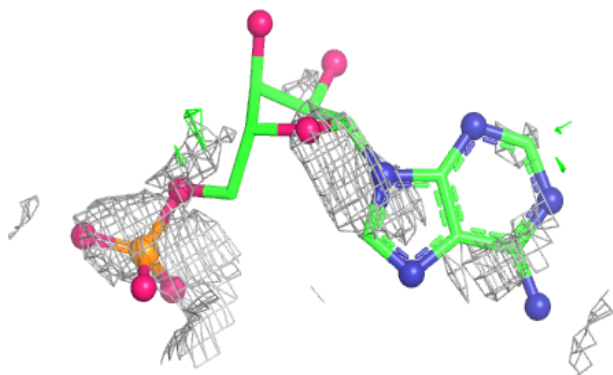
**Electron density around AMP F 1003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

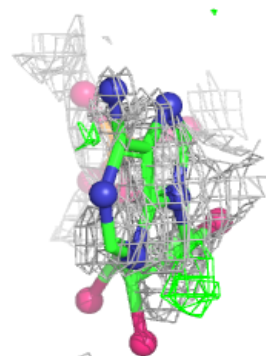
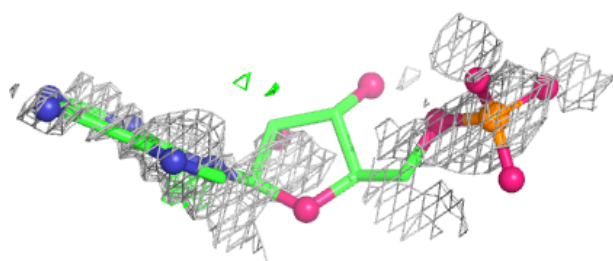
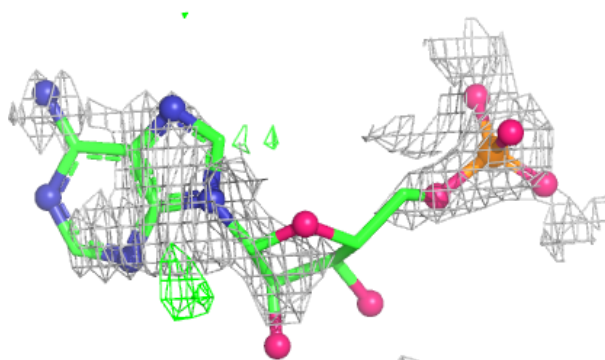


Electron density around AMP E 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around AMP B 1003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.