Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2023 – 04:11 AM EDT

PDB ID	:	2GR9
Title	:	Crystal structure of P5CR complexed with NADH
Authors	:	Meng, Z.; Lou, Z.; Liu, Z.; Rao, Z.
Deposited on	:	2006-04-23
Resolution	:	3.10 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

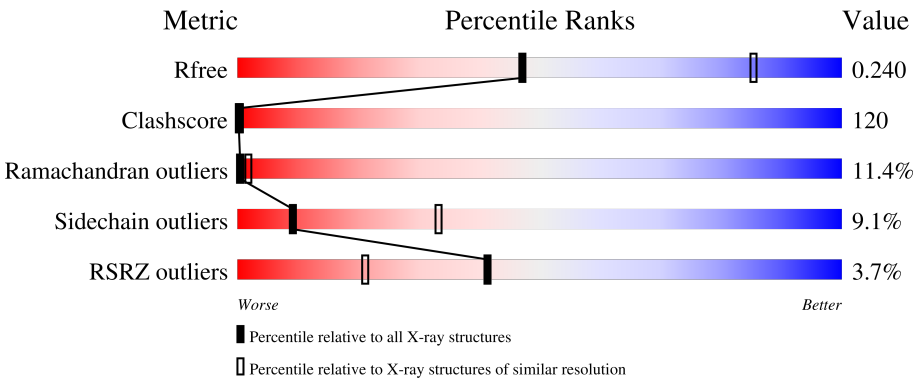
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 <=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	277	19% 63% 16% •
1	B	277	8% 18% 65% 14% •
1	C	277	7% 19% 68% 13%
1	D	277	% 21% 67% 11% •
1	E	277	2% 17% 67% 15% •

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
2	NAI	A	1300	X	-	X	X
2	NAI	B	2300	X	-	X	X
2	NAI	C	3300	X	-	X	X
2	NAI	D	4300	X	-	X	X
2	NAI	E	5300	X	-	X	-
3	GLU	A	1301	-	-	X	X
3	GLU	B	2301	-	-	X	X
3	GLU	C	3301	-	-	X	X
3	GLU	D	4301	-	-	X	X
3	GLU	E	5301	-	-	X	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11077 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 Pyrroline-5-carboxylate reductase 1.

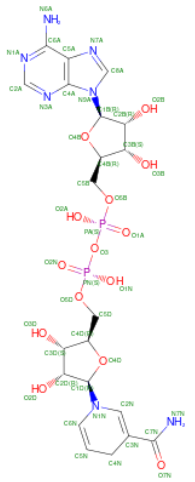
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	277	2038	1279	363	383	13	0	0	0
1	B	276	2023	1270	358	382	13	0	0	0
1	C	277	2032	1276	360	383	13	0	0	0
1	D	277	2038	1279	363	383	13	0	0	0
1	E	277	2038	1279	363	383	13	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	cloning artifact	UNP P32322
A	0	GLY	-	cloning artifact	UNP P32322
B	-1	ARG	-	cloning artifact	UNP P32322
B	0	GLY	-	cloning artifact	UNP P32322
C	-1	ARG	-	cloning artifact	UNP P32322
C	0	GLY	-	cloning artifact	UNP P32322
D	-1	ARG	-	cloning artifact	UNP P32322
D	0	GLY	-	cloning artifact	UNP P32322
E	-1	ARG	-	cloning artifact	UNP P32322
E	0	GLY	-	cloning artifact	UNP P32322

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).

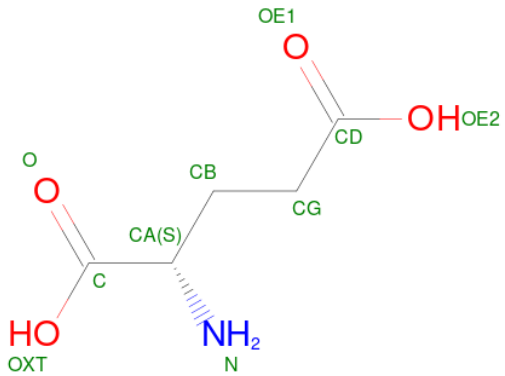
NAI



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	43	21	6	14	2	0	0
2	B	1	43	21	6	14	2	0	0
2	C	1	43	21	6	14	2	0	0
2	D	1	43	21	6	14	2	0	0
2	E	1	43	21	6	14	2	0	0

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).

GLU



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	10	5	1	4	0	0
3	B	1	10	5	1	4	0	0
3	C	1	10	5	1	4	0	0
3	D	1	10	5	1	4	0	0
3	E	1	10	5	1	4	0	0

- Molecule 4 is water.

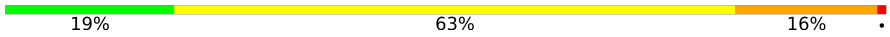
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	141	141	141	0	0
4	B	93	93	93	0	0
4	C	116	116	116	0	0
4	D	155	155	155	0	0
4	E	138	138	138	0	0

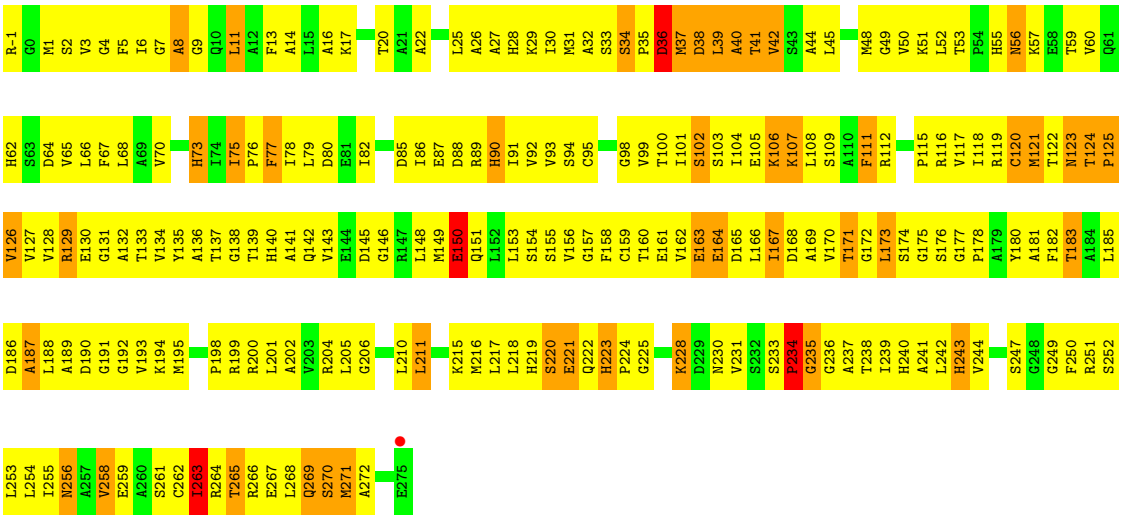
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Pyrroline-5-carboxylate reductase 1

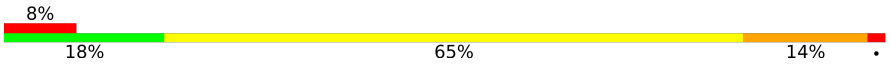
Chain A:

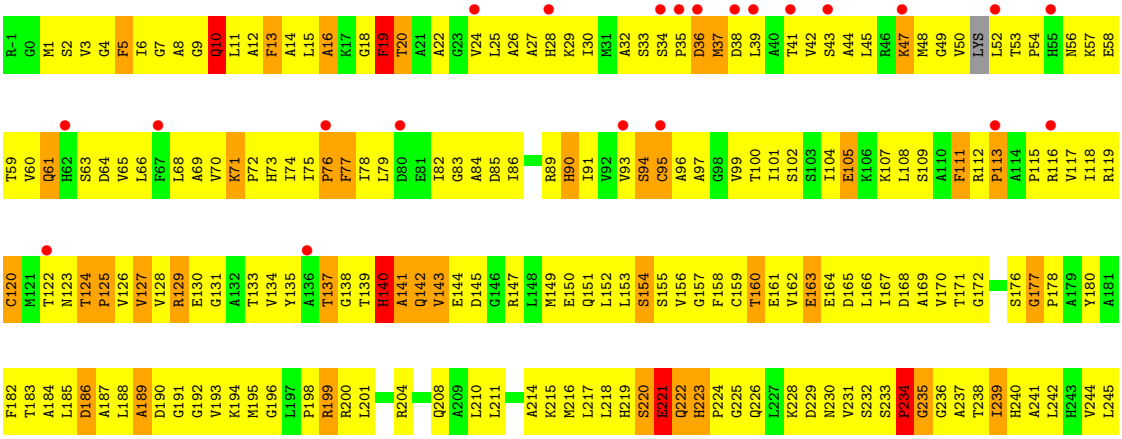


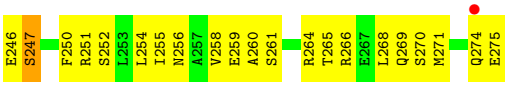


• Molecule 1: Pyrroline-5-carboxylate reductase 1

Chain B:

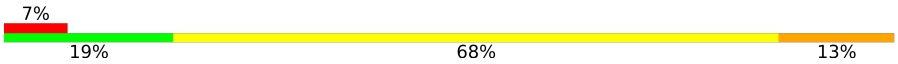


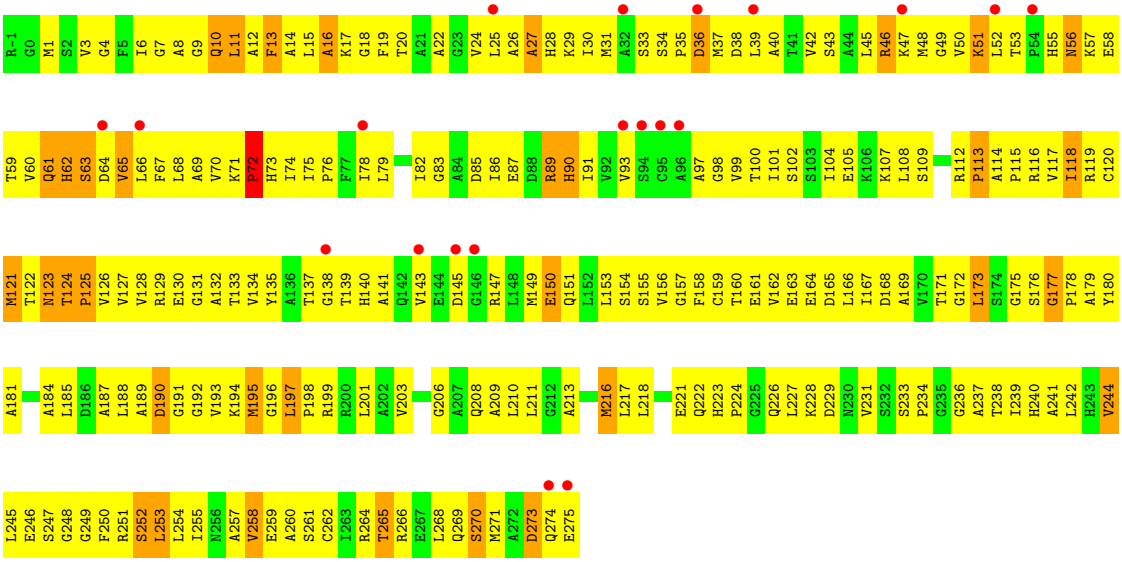




• Molecule 1: Pyrroline-5-carboxylate reductase 1

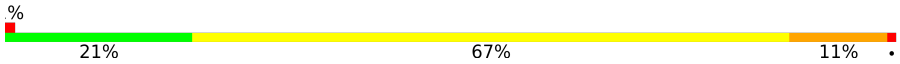
Chain C:

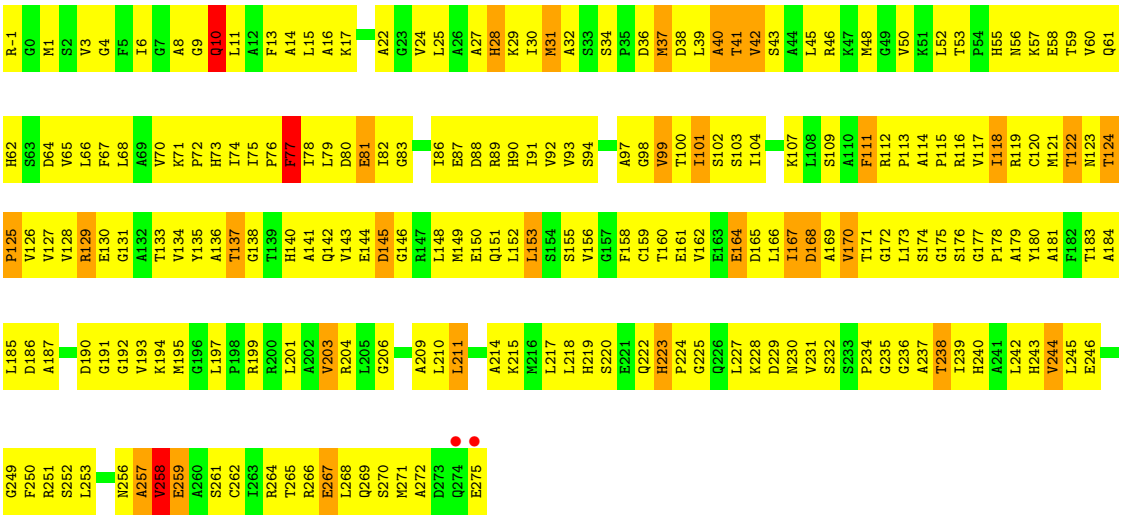




• Molecule 1: Pyrroline-5-carboxylate reductase 1

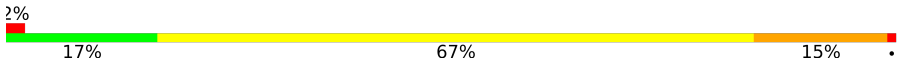
Chain D:

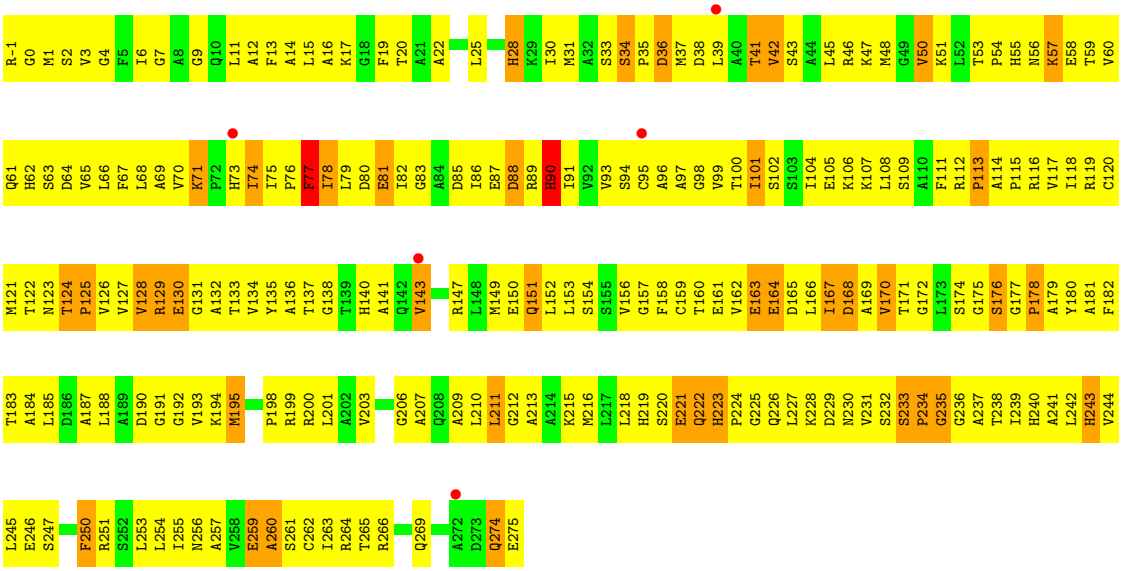




• Molecule 1: Pyrroline-5-carboxylate reductase 1

Chain E:




R-1 G0 M1 S2 V3 G4 F5 I6 G7 A8 G9 Q10 L11 A12 F13 A14 L15 A16 K17 G18 F19 T20 A21 A22 L25 H28 K29 I30 M31 A32 S33 S34 P35 D36 M37 D38 L39 A40 T41 V42 S43 A44 L45 R46 K47 M48 G49 V50 K51 L52 T53 P54 H55 N56 K57 E58 T59 V60
Q61 H62 S63 D64 V65 L66 F67 L68 A69 V70 K71 F72 H73 I74 I75 P76 F77 I78 L79 D80 E81 I82 G83 A84 D85 I86 E87 D88 R89 H90 I91 V92 V93 S94 C95 A96 A97 G98 V99 T100 I101 S102 S103 I104 E105 K106 K107 L108 S109 A110 F111 R112 P113 A114 P115 R116 V117 I118 R119 C120
M121 T122 N123 T124 P125 V126 V127 V128 R129 E130 G131 A132 T133 V134 Y135 A136 T137 G138 T139 H140 A141 Q142 V143 R147 L148 M149 E150 Q151 L152 L153 S154 S155 V156 G157 F158 C159 T160 E161 V162 E163 E164 D165 L166 I167 D168 A169 V170 T171 G172 L173 S174 G175 S176 G177 P178 A179 Y180 A181 F182
T183 A184 L185 D186 A187 L188 A189 D190 G191 G192 V193 K194 M195 P198 R199 R200 L201 A202 V203 G206 A207 Q208 A209 L210 L211 G212 A213 A214 K215 M216 L217 L218 H219 S220 E221 Q222 H223 P224 G225 Q226 L227 K228 D229 N230 V231 S232 S233 P234 G235 G236 A237 T238 I239 H240 A241 L242 H243 V244
L245 E246 S247 F250 R251 S252 L253 L254 I255 N256 A257 V258 E259 A260 S261 C262 I263 R264 T265 R266 Q269 A272 D273 Q274 E275

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	208.18Å 122.64Å 120.71Å 90.00° 122.03° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 28.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 94.9 (28.96-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.278 0.236 , 0.240	Depositor DCC
R_{free} test set	3139 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	61.4	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 96.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.017 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.026 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11077	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: NAI

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	0.41	0/2069	0.72	1/2800 (0.0%)
1	B	0.37	0/2053	0.71	1/2779 (0.0%)
1	C	0.38	0/2063	0.70	1/2793 (0.0%)
1	D	0.42	0/2069	0.69	0/2800
1	E	0.49	2/2069 (0.1%)	0.86	6/2800 (0.2%)
All	All	0.41	2/10323 (0.0%)	0.74	9/13972 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	129	ARG	C-N	11.03	1.59	1.34
1	E	128	VAL	C-N	-5.02	1.22	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	128	VAL	O-C-N	14.89	146.53	122.70
1	E	128	VAL	CA-C-N	-11.74	91.36	117.20
1	E	129	ARG	O-C-N	-10.77	105.48	122.70
1	E	128	VAL	C-N-CA	-8.96	99.30	121.70
1	E	129	ARG	CA-C-N	6.87	132.32	117.20
1	A	221	GLU	CB-CA-C	5.99	122.37	110.40
1	B	221	GLU	CB-CA-C	5.31	121.02	110.40
1	E	129	ARG	C-N-CA	5.28	134.90	121.70
1	C	191	GLY	N-CA-C	-5.04	100.49	113.10

There are no chirality outliers.

There are no planarity outliers.

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	A	2038	0	2084	489	6
1	B	2023	0	2059	491	5
1	C	2032	0	2072	530	2
1	D	2038	0	2084	436	2
1	E	2038	0	2084	492	1
2	A	43	0	23	26	0
2	B	43	0	24	67	5
2	C	43	0	23	39	4
2	D	43	0	24	40	0
2	E	43	0	21	32	1
3	A	10	0	5	8	0
3	B	10	0	5	17	0
3	C	10	0	5	12	0
3	D	10	0	5	21	0
3	E	10	0	5	11	0
4	A	141	0	0	262	6
4	B	93	0	0	169	3
4	C	116	0	0	256	4
4	D	155	0	0	247	2
4	E	138	0	0	298	1
All	All	11077	0	10523	2520	22

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 120.

All (2520) 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:A:1300:NAI:C1D	2:A:1300:NAI:N1N	1.68	1.55
2:E:5300:NAI:O3	2:E:5300:NAI:PN	1.13	1.50
1:B:129:ARG:CZ	2:B:2300:NAI:H2N	1.48	1.40
2:E:5300:NAI:O5B	2:E:5300:NAI:C5B	1.71	1.36
2:D:4300:NAI:H1D	3:D:4301:GLU:N	1.41	1.36
1:E:199:ARG:HG3	4:E:5320:HOH:O	1.21	1.35
1:B:129:ARG:HH22	3:B:2301:GLU:CB	1.40	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:ARG:HB3	4:E:5348:HOH:O	1.27	1.34
1:A:42:VAL:HG23	4:A:1349:HOH:O	1.19	1.33
1:E:111:PHE:HB3	4:E:5422:HOH:O	1.26	1.32
1:D:265:THR:HB	4:D:4360:HOH:O	1.23	1.31
1:E:150:GLU:HB3	4:E:5327:HOH:O	1.15	1.31
1:B:129:ARG:NH1	2:B:2300:NAI:H2N	1.42	1.31
1:A:141:ALA:HA	4:A:1390:HOH:O	1.25	1.30
1:E:38:ASP:HA	4:E:5427:HOH:O	1.27	1.30
1:B:129:ARG:NH2	2:B:2300:NAI:O7N	1.65	1.29
1:B:37:MET:HB2	4:B:2393:HOH:O	1.12	1.28
1:D:214:ALA:HA	4:D:4323:HOH:O	1.29	1.28
1:A:82:ILE:HA	4:A:1437:HOH:O	1.30	1.28
1:C:259:GLU:HB3	4:C:3381:HOH:O	1.33	1.28
1:A:11:LEU:HB2	4:A:1389:HOH:O	1.30	1.27
1:B:99:VAL:HG21	4:B:2309:HOH:O	1.33	1.26
1:A:258:VAL:HA	4:A:1302:HOH:O	1.19	1.26
1:E:91:ILE:HB	4:E:5344:HOH:O	1.30	1.26
1:E:185:LEU:HG	4:E:5383:HOH:O	1.29	1.26
1:C:180:TYR:HB2	4:C:3336:HOH:O	1.28	1.26
1:E:188:LEU:HD23	4:E:5343:HOH:O	1.12	1.25
2:A:1300:NAI:C2N	3:A:1301:GLU:HB3	1.65	1.24
1:B:238:THR:HG22	4:B:2352:HOH:O	1.37	1.24
2:B:2300:NAI:C2N	3:B:2301:GLU:HB3	1.65	1.24
1:C:31:MET:HE2	4:C:3362:HOH:O	1.32	1.24
2:C:3300:NAI:C2N	3:C:3301:GLU:HB3	1.65	1.24
1:E:134:VAL:HG13	4:E:5413:HOH:O	1.36	1.24
1:A:182:PHE:HA	4:A:1419:HOH:O	1.38	1.24
1:D:126:VAL:HA	4:D:4331:HOH:O	1.11	1.24
1:D:227:LEU:HB2	4:D:4363:HOH:O	1.28	1.24
1:D:195:MET:HE2	4:D:4366:HOH:O	1.32	1.23
1:A:157:GLY:O	2:A:1300:NAI:H42N	1.32	1.23
2:E:5300:NAI:O5D	3:E:5301:GLU:O	1.54	1.22
1:A:272:ALA:HB3	4:A:1407:HOH:O	1.35	1.22
1:B:158:PHE:CZ	2:B:2300:NAI:H4B	1.73	1.22
2:E:5300:NAI:O1N	3:E:5301:GLU:HA	1.38	1.22
1:E:179:ALA:HA	4:E:5369:HOH:O	1.38	1.22
1:E:163:GLU:HG3	4:E:5399:HOH:O	1.39	1.22
1:D:186:ASP:HA	4:D:4361:HOH:O	1.34	1.21
1:B:129:ARG:NH2	3:B:2301:GLU:CB	2.02	1.21
1:B:129:ARG:NH2	2:B:2300:NAI:H2N	1.55	1.20
1:C:122:THR:HB	4:C:3317:HOH:O	1.41	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:HIS:HA	4:D:4320:HOH:O	1.37	1.20
1:C:29:LYS:HG3	4:C:3344:HOH:O	1.39	1.19
1:A:199:ARG:HA	4:A:1369:HOH:O	1.38	1.19
1:A:171:THR:HA	4:A:1402:HOH:O	1.36	1.19
1:D:231:VAL:HG12	4:D:4401:HOH:O	1.37	1.19
1:C:180:TYR:HA	4:C:3302:HOH:O	1.43	1.18
1:C:257:ALA:HA	4:C:3378:HOH:O	1.39	1.18
1:C:261:SER:HA	4:C:3354:HOH:O	1.40	1.18
1:E:251:ARG:HG2	4:E:5317:HOH:O	1.43	1.17
1:A:191:GLY:HA2	4:A:1420:HOH:O	1.44	1.17
1:B:129:ARG:HH22	3:B:2301:GLU:HB3	1.00	1.17
1:D:167:ILE:HG22	4:D:4440:HOH:O	1.40	1.17
1:A:217:LEU:HB3	4:A:1312:HOH:O	1.43	1.16
1:C:122:THR:HB	4:C:3331:HOH:O	1.37	1.16
1:D:99:VAL:HA	4:D:4445:HOH:O	1.41	1.16
1:B:129:ARG:CZ	2:B:2300:NAI:O7N	1.92	1.16
1:E:176:SER:HA	4:E:5333:HOH:O	1.44	1.16
1:B:119:ARG:HG3	4:B:2333:HOH:O	1.42	1.16
1:D:122:THR:HG23	1:D:133:THR:HB	1.25	1.16
1:D:217:LEU:HD13	4:D:4372:HOH:O	1.45	1.16
1:E:158:PHE:HA	4:E:5425:HOH:O	1.43	1.15
1:E:229:ASP:HA	4:E:5337:HOH:O	1.46	1.15
1:A:254:LEU:HB3	4:A:1360:HOH:O	1.47	1.15
1:B:129:ARG:NH2	2:B:2300:NAI:C2N	2.09	1.15
1:C:157:GLY:O	2:C:3300:NAI:H42N	1.45	1.15
1:D:119:ARG:HD2	4:D:4422:HOH:O	1.47	1.15
1:D:239:ILE:HG13	4:D:4429:HOH:O	1.45	1.15
1:E:80:ASP:HB2	4:E:5336:HOH:O	1.47	1.14
1:D:180:TYR:HA	4:D:4308:HOH:O	1.45	1.14
1:C:158:PHE:CZ	2:C:3300:NAI:O3B	1.99	1.14
1:C:255:ILE:HB	4:C:3364:HOH:O	1.48	1.14
1:E:238:THR:HG21	4:E:5321:HOH:O	1.45	1.14
1:A:162:VAL:HA	4:A:1355:HOH:O	1.46	1.14
1:D:267:GLU:HB2	4:D:4338:HOH:O	1.46	1.14
1:D:251:ARG:HB2	4:D:4342:HOH:O	1.46	1.13
1:A:40:ALA:HB3	4:A:1336:HOH:O	1.49	1.12
1:A:86:ILE:HD12	1:A:108:LEU:HD11	1.28	1.13
1:E:194:LYS:HA	4:E:5303:HOH:O	1.48	1.12
1:C:244:VAL:HA	4:C:3321:HOH:O	1.44	1.12
1:D:224:PRO:HD2	4:D:4355:HOH:O	1.47	1.12
1:B:129:ARG:CZ	2:B:2300:NAI:C2N	2.27	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLU:HB2	4:A:1344:HOH:O	1.43	1.12
1:B:228:LYS:HA	4:B:2364:HOH:O	1.50	1.12
1:C:48:MET:HB2	4:C:3371:HOH:O	1.49	1.12
1:C:126:VAL:HA	4:C:3307:HOH:O	1.46	1.12
2:E:5300:NAI:PN	3:E:5301:GLU:O	2.07	1.12
1:B:259:GLU:HB3	4:B:2381:HOH:O	1.46	1.11
1:B:228:LYS:HE3	4:B:2386:HOH:O	1.48	1.11
4:A:1352:HOH:O	1:C:194:LYS:HG3	1.48	1.10
1:A:259:GLU:HA	4:A:1366:HOH:O	1.51	1.10
1:C:75:ILE:HD12	4:C:3415:HOH:O	1.51	1.09
2:D:4300:NAI:H4N	3:D:4301:GLU:O	1.50	1.09
2:E:5300:NAI:H8A	2:E:5300:NAI:O2B	1.36	1.09
1:D:135:TYR:HE1	4:D:4398:HOH:O	1.36	1.09
1:C:218:LEU:HD13	2:C:3300:NAI:C5D	1.83	1.09
1:E:262:CYS:SG	4:E:5342:HOH:O	2.09	1.09
1:A:210:LEU:HD21	4:A:1380:HOH:O	1.52	1.08
1:E:134:VAL:HB	4:E:5407:HOH:O	1.50	1.08
1:A:218:LEU:HD22	2:A:1300:NAI:H52A	1.31	1.07
1:A:1:MET:HB3	4:A:1427:HOH:O	1.53	1.07
1:D:124:THR:HG23	4:D:4375:HOH:O	1.53	1.07
1:D:218:LEU:HD22	2:D:4300:NAI:H52A	1.29	1.07
2:D:4300:NAI:N1N	3:D:4301:GLU:N	2.01	1.07
1:D:91:ILE:HA	4:D:4455:HOH:O	1.55	1.06
1:D:229:ASP:HB2	4:D:4393:HOH:O	1.55	1.06
2:D:4300:NAI:C4N	3:D:4301:GLU:O	2.02	1.06
1:A:182:PHE:CE1	4:A:1324:HOH:O	2.08	1.06
1:B:142:GLN:HG2	1:B:143:VAL:H	1.14	1.06
1:D:185:LEU:HG	4:D:4330:HOH:O	1.52	1.06
1:D:37:MET:HG2	4:D:4306:HOH:O	1.51	1.06
1:C:129:ARG:HH12	3:C:3301:GLU:HG3	1.17	1.06
2:D:4300:NAI:C2N	3:D:4301:GLU:CA	2.34	1.06
1:B:29:LYS:HB3	4:B:2332:HOH:O	1.56	1.05
1:C:60:VAL:HG23	4:C:3383:HOH:O	1.51	1.05
1:C:218:LEU:HD22	2:C:3300:NAI:PA	1.96	1.05
2:D:4300:NAI:C1D	3:D:4301:GLU:N	2.20	1.05
2:A:1300:NAI:C6N	3:A:1301:GLU:OXT	2.04	1.05
1:A:133:THR:HG21	1:A:153:LEU:HD13	1.37	1.04
1:B:129:ARG:NH2	2:B:2300:NAI:C7N	2.19	1.04
1:B:154:SER:O	2:B:2300:NAI:N7N	1.91	1.04
1:D:64:ASP:HB3	4:D:4353:HOH:O	1.55	1.04
1:D:78:ILE:HD11	4:D:4446:HOH:O	1.55	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:CYS:HB2	4:A:1337:HOH:O	1.56	1.04
1:C:218:LEU:HD13	2:C:3300:NAI:H52N	1.40	1.04
2:E:5300:NAI:C5B	2:E:5300:NAI:PA	2.45	1.04
1:B:129:ARG:NE	2:B:2300:NAI:O7N	1.89	1.04
1:D:141:ALA:HB2	4:D:4364:HOH:O	1.58	1.04
1:A:95:CYS:CB	4:A:1337:HOH:O	2.07	1.03
1:A:183:THR:HA	4:A:1354:HOH:O	1.58	1.03
1:B:129:ARG:NH2	3:B:2301:GLU:HB3	1.64	1.03
1:B:259:GLU:HA	4:B:2307:HOH:O	1.58	1.03
1:B:219:HIS:CE1	2:B:2300:NAI:O5D	2.12	1.03
1:C:29:LYS:CD	4:C:3404:HOH:O	2.06	1.03
1:E:122:THR:HB	1:E:133:THR:HG22	1.41	1.03
1:A:178:PRO:HD2	4:A:1436:HOH:O	1.59	1.02
1:C:70:VAL:HB	4:C:3407:HOH:O	1.58	1.02
1:D:107:LYS:HD2	4:D:4370:HOH:O	1.59	1.02
1:B:176:SER:HB2	4:B:2324:HOH:O	1.55	1.02
1:B:158:PHE:CE1	2:B:2300:NAI:H4B	1.93	1.02
1:B:158:PHE:CE2	2:B:2300:NAI:O3B	2.12	1.01
1:D:30:ILE:HB	4:D:4425:HOH:O	1.62	1.00
1:C:237:ALA:HA	4:C:3411:HOH:O	1.59	1.00
1:E:187:ALA:HB2	4:E:5363:HOH:O	1.58	1.00
1:A:112:ARG:CD	4:A:1392:HOH:O	2.08	1.00
1:B:75:ILE:HB	1:B:76:PRO:HD3	1.40	1.00
2:A:1300:NAI:H5N	4:A:1412:HOH:O	1.61	1.00
2:C:3300:NAI:C6N	3:C:3301:GLU:OXT	2.10	1.00
1:A:16:ALA:HB3	4:A:1387:HOH:O	1.62	1.00
2:E:5300:NAI:O2B	2:E:5300:NAI:C8A	2.08	0.99
2:D:4300:NAI:C3N	3:D:4301:GLU:O	2.10	0.99
2:B:2300:NAI:C6N	3:B:2301:GLU:OXT	2.10	0.99
1:A:161:GLU:HB3	4:A:1364:HOH:O	1.61	0.99
1:B:71:LYS:HB3	1:B:72:PRO:HD2	1.43	0.99
1:C:168:ASP:HA	4:C:3380:HOH:O	1.61	0.99
1:E:112:ARG:HG3	4:E:5328:HOH:O	1.61	0.99
2:D:4300:NAI:C2N	3:D:4301:GLU:HA	1.92	0.99
1:C:22:ALA:HB3	4:C:3369:HOH:O	1.61	0.99
1:C:129:ARG:HD2	2:C:3300:NAI:O7N	1.62	0.99
1:C:213:ALA:HB2	4:C:3386:HOH:O	1.63	0.99
1:B:155:SER:HA	2:B:2300:NAI:H72N	1.25	0.98
1:E:185:LEU:HA	4:E:5323:HOH:O	1.61	0.98
1:C:129:ARG:NH1	3:C:3301:GLU:HG3	1.76	0.98
1:B:189:ALA:C	4:B:2302:HOH:O	2.00	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:PRO:HB2	4:D:4454:HOH:O	1.62	0.98
1:A:98:GLY:HA2	4:A:1328:HOH:O	1.62	0.98
1:E:17:LYS:HB2	4:E:5306:HOH:O	1.61	0.98
1:A:234:PRO:HB3	1:C:196:GLY:O	1.62	0.98
1:C:151:GLN:HA	4:C:3319:HOH:O	1.64	0.98
1:B:129:ARG:NH1	2:B:2300:NAI:C2N	2.27	0.97
1:B:183:THR:HA	4:B:2305:HOH:O	1.61	0.97
1:D:122:THR:CG2	1:D:133:THR:HB	1.93	0.97
1:B:158:PHE:CZ	2:B:2300:NAI:O3B	2.18	0.97
1:D:194:LYS:HB3	4:D:4366:HOH:O	1.64	0.96
2:E:5300:NAI:H51N	4:E:5404:HOH:O	1.63	0.96
1:C:176:SER:HA	4:C:3330:HOH:O	1.66	0.96
1:E:9:GLY:H	1:E:41:THR:HG21	1.28	0.96
1:E:188:LEU:HA	4:E:5343:HOH:O	1.65	0.96
1:B:218:LEU:HD22	2:B:2300:NAI:PA	2.04	0.96
1:C:48:MET:CB	4:C:3371:HOH:O	2.06	0.96
1:D:122:THR:HG23	1:D:133:THR:CB	1.96	0.96
1:B:45:LEU:HD11	4:B:2314:HOH:O	1.62	0.96
1:C:112:ARG:HH11	1:C:113:PRO:HD2	1.27	0.96
1:E:163:GLU:CG	4:E:5399:HOH:O	2.02	0.96
1:C:108:LEU:HB3	4:C:3358:HOH:O	1.65	0.96
1:B:33:SER:HB2	1:B:59:THR:OG1	1.66	0.95
1:B:218:LEU:HD13	2:B:2300:NAI:H52N	1.46	0.95
1:D:219:HIS:HE1	2:D:4300:NAI:C5D	1.79	0.95
1:E:17:LYS:CB	4:E:5306:HOH:O	2.14	0.95
1:A:13:PHE:HA	4:A:1387:HOH:O	1.64	0.95
1:D:165:ASP:HB2	4:D:4368:HOH:O	1.67	0.95
1:A:182:PHE:CA	4:A:1419:HOH:O	2.01	0.95
1:E:188:LEU:HD12	4:E:5439:HOH:O	1.65	0.95
1:E:47:LYS:HE2	4:E:5338:HOH:O	1.65	0.95
1:B:9:GLY:H	1:B:12:ALA:HB3	1.28	0.95
1:E:225:GLY:CA	4:E:5353:HOH:O	2.14	0.95
1:C:178:PRO:HB2	4:C:3396:HOH:O	1.65	0.94
1:C:29:LYS:HD3	4:C:3404:HOH:O	1.65	0.94
1:C:122:THR:CB	4:C:3317:HOH:O	2.03	0.94
1:D:180:TYR:CA	4:D:4308:HOH:O	2.09	0.94
1:C:101:ILE:HG12	4:C:3394:HOH:O	1.66	0.94
1:D:118:ILE:HB	4:D:4408:HOH:O	1.67	0.94
1:B:14:ALA:HA	1:B:127:VAL:HG22	1.49	0.94
1:E:101:ILE:HG13	4:E:5418:HOH:O	1.66	0.94
1:C:213:ALA:N	4:C:3386:HOH:O	2.01	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:ARG:HD2	4:C:3303:HOH:O	1.68	0.94
1:D:-1:ARG:HG3	4:D:4424:HOH:O	1.68	0.94
1:E:132:ALA:HB3	4:E:5335:HOH:O	1.67	0.94
1:C:89:ARG:HD2	1:C:90:HIS:N	1.83	0.94
1:B:155:SER:CA	2:B:2300:NAI:H72N	1.81	0.94
1:C:122:THR:HB	1:C:133:THR:HG22	1.48	0.94
1:C:179:ALA:N	4:C:3396:HOH:O	2.01	0.94
1:B:89:ARG:NH2	4:B:2325:HOH:O	2.00	0.93
1:B:236:GLY:HA2	1:B:239:ILE:HG22	1.49	0.93
1:E:132:ALA:HB1	4:E:5391:HOH:O	1.67	0.93
1:A:9:GLY:H	1:A:41:THR:HG21	1.33	0.93
1:A:250:PHE:N	4:A:1314:HOH:O	2.02	0.93
4:C:3375:HOH:O	1:D:199:ARG:HD3	1.67	0.93
1:A:186:ASP:N	4:A:1370:HOH:O	2.01	0.93
1:C:237:ALA:CB	4:C:3411:HOH:O	2.16	0.93
1:A:121:MET:HB2	4:A:1327:HOH:O	1.68	0.92
1:C:167:ILE:CG2	4:C:3345:HOH:O	2.16	0.92
1:D:98:GLY:N	4:D:4333:HOH:O	2.01	0.92
1:A:210:LEU:HG	4:A:1421:HOH:O	1.68	0.92
1:E:-1:ARG:CD	4:E:5319:HOH:O	2.17	0.92
1:E:63:SER:N	4:E:5372:HOH:O	2.00	0.92
1:A:95:CYS:N	4:A:1337:HOH:O	2.03	0.92
1:A:266:ARG:CD	4:A:1331:HOH:O	2.16	0.92
1:D:62:HIS:C	4:D:4448:HOH:O	2.08	0.92
1:E:3:VAL:N	4:E:5387:HOH:O	2.01	0.92
1:B:247:SER:HA	4:B:2350:HOH:O	1.70	0.92
1:D:174:SER:C	4:D:4315:HOH:O	2.07	0.92
1:A:222:GLN:HG2	4:A:1441:HOH:O	1.69	0.92
1:C:4:GLY:N	4:C:3356:HOH:O	2.02	0.92
1:C:108:LEU:HD23	4:C:3329:HOH:O	1.70	0.92
1:E:69:ALA:HB3	4:E:5379:HOH:O	1.70	0.92
1:E:107:LYS:N	4:E:5384:HOH:O	2.01	0.92
1:B:153:LEU:CA	4:B:2392:HOH:O	2.16	0.92
1:C:7:GLY:N	4:C:3322:HOH:O	2.03	0.92
1:E:241:ALA:O	1:E:244:VAL:HG12	1.69	0.92
1:B:29:LYS:HE2	4:B:2332:HOH:O	1.68	0.91
1:C:45:LEU:HA	4:C:3371:HOH:O	1.71	0.91
1:C:129:ARG:HH12	3:C:3301:GLU:CG	1.83	0.91
1:E:63:SER:C	4:E:5417:HOH:O	2.08	0.91
1:B:5:PHE:HZ	1:B:15:LEU:HB2	1.34	0.91
1:C:171:THR:O	1:C:175:GLY:HA3	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:GLU:N	4:E:5401:HOH:O	2.02	0.91
1:C:49:GLY:C	4:C:3363:HOH:O	2.09	0.91
1:C:259:GLU:N	4:C:3391:HOH:O	2.03	0.91
1:C:266:ARG:CD	4:C:3303:HOH:O	2.19	0.91
1:D:225:GLY:HA2	4:D:4397:HOH:O	1.68	0.91
1:A:119:ARG:CG	4:A:1372:HOH:O	2.18	0.90
1:A:119:ARG:NH2	4:A:1328:HOH:O	2.03	0.90
1:D:219:HIS:CE1	2:D:4300:NAI:O5D	2.24	0.90
1:E:122:THR:HB	4:E:5385:HOH:O	1.70	0.90
1:B:176:SER:CB	4:B:2324:HOH:O	2.14	0.90
2:B:2300:NAI:C3N	3:B:2301:GLU:HB3	2.00	0.90
1:E:215:LYS:CE	4:E:5430:HOH:O	2.18	0.90
1:E:185:LEU:HD23	4:E:5323:HOH:O	1.71	0.90
1:A:29:LYS:NZ	4:A:1400:HOH:O	2.04	0.90
2:E:5300:NAI:O1N	3:E:5301:GLU:CA	2.18	0.90
1:A:121:MET:HE1	4:A:1346:HOH:O	1.70	0.90
1:B:153:LEU:C	4:B:2392:HOH:O	2.10	0.90
2:C:3300:NAI:C3N	3:C:3301:GLU:HB3	2.00	0.90
1:B:218:LEU:HD13	2:B:2300:NAI:C5D	2.01	0.90
1:D:1:MET:HE2	1:D:25:LEU:HD21	1.54	0.90
1:D:78:ILE:CD1	4:D:4446:HOH:O	2.14	0.90
1:B:129:ARG:NH2	3:B:2301:GLU:HB2	1.86	0.90
1:B:129:ARG:HH12	2:B:2300:NAI:H2N	1.30	0.90
1:D:141:ALA:HA	4:D:4386:HOH:O	1.69	0.90
4:B:2308:HOH:O	1:D:239:ILE:CG2	2.18	0.89
1:C:105:GLU:HG2	4:C:3315:HOH:O	1.71	0.89
1:D:87:GLU:HB3	4:D:4322:HOH:O	1.71	0.89
1:A:7:GLY:N	4:A:1305:HOH:O	2.05	0.89
1:A:88:ASP:HB2	1:A:112:ARG:HH21	1.38	0.89
1:A:239:ILE:HG12	4:C:3309:HOH:O	1.73	0.89
1:E:122:THR:HG22	1:E:133:THR:HB	1.54	0.89
1:E:246:GLU:HB3	4:E:5312:HOH:O	1.70	0.89
1:A:256:ASN:N	4:A:1335:HOH:O	2.06	0.89
1:C:237:ALA:N	4:C:3398:HOH:O	2.06	0.89
1:C:266:ARG:HA	4:C:3340:HOH:O	1.72	0.89
1:C:129:ARG:CZ	2:C:3300:NAI:H2N	2.02	0.89
1:E:65:VAL:HA	4:E:5344:HOH:O	1.72	0.89
1:E:162:VAL:HG13	1:E:166:LEU:HD12	1.55	0.89
1:C:133:THR:HG22	4:C:3317:HOH:O	1.71	0.88
1:C:203:VAL:HA	4:C:3355:HOH:O	1.73	0.88
1:B:73:HIS:CD2	4:B:2320:HOH:O	2.26	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:NH1	2:B:2300:NAI:O2D	2.07	0.88
1:D:53:THR:HB	4:D:4404:HOH:O	1.73	0.88
1:A:102:SER:HB2	4:A:1358:HOH:O	1.72	0.88
1:E:187:ALA:HA	4:E:5381:HOH:O	1.70	0.88
1:B:73:HIS:HD2	4:B:2320:HOH:O	1.56	0.88
1:E:122:THR:CB	4:E:5385:HOH:O	2.21	0.88
1:A:154:SER:O	2:A:1300:NAI:N7N	2.05	0.88
1:B:50:VAL:HB	4:B:2385:HOH:O	1.73	0.88
1:C:160:THR:CG2	4:C:3323:HOH:O	2.22	0.88
2:E:5300:NAI:O3	2:E:5300:NAI:O5D	1.92	0.88
1:C:192:GLY:CA	4:C:3367:HOH:O	2.20	0.88
1:E:200:ARG:HG3	4:E:5416:HOH:O	1.74	0.87
1:B:95:CYS:HA	4:B:2349:HOH:O	1.73	0.87
1:B:129:ARG:NH2	2:B:2300:NAI:C3N	2.36	0.87
1:E:123:ASN:ND2	4:E:5335:HOH:O	2.07	0.87
2:E:5300:NAI:C5D	3:E:5301:GLU:O	2.22	0.87
1:A:112:ARG:NE	4:A:1392:HOH:O	2.08	0.87
1:C:112:ARG:HG3	1:C:113:PRO:HD2	1.54	0.87
1:A:124:THR:O	1:A:127:VAL:HG23	1.75	0.87
1:B:122:THR:HG22	1:B:133:THR:CB	2.04	0.87
1:D:64:ASP:CB	4:D:4353:HOH:O	2.15	0.87
1:D:272:ALA:HB1	4:D:4328:HOH:O	1.71	0.87
1:B:158:PHE:CZ	2:B:2300:NAI:C4B	2.57	0.87
1:B:12:ALA:HB3	4:B:2314:HOH:O	1.75	0.87
1:B:190:ASP:N	4:B:2302:HOH:O	2.06	0.86
1:C:33:SER:HB2	1:C:59:THR:OG1	1.75	0.86
1:B:236:GLY:HA3	4:B:2318:HOH:O	1.75	0.86
1:A:102:SER:N	4:A:1358:HOH:O	2.08	0.86
1:B:228:LYS:CE	4:B:2386:HOH:O	2.12	0.86
1:C:28:HIS:HA	1:C:51:LYS:HE3	1.58	0.86
1:C:155:SER:HA	2:C:3300:NAI:H72N	1.37	0.86
1:B:73:HIS:CE1	4:B:2390:HOH:O	2.28	0.86
1:D:224:PRO:CD	4:D:4355:HOH:O	2.14	0.86
1:D:30:ILE:HB	1:D:50:VAL:HG22	1.55	0.86
1:C:69:ALA:N	4:C:3322:HOH:O	2.07	0.86
1:B:228:LYS:CA	4:B:2364:HOH:O	2.12	0.86
1:E:73:HIS:HB2	4:E:5415:HOH:O	1.75	0.86
1:E:88:ASP:N	4:E:5318:HOH:O	2.03	0.86
1:A:122:THR:C	4:A:1428:HOH:O	2.14	0.86
1:A:259:GLU:CA	4:A:1366:HOH:O	2.17	0.86
1:E:53:THR:HG22	1:E:55:HIS:H	1.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:SER:CB	4:A:1358:HOH:O	2.24	0.85
1:B:129:ARG:HH22	3:B:2301:GLU:CG	1.89	0.85
1:C:247:SER:C	4:C:3402:HOH:O	2.15	0.85
1:D:57:LYS:CE	4:D:4376:HOH:O	2.21	0.85
1:E:115:PRO:HA	4:E:5436:HOH:O	1.76	0.85
1:C:251:ARG:HA	4:C:3359:HOH:O	1.76	0.85
1:B:193:VAL:HG12	1:D:239:ILE:HD13	1.58	0.85
1:E:53:THR:HG21	4:E:5332:HOH:O	1.75	0.85
1:B:10:GLN:NE2	4:B:2354:HOH:O	2.08	0.85
1:B:185:LEU:HD21	1:B:210:LEU:HD12	1.58	0.85
1:E:174:SER:HB2	4:E:5335:HOH:O	1.76	0.85
1:E:55:HIS:HB2	4:E:5332:HOH:O	1.75	0.85
1:E:111:PHE:HE1	4:E:5326:HOH:O	1.58	0.85
1:A:138:GLY:HA3	4:A:1310:HOH:O	1.75	0.85
1:D:39:LEU:HD23	4:D:4405:HOH:O	1.77	0.85
1:D:219:HIS:CE1	2:D:4300:NAI:C5D	2.59	0.85
1:C:53:THR:HG21	1:C:58:GLU:HB2	1.58	0.85
1:C:123:ASN:HD21	1:C:132:ALA:HB3	1.42	0.85
1:C:237:ALA:CA	4:C:3411:HOH:O	2.21	0.85
1:B:155:SER:HA	2:B:2300:NAI:N7N	1.90	0.85
1:A:266:ARG:CZ	4:A:1440:HOH:O	2.24	0.84
1:B:95:CYS:N	4:B:2349:HOH:O	2.09	0.84
1:B:241:ALA:HA	4:B:2329:HOH:O	1.75	0.84
1:E:231:VAL:HG12	4:E:5321:HOH:O	1.77	0.84
1:C:236:GLY:C	4:C:3398:HOH:O	2.14	0.84
1:E:183:THR:CB	4:E:5370:HOH:O	2.24	0.84
1:A:259:GLU:O	1:A:263:ILE:HD13	1.76	0.84
1:D:178:PRO:C	4:D:4454:HOH:O	2.16	0.84
1:E:96:ALA:N	4:E:5423:HOH:O	2.07	0.84
1:A:118:ILE:HG22	1:A:137:THR:HA	1.60	0.84
1:A:119:ARG:HG3	4:A:1372:HOH:O	1.77	0.84
1:B:129:ARG:HH22	2:B:2300:NAI:C2N	1.86	0.84
1:B:160:THR:CG2	4:B:2360:HOH:O	2.26	0.84
1:E:183:THR:HG22	4:E:5370:HOH:O	1.76	0.84
1:A:210:LEU:CD2	4:A:1380:HOH:O	2.16	0.84
1:B:74:ILE:HG13	4:B:2309:HOH:O	1.77	0.84
1:C:162:VAL:HB	1:C:166:LEU:HD12	1.57	0.84
1:E:188:LEU:CA	4:E:5343:HOH:O	2.21	0.84
1:B:138:GLY:HA3	4:B:2370:HOH:O	1.77	0.84
1:E:243:HIS:CE1	4:E:5357:HOH:O	2.30	0.84
1:C:247:SER:HA	4:C:3402:HOH:O	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:THR:HG22	1:D:55:HIS:H	1.41	0.84
1:D:118:ILE:HG23	1:D:137:THR:HA	1.60	0.84
1:B:45:LEU:HB2	1:B:52:LEU:HD21	1.58	0.84
1:B:129:ARG:HH22	2:B:2300:NAI:H2N	1.43	0.84
1:C:194:LYS:HA	4:C:3309:HOH:O	1.77	0.84
1:A:-1:ARG:CG	4:A:1332:HOH:O	2.26	0.83
1:E:182:PHE:HB2	4:E:5369:HOH:O	1.77	0.83
1:A:28:HIS:ND1	4:A:1382:HOH:O	2.10	0.83
1:D:9:GLY:N	1:D:41:THR:HG21	1.93	0.83
1:D:228:LYS:HE2	4:D:4414:HOH:O	1.78	0.83
1:A:255:ILE:HG22	4:A:1335:HOH:O	1.79	0.83
1:B:11:LEU:HD23	4:B:2343:HOH:O	1.78	0.83
1:B:160:THR:HG23	4:B:2360:HOH:O	1.79	0.83
1:B:250:PHE:HB2	4:B:2353:HOH:O	1.77	0.83
1:C:171:THR:CA	4:C:3351:HOH:O	2.26	0.83
1:D:126:VAL:HG13	1:D:156:VAL:HG11	1.60	0.83
2:D:4300:NAI:C4N	3:D:4301:GLU:C	2.45	0.83
1:C:199:ARG:CD	4:C:3392:HOH:O	2.27	0.83
1:C:133:THR:CG2	4:C:3317:HOH:O	2.25	0.83
1:E:212:GLY:HA2	4:E:5314:HOH:O	1.76	0.83
1:B:245:LEU:HA	4:B:2353:HOH:O	1.79	0.83
1:C:89:ARG:HD2	1:C:90:HIS:H	1.39	0.83
1:C:213:ALA:CA	4:C:3386:HOH:O	2.27	0.83
1:D:136:ALA:HA	4:D:4394:HOH:O	1.78	0.83
1:A:194:LYS:NZ	4:A:1381:HOH:O	2.12	0.82
1:A:161:GLU:CD	4:A:1364:HOH:O	2.16	0.82
1:C:171:THR:N	4:C:3351:HOH:O	2.11	0.82
1:E:-1:ARG:HD3	4:E:5319:HOH:O	1.76	0.82
1:B:79:LEU:HD11	1:B:104:ILE:HG12	1.61	0.82
1:D:251:ARG:NH1	4:D:4427:HOH:O	2.12	0.82
1:D:123:ASN:HB3	4:D:4309:HOH:O	1.78	0.82
1:D:211:LEU:HD12	4:D:4406:HOH:O	1.79	0.82
1:E:274:GLN:HG3	1:E:275:GLU:H	1.41	0.82
1:A:120:CYS:HA	4:A:1368:HOH:O	1.79	0.82
1:D:228:LYS:C	4:D:4310:HOH:O	2.16	0.82
1:D:266:ARG:NH2	4:D:4378:HOH:O	2.05	0.82
1:E:31:MET:HG2	1:E:51:LYS:HB2	1.61	0.82
1:D:107:LYS:CD	4:D:4370:HOH:O	2.22	0.82
1:E:262:CYS:SG	4:E:5375:HOH:O	2.38	0.82
1:D:246:GLU:HG3	4:D:4383:HOH:O	1.80	0.82
1:B:164:GLU:HG3	1:B:167:ILE:HD12	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:GLY:HA3	4:C:3307:HOH:O	1.78	0.82
1:A:258:VAL:CG2	4:A:1302:HOH:O	2.27	0.81
1:C:7:GLY:CA	4:C:3322:HOH:O	2.25	0.81
1:C:134:VAL:HB	4:C:3327:HOH:O	1.80	0.81
1:C:258:VAL:HG12	1:C:258:VAL:O	1.79	0.81
1:D:158:PHE:CZ	2:D:4300:NAI:O3B	2.33	0.81
1:D:223:HIS:N	4:D:4384:HOH:O	2.01	0.81
2:A:1300:NAI:H51N	4:A:1431:HOH:O	1.78	0.81
1:B:82:ILE:HA	4:B:2376:HOH:O	1.78	0.81
1:B:82:ILE:HG22	1:B:86:ILE:HD11	1.61	0.81
1:D:272:ALA:HA	4:D:4400:HOH:O	1.80	0.81
1:A:9:GLY:N	1:A:41:THR:HG21	1.94	0.81
1:A:266:ARG:NH1	4:A:1308:HOH:O	2.14	0.81
1:B:7:GLY:O	1:B:12:ALA:HB2	1.80	0.81
1:B:142:GLN:HG2	1:B:143:VAL:N	1.94	0.81
1:C:7:GLY:HA3	4:C:3322:HOH:O	1.80	0.81
1:C:247:SER:CA	4:C:3402:HOH:O	2.27	0.81
1:D:31:MET:HG2	1:D:59:THR:HA	1.62	0.81
1:D:257:ALA:C	4:D:4349:HOH:O	2.17	0.81
1:D:121:MET:HG2	4:D:4324:HOH:O	1.79	0.81
1:B:6:ILE:HD12	1:B:56:ASN:O	1.81	0.81
1:B:122:THR:HG22	1:B:133:THR:HB	1.59	0.81
1:C:240:HIS:HB2	4:C:3398:HOH:O	1.80	0.81
1:A:239:ILE:HG21	4:C:3309:HOH:O	1.81	0.81
1:A:202:ALA:HB3	4:A:1369:HOH:O	1.80	0.81
1:B:63:SER:HB2	1:B:89:ARG:HH12	1.45	0.81
1:D:133:THR:O	1:D:159:CYS:HA	1.81	0.81
1:E:153:LEU:HB2	4:E:5432:HOH:O	1.80	0.81
2:A:1300:NAI:N1N	3:A:1301:GLU:OXT	2.14	0.81
1:D:211:LEU:HD12	1:D:211:LEU:O	1.80	0.81
1:C:262:CYS:SG	4:C:3320:HOH:O	2.39	0.80
1:E:138:GLY:HA2	4:E:5418:HOH:O	1.79	0.80
1:E:183:THR:HB	4:E:5370:HOH:O	1.80	0.80
1:B:5:PHE:CZ	1:B:15:LEU:HB2	2.16	0.80
1:A:123:ASN:HD21	1:A:132:ALA:H	1.30	0.80
1:B:251:ARG:HD3	4:B:2330:HOH:O	1.80	0.80
1:D:60:VAL:HG21	1:D:82:ILE:HG23	1.63	0.80
1:E:60:VAL:HG21	1:E:82:ILE:HD12	1.63	0.80
1:C:87:GLU:HG3	4:C:3382:HOH:O	1.80	0.80
1:C:218:LEU:CD1	2:C:3300:NAI:C5D	2.59	0.80
1:D:91:ILE:CA	4:D:4455:HOH:O	2.19	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:LYS:HE2	4:E:5430:HOH:O	1.77	0.80
4:B:2308:HOH:O	1:D:239:ILE:HG23	1.82	0.80
1:C:192:GLY:C	4:C:3367:HOH:O	2.19	0.80
1:A:181:ALA:C	4:A:1419:HOH:O	2.20	0.80
1:C:158:PHE:CE1	2:C:3300:NAI:H4B	2.17	0.80
1:C:236:GLY:CA	4:C:3398:HOH:O	2.30	0.80
1:D:124:THR:CB	4:D:4375:HOH:O	2.30	0.80
2:A:1300:NAI:C1D	2:A:1300:NAI:C2N	2.60	0.80
1:C:218:LEU:CD1	2:C:3300:NAI:H52N	2.12	0.80
1:D:88:ASP:CA	4:D:4432:HOH:O	2.29	0.80
1:D:219:HIS:HE1	2:D:4300:NAI:H51N	1.45	0.80
1:C:226:GLN:HG2	4:C:3366:HOH:O	1.82	0.79
1:E:9:GLY:N	1:E:41:THR:HG21	1.96	0.79
1:A:79:LEU:HD11	1:A:104:ILE:HD12	1.63	0.79
1:A:94:SER:O	4:A:1372:HOH:O	2.00	0.79
1:C:167:ILE:HG21	4:C:3345:HOH:O	1.80	0.79
1:D:118:ILE:CB	4:D:4408:HOH:O	2.27	0.79
1:B:142:GLN:HB2	4:B:2339:HOH:O	1.83	0.79
1:C:178:PRO:HG3	4:C:3346:HOH:O	1.83	0.79
1:C:199:ARG:HD3	4:C:3392:HOH:O	1.81	0.79
2:D:4300:NAI:C3N	3:D:4301:GLU:C	2.50	0.79
1:E:183:THR:CG2	4:E:5370:HOH:O	2.28	0.79
1:E:199:ARG:C	4:E:5320:HOH:O	2.21	0.79
1:A:8:ALA:O	4:A:1333:HOH:O	2.01	0.79
1:E:121:MET:HE2	1:E:122:THR:N	1.98	0.79
1:B:95:CYS:CA	4:B:2349:HOH:O	2.27	0.79
1:A:45:LEU:HD11	4:A:1379:HOH:O	1.82	0.79
1:D:113:PRO:N	4:D:4329:HOH:O	2.15	0.79
1:C:266:ARG:HH11	1:C:266:ARG:HG2	1.47	0.79
1:A:37:MET:HA	1:A:42:VAL:HG21	1.64	0.79
1:A:178:PRO:O	4:A:1324:HOH:O	2.01	0.79
1:C:266:ARG:CA	4:C:3340:HOH:O	2.29	0.79
1:D:56:ASN:ND2	4:D:4446:HOH:O	2.16	0.79
1:E:94:SER:C	4:E:5423:HOH:O	2.20	0.79
1:B:60:VAL:HG12	1:B:89:ARG:HH22	1.49	0.79
1:C:129:ARG:NH1	3:C:3301:GLU:CG	2.45	0.79
1:D:112:ARG:HD2	4:D:4347:HOH:O	1.81	0.79
1:E:132:ALA:HA	4:E:5351:HOH:O	1.82	0.79
1:E:61:GLN:O	4:E:5324:HOH:O	2.00	0.78
1:E:159:CYS:SG	4:E:5432:HOH:O	2.41	0.78
1:E:179:ALA:HB1	4:E:5322:HOH:O	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:LEU:N	4:E:5343:HOH:O	2.15	0.78
1:C:98:GLY:HA2	4:C:3310:HOH:O	1.83	0.78
1:A:120:CYS:CA	4:A:1368:HOH:O	2.31	0.78
1:A:238:THR:N	4:A:1391:HOH:O	2.14	0.78
1:B:187:ALA:HA	4:B:2341:HOH:O	1.83	0.78
1:D:94:SER:OG	4:D:4344:HOH:O	2.01	0.78
1:D:162:VAL:HG13	1:D:166:LEU:HD12	1.63	0.78
1:C:48:MET:HG3	4:C:3363:HOH:O	1.83	0.78
2:D:4300:NAI:H3D	4:D:4410:HOH:O	1.82	0.78
2:D:4300:NAI:O1N	3:D:4301:GLU:N	2.15	0.78
2:E:5300:NAI:C1D	3:E:5301:GLU:N	2.47	0.78
1:B:228:LYS:O	4:B:2364:HOH:O	2.02	0.78
1:C:128:VAL:HG12	1:C:129:ARG:H	1.49	0.78
1:E:185:LEU:CA	4:E:5323:HOH:O	2.25	0.78
1:D:275:GLU:O	4:D:4456:HOH:O	2.00	0.78
1:E:-1:ARG:NE	4:E:5319:HOH:O	2.14	0.78
2:A:1300:NAI:H2N	3:A:1301:GLU:HB3	1.63	0.78
1:B:108:LEU:O	4:B:2328:HOH:O	2.02	0.78
1:B:129:ARG:HH21	2:B:2300:NAI:C7N	1.91	0.78
1:B:256:ASN:HB3	4:B:2369:HOH:O	1.82	0.78
1:D:158:PHE:CE2	2:D:4300:NAI:O3B	2.36	0.78
1:D:179:ALA:O	4:D:4335:HOH:O	2.01	0.78
1:E:207:ALA:N	4:E:5408:HOH:O	2.15	0.78
1:A:155:SER:O	4:A:1425:HOH:O	2.01	0.78
1:D:223:HIS:CD2	4:D:4321:HOH:O	2.37	0.78
1:B:161:GLU:OE2	4:B:2346:HOH:O	2.00	0.77
1:A:112:ARG:HD3	4:A:1392:HOH:O	1.77	0.77
1:C:53:THR:HG22	1:C:55:HIS:H	1.46	0.77
1:D:146:GLY:O	4:D:4443:HOH:O	2.01	0.77
1:E:53:THR:CG2	4:E:5332:HOH:O	2.29	0.77
1:B:141:ALA:O	1:B:145:ASP:HB3	1.85	0.77
1:B:155:SER:CA	2:B:2300:NAI:N7N	2.47	0.77
1:D:4:GLY:O	4:D:4327:HOH:O	2.02	0.77
1:D:43:SER:HB2	4:D:4405:HOH:O	1.83	0.77
1:E:105:GLU:OE1	4:E:5437:HOH:O	2.02	0.77
1:A:102:SER:CA	4:A:1358:HOH:O	2.33	0.77
1:B:135:TYR:CE1	1:B:161:GLU:HB3	2.20	0.77
1:B:153:LEU:HA	4:B:2392:HOH:O	1.80	0.77
1:C:160:THR:HG22	4:C:3323:HOH:O	1.82	0.77
1:D:204:ARG:NH2	4:D:4411:HOH:O	2.17	0.77
1:E:137:THR:HG23	4:E:5426:HOH:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LEU:C	4:A:1370:HOH:O	2.21	0.77
1:C:271:MET:HA	1:C:274:GLN:HB3	1.67	0.77
1:D:30:ILE:HA	4:D:4365:HOH:O	1.83	0.77
1:D:88:ASP:O	4:D:4432:HOH:O	2.02	0.77
1:E:172:GLY:HA2	1:E:261:SER:OG	1.85	0.77
1:E:80:ASP:CB	4:E:5336:HOH:O	2.18	0.77
2:E:5300:NAI:C5B	2:E:5300:NAI:O2A	2.32	0.77
1:E:59:THR:O	4:E:5372:HOH:O	2.03	0.77
1:B:11:LEU:N	4:B:2343:HOH:O	2.18	0.76
1:C:86:ILE:C	4:C:3382:HOH:O	2.24	0.76
1:C:248:GLY:N	4:C:3402:HOH:O	2.16	0.76
1:C:255:ILE:HA	4:C:3332:HOH:O	1.85	0.76
1:D:115:PRO:HA	4:D:4374:HOH:O	1.85	0.76
1:B:74:ILE:HD12	4:B:2306:HOH:O	1.84	0.76
1:D:64:ASP:OD2	4:D:4353:HOH:O	2.03	0.76
1:D:115:PRO:O	4:D:4304:HOH:O	2.02	0.76
1:E:129:ARG:HB3	4:E:5401:HOH:O	1.85	0.76
1:A:75:ILE:HG22	1:A:76:PRO:HD3	1.67	0.76
1:A:168:ASP:OD1	4:A:1328:HOH:O	2.03	0.76
1:D:27:ALA:O	4:D:4425:HOH:O	2.02	0.76
3:A:1301:GLU:HB2	4:A:1408:HOH:O	1.86	0.76
1:B:1:MET:O	4:B:2332:HOH:O	2.04	0.76
1:A:122:THR:HG22	1:A:123:ASN:N	1.99	0.76
1:B:251:ARG:CD	4:B:2330:HOH:O	2.34	0.76
1:D:57:LYS:HE2	4:D:4376:HOH:O	1.79	0.76
1:D:156:VAL:O	1:D:156:VAL:HG12	1.83	0.76
1:E:185:LEU:N	4:E:5323:HOH:O	2.19	0.76
1:A:218:LEU:HD22	2:A:1300:NAI:C5B	2.14	0.76
1:C:15:LEU:CD1	4:C:3348:HOH:O	2.34	0.76
1:C:71:LYS:H	1:C:71:LYS:HD3	1.48	0.76
1:E:236:GLY:O	4:E:5307:HOH:O	2.03	0.76
1:D:220:SER:HB2	4:D:4419:HOH:O	1.83	0.76
1:E:58:GLU:HB2	4:E:5332:HOH:O	1.85	0.76
1:E:199:ARG:O	4:E:5320:HOH:O	2.02	0.76
1:A:-1:ARG:HG3	4:A:1424:HOH:O	1.85	0.76
1:D:224:PRO:CG	4:D:4355:HOH:O	2.33	0.76
1:E:169:ALA:CA	4:E:5375:HOH:O	2.34	0.76
1:A:89:ARG:NH1	4:A:1316:HOH:O	2.18	0.76
2:A:1300:NAI:C3N	3:A:1301:GLU:HB3	2.15	0.76
1:B:45:LEU:O	4:B:2385:HOH:O	2.03	0.76
1:C:163:GLU:HB2	4:C:3397:HOH:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:ALA:C	4:C:3352:HOH:O	2.24	0.76
2:C:3300:NAI:O4D	2:C:3300:NAI:PN	2.44	0.76
1:E:231:VAL:O	4:E:5321:HOH:O	2.03	0.76
1:E:263:ILE:N	4:E:5342:HOH:O	2.18	0.76
2:E:5300:NAI:O1N	3:E:5301:GLU:O	2.03	0.76
1:A:130:GLU:OE1	2:A:1300:NAI:H2D	1.85	0.76
1:B:6:ILE:HA	1:B:33:SER:HB3	1.66	0.76
1:B:129:ARG:HH22	3:B:2301:GLU:HG3	1.51	0.76
1:B:152:LEU:O	4:B:2392:HOH:O	2.04	0.76
1:C:198:PRO:N	4:C:3361:HOH:O	2.19	0.76
1:D:9:GLY:H	1:D:41:THR:HG21	1.48	0.76
1:A:3:VAL:HG22	1:A:65:VAL:HB	1.66	0.75
1:B:10:GLN:HB3	4:B:2343:HOH:O	1.85	0.75
1:B:195:MET:HE2	1:B:195:MET:HA	1.67	0.75
1:E:206:GLY:HA3	4:E:5408:HOH:O	1.85	0.75
1:C:217:LEU:CD1	4:C:3417:HOH:O	2.33	0.75
1:D:223:HIS:C	4:D:4372:HOH:O	2.24	0.75
1:E:134:VAL:CG1	4:E:5413:HOH:O	2.11	0.75
1:B:259:GLU:HA	4:B:2382:HOH:O	1.83	0.75
1:C:252:SER:O	1:C:254:LEU:N	2.18	0.75
1:D:3:VAL:O	4:D:4365:HOH:O	2.03	0.75
1:A:-1:ARG:HG3	4:A:1332:HOH:O	1.87	0.75
1:B:232:SER:OG	4:B:2352:HOH:O	2.03	0.75
1:C:154:SER:O	2:C:3300:NAI:N7N	2.19	0.75
1:E:91:ILE:CA	4:E:5344:HOH:O	2.28	0.75
1:E:178:PRO:N	4:E:5315:HOH:O	2.19	0.75
1:D:257:ALA:O	4:D:4349:HOH:O	2.03	0.75
1:E:158:PHE:HB3	4:E:5351:HOH:O	1.86	0.75
1:A:183:THR:CA	4:A:1354:HOH:O	2.21	0.75
1:D:218:LEU:CD2	2:D:4300:NAI:H52A	2.13	0.75
2:D:4300:NAI:C2N	3:D:4301:GLU:N	2.47	0.75
1:B:178:PRO:C	4:B:2373:HOH:O	2.25	0.75
1:E:121:MET:HB3	4:E:5407:HOH:O	1.85	0.75
1:A:33:SER:O	1:A:35:PRO:HD3	1.87	0.75
1:D:223:HIS:NE2	4:D:4321:HOH:O	2.18	0.75
1:E:253:LEU:HD23	4:E:5364:HOH:O	1.85	0.75
1:A:64:ASP:OD2	4:A:1403:HOH:O	2.03	0.74
1:B:9:GLY:N	4:B:2314:HOH:O	2.19	0.74
1:C:82:ILE:HG22	1:C:86:ILE:HD13	1.68	0.74
1:E:221:GLU:O	1:E:223:HIS:N	2.19	0.74
1:A:29:LYS:HA	4:A:1329:HOH:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ASP:CA	4:A:1370:HOH:O	2.34	0.74
2:B:2300:NAI:O4D	2:B:2300:NAI:PN	2.44	0.74
1:B:228:LYS:C	4:B:2364:HOH:O	2.26	0.74
1:C:163:GLU:CB	4:C:3397:HOH:O	2.36	0.74
1:C:195:MET:HA	1:C:195:MET:HE2	1.70	0.74
1:D:124:THR:OG1	4:D:4312:HOH:O	2.04	0.74
1:D:173:LEU:O	4:D:4315:HOH:O	2.05	0.74
1:A:182:PHE:N	4:A:1419:HOH:O	2.13	0.74
1:C:137:THR:OG1	4:C:3384:HOH:O	2.04	0.74
1:E:162:VAL:HB	4:E:5413:HOH:O	1.87	0.74
1:E:183:THR:OG1	4:E:5390:HOH:O	2.04	0.74
1:A:188:LEU:N	4:A:1303:HOH:O	2.21	0.74
1:A:199:ARG:HD3	4:A:1351:HOH:O	1.87	0.74
1:C:158:PHE:CE2	2:C:3300:NAI:O3B	2.39	0.74
1:E:162:VAL:N	4:E:5413:HOH:O	2.19	0.74
1:A:77:PHE:C	4:A:1356:HOH:O	2.25	0.74
1:B:12:ALA:CB	4:B:2314:HOH:O	2.32	0.74
1:B:129:ARG:CZ	2:B:2300:NAI:C7N	2.63	0.74
1:E:111:PHE:CE1	4:E:5326:HOH:O	2.36	0.74
1:C:178:PRO:CB	4:C:3396:HOH:O	2.29	0.74
1:A:13:PHE:HB2	4:A:1379:HOH:O	1.87	0.74
1:B:239:ILE:HG21	4:E:5303:HOH:O	1.87	0.74
1:D:229:ASP:CB	4:D:4393:HOH:O	2.22	0.74
1:B:45:LEU:HA	1:B:48:MET:SD	2.28	0.73
1:B:258:VAL:C	4:B:2382:HOH:O	2.25	0.73
1:A:163:GLU:HG3	4:A:1417:HOH:O	1.87	0.73
1:A:186:ASP:HB3	4:A:1354:HOH:O	1.89	0.73
1:B:222:GLN:O	1:B:223:HIS:HB2	1.88	0.73
2:D:4300:NAI:O4D	2:D:4300:NAI:PN	2.44	0.73
1:A:137:THR:O	4:A:1367:HOH:O	2.05	0.73
1:B:75:ILE:H	1:B:75:ILE:HD12	1.53	0.73
1:C:75:ILE:HD13	4:C:3377:HOH:O	1.87	0.73
1:A:171:THR:CA	4:A:1402:HOH:O	2.11	0.73
1:C:1:MET:O	4:C:3306:HOH:O	2.06	0.73
1:C:29:LYS:HE3	4:C:3404:HOH:O	1.88	0.73
1:A:35:PRO:O	1:A:36:ASP:HB2	1.88	0.73
1:A:122:THR:O	4:A:1428:HOH:O	2.05	0.73
1:D:112:ARG:HB3	4:D:4329:HOH:O	1.88	0.73
1:E:179:ALA:CA	4:E:5369:HOH:O	2.14	0.73
1:A:125:PRO:HG2	1:A:131:GLY:HA2	1.68	0.73
1:C:62:HIS:ND1	4:C:3362:HOH:O	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ASN:HB2	1:C:125:PRO:HD2	1.69	0.73
1:A:2:SER:OG	4:A:1403:HOH:O	2.07	0.73
1:A:183:THR:O	4:A:1354:HOH:O	2.07	0.73
1:A:266:ARG:HG2	1:A:266:ARG:HH11	1.54	0.73
1:A:269:GLN:HG2	1:A:270:SER:N	2.02	0.73
1:B:65:VAL:HG22	1:B:91:ILE:HD13	1.70	0.73
1:B:85:ASP:HB2	4:B:2376:HOH:O	1.89	0.73
1:B:120:CYS:N	4:B:2349:HOH:O	2.10	0.73
1:B:153:LEU:O	4:B:2392:HOH:O	2.07	0.73
1:D:246:GLU:OE2	4:D:4417:HOH:O	2.07	0.73
2:D:4300:NAI:C2N	3:D:4301:GLU:C	2.57	0.73
1:D:178:PRO:CB	4:D:4454:HOH:O	2.27	0.72
1:E:73:HIS:CB	4:E:5415:HOH:O	2.30	0.72
1:B:157:GLY:O	2:B:2300:NAI:H42N	1.89	0.72
1:C:135:TYR:CE1	1:C:161:GLU:HB3	2.23	0.72
1:C:193:VAL:HG12	4:C:3309:HOH:O	1.88	0.72
1:D:180:TYR:N	4:D:4308:HOH:O	2.18	0.72
1:B:60:VAL:HG12	1:B:89:ARG:NH2	2.03	0.72
2:D:4300:NAI:C5N	3:D:4301:GLU:C	2.57	0.72
1:E:211:LEU:O	4:E:5314:HOH:O	2.08	0.72
1:A:126:VAL:HG22	1:A:156:VAL:HG12	1.71	0.72
1:B:4:GLY:HA3	1:B:66:LEU:HD23	1.72	0.72
1:B:160:THR:HG22	1:B:161:GLU:N	2.04	0.72
2:E:5300:NAI:PA	2:E:5300:NAI:C4B	2.78	0.72
1:D:100:THR:HA	4:D:4422:HOH:O	1.89	0.72
1:E:234:PRO:O	4:E:5309:HOH:O	2.08	0.72
1:B:186:ASP:OD2	4:B:2356:HOH:O	2.07	0.72
1:C:209:ALA:O	4:C:3386:HOH:O	2.08	0.72
1:D:231:VAL:HB	4:D:4402:HOH:O	1.89	0.72
1:E:126:VAL:HG21	4:E:5385:HOH:O	1.88	0.72
1:A:186:ASP:HA	4:A:1370:HOH:O	1.88	0.72
1:D:101:ILE:HB	1:D:164:GLU:OE1	1.90	0.72
1:C:171:THR:OG1	4:C:3351:HOH:O	2.08	0.72
1:E:153:LEU:CB	4:E:5432:HOH:O	2.38	0.72
1:A:201:LEU:O	1:A:205:LEU:HG	1.89	0.72
1:B:142:GLN:CG	1:B:143:VAL:H	1.91	0.72
1:D:100:THR:HG22	1:D:102:SER:H	1.55	0.72
1:D:246:GLU:OE1	4:D:4383:HOH:O	2.08	0.72
1:E:91:ILE:CB	4:E:5344:HOH:O	2.02	0.72
1:E:246:GLU:OE2	4:E:5312:HOH:O	2.07	0.72
1:C:163:GLU:HG3	4:C:3397:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ILE:HD12	1:D:66:LEU:HD21	1.71	0.71
1:D:211:LEU:O	4:D:4406:HOH:O	2.07	0.71
1:E:141:ALA:HB2	4:E:5388:HOH:O	1.89	0.71
1:E:158:PHE:CD1	2:E:5300:NAI:H4B	2.25	0.71
1:E:251:ARG:NH1	4:E:5366:HOH:O	2.22	0.71
1:B:150:GLU:OE1	4:B:2312:HOH:O	2.08	0.71
1:D:11:LEU:N	4:D:4387:HOH:O	2.23	0.71
1:D:174:SER:CA	4:D:4315:HOH:O	2.39	0.71
1:E:130:GLU:OE2	2:E:5300:NAI:H2D	1.90	0.71
1:D:97:ALA:HB1	1:D:265:THR:HG23	1.72	0.71
1:D:124:THR:O	1:D:127:VAL:HG23	1.89	0.71
1:E:57:LYS:H	1:E:57:LYS:HD3	1.56	0.71
1:E:58:GLU:OE1	4:E:5332:HOH:O	2.07	0.71
1:A:27:ALA:N	4:A:1382:HOH:O	2.21	0.71
1:A:89:ARG:NH2	4:A:1395:HOH:O	2.23	0.71
1:B:28:HIS:O	4:B:2344:HOH:O	2.08	0.71
1:A:2:SER:HB3	4:A:1334:HOH:O	1.89	0.71
1:C:126:VAL:HG11	4:C:3317:HOH:O	1.89	0.71
1:D:83:GLY:O	1:D:86:ILE:HG22	1.89	0.71
1:E:206:GLY:CA	4:E:5408:HOH:O	2.36	0.71
1:D:37:MET:CG	4:D:4306:HOH:O	2.22	0.71
1:E:70:VAL:N	4:E:5305:HOH:O	2.15	0.71
1:A:3:VAL:N	4:A:1334:HOH:O	2.22	0.71
1:A:88:ASP:HB2	1:A:112:ARG:NH2	2.05	0.71
1:B:2:SER:HA	1:B:30:ILE:HG12	1.72	0.71
1:D:124:THR:CA	4:D:4375:HOH:O	2.39	0.71
1:A:86:ILE:CD1	1:A:108:LEU:HD11	2.15	0.71
1:E:199:ARG:HB3	4:E:5416:HOH:O	1.90	0.71
1:B:117:VAL:O	4:B:2370:HOH:O	2.09	0.71
1:C:222:GLN:HA	4:C:3304:HOH:O	1.89	0.71
1:D:161:GLU:OE2	4:D:4398:HOH:O	2.08	0.71
1:C:3:VAL:HB	1:C:30:ILE:CG1	2.21	0.71
1:D:185:LEU:HD21	1:D:210:LEU:HD12	1.72	0.71
1:C:91:ILE:HG23	1:C:116:ARG:HB2	1.73	0.70
1:D:32:ALA:HB3	1:D:52:LEU:HD23	1.72	0.70
1:D:150:GLU:OE2	4:D:4390:HOH:O	2.09	0.70
1:E:121:MET:HE2	1:E:122:THR:H	1.55	0.70
1:E:153:LEU:CA	4:E:5432:HOH:O	2.39	0.70
1:E:215:LYS:HE3	4:E:5430:HOH:O	1.84	0.70
1:A:190:ASP:O	4:A:1420:HOH:O	2.09	0.70
1:A:269:GLN:HA	4:A:1407:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-1:ARG:HB3	4:A:1342:HOH:O	1.90	0.70
1:C:126:VAL:HG12	4:C:3307:HOH:O	1.89	0.70
1:C:218:LEU:HB3	2:C:3300:NAI:H52N	1.73	0.70
1:C:264:ARG:NE	4:C:3353:HOH:O	2.10	0.70
1:A:75:ILE:HG22	1:A:76:PRO:CD	2.21	0.70
1:B:19:PHE:HA	1:B:22:ALA:HB3	1.73	0.70
1:B:100:THR:HG22	1:B:101:ILE:N	2.06	0.70
1:B:187:ALA:O	1:B:190:ASP:HB2	1.91	0.70
1:C:6:ILE:HD12	1:C:56:ASN:HB3	1.73	0.70
1:C:122:THR:CB	1:C:133:THR:HG22	2.19	0.70
1:D:128:VAL:O	1:D:129:ARG:HB2	1.92	0.70
1:A:122:THR:CG2	1:A:123:ASN:H	2.04	0.70
1:A:124:THR:N	4:A:1325:HOH:O	2.15	0.70
1:A:158:PHE:HA	4:A:1412:HOH:O	1.91	0.70
1:A:266:ARG:HD2	4:A:1331:HOH:O	1.82	0.70
1:D:116:ARG:HA	4:D:4389:HOH:O	1.91	0.70
1:D:168:ASP:OD1	4:D:4337:HOH:O	2.09	0.70
1:E:100:THR:HG22	1:E:102:SER:H	1.56	0.70
1:B:218:LEU:CD2	2:B:2300:NAI:H52A	2.21	0.70
1:C:15:LEU:HD11	4:C:3348:HOH:O	1.88	0.70
1:C:274:GLN:NE2	4:C:3339:HOH:O	2.22	0.70
1:D:184:ALA:HB2	4:D:4340:HOH:O	1.92	0.70
1:E:57:LYS:HD3	1:E:57:LYS:N	2.07	0.70
1:E:165:ASP:O	4:E:5349:HOH:O	2.09	0.70
1:A:161:GLU:CB	4:A:1364:HOH:O	2.26	0.70
1:C:29:LYS:CB	4:C:3306:HOH:O	2.39	0.70
1:C:195:MET:HA	1:C:195:MET:CE	2.21	0.70
1:E:156:VAL:O	1:E:156:VAL:HG12	1.90	0.70
1:A:130:GLU:O	4:A:1307:HOH:O	2.10	0.70
1:C:266:ARG:NE	4:C:3303:HOH:O	2.24	0.70
1:E:60:VAL:HG21	1:E:82:ILE:HG23	1.71	0.70
1:C:7:GLY:HA2	1:C:70:VAL:HG22	1.74	0.70
1:C:165:ASP:O	4:C:3311:HOH:O	2.10	0.70
1:E:194:LYS:CA	4:E:5303:HOH:O	2.19	0.70
1:B:208:GLN:OE1	4:B:2359:HOH:O	2.09	0.70
1:D:56:ASN:ND2	4:D:4369:HOH:O	2.25	0.70
1:E:174:SER:CB	4:E:5391:HOH:O	2.40	0.70
1:B:208:GLN:HB2	4:B:2359:HOH:O	1.91	0.69
1:C:27:ALA:HB1	4:C:3363:HOH:O	1.92	0.69
1:D:97:ALA:HA	4:D:4333:HOH:O	1.91	0.69
1:D:103:SER:HA	4:D:4449:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:ALA:O	4:E:5434:HOH:O	2.09	0.69
1:B:100:THR:HG22	1:B:101:ILE:H	1.55	0.69
1:C:56:ASN:O	4:C:3383:HOH:O	2.10	0.69
1:C:85:ASP:O	4:C:3382:HOH:O	2.10	0.69
1:A:106:LYS:O	4:A:1432:HOH:O	2.09	0.69
1:C:10:GLN:NE2	4:C:3390:HOH:O	2.25	0.69
1:C:198:PRO:HG2	1:C:201:LEU:HB3	1.75	0.69
1:D:231:VAL:O	4:D:4401:HOH:O	2.09	0.69
1:B:8:ALA:HA	1:B:12:ALA:CB	2.22	0.69
1:D:124:THR:CG2	4:D:4375:HOH:O	2.20	0.69
1:E:91:ILE:N	4:E:5344:HOH:O	2.26	0.69
1:E:169:ALA:HA	4:E:5375:HOH:O	1.92	0.69
1:A:130:GLU:OE2	2:A:1300:NAI:H2D	1.92	0.69
1:A:168:ASP:HB2	4:A:1338:HOH:O	1.92	0.69
1:C:115:PRO:HB3	4:C:3358:HOH:O	1.93	0.69
1:A:162:VAL:HG13	1:A:166:LEU:HD12	1.75	0.69
1:A:193:VAL:CG2	4:A:1369:HOH:O	2.40	0.69
1:B:37:MET:HE3	4:B:2393:HOH:O	1.92	0.69
1:C:128:VAL:HG12	1:C:129:ARG:N	2.06	0.69
1:D:125:PRO:O	1:D:128:VAL:HG12	1.92	0.69
1:E:102:SER:HB3	4:E:5347:HOH:O	1.91	0.69
2:E:5300:NAI:PN	2:E:5300:NAI:PA	2.89	0.69
2:E:5300:NAI:O2A	2:E:5300:NAI:O4B	2.11	0.69
1:A:122:THR:CG2	1:A:123:ASN:N	2.56	0.69
1:B:231:VAL:CG1	4:B:2363:HOH:O	2.40	0.69
1:C:100:THR:HG22	1:C:102:SER:H	1.57	0.69
1:C:118:ILE:H	1:C:118:ILE:HD13	1.57	0.69
1:C:140:HIS:HB2	4:C:3385:HOH:O	1.91	0.69
1:E:164:GLU:O	4:E:5395:HOH:O	2.11	0.69
1:A:29:LYS:CA	4:A:1329:HOH:O	2.41	0.69
1:D:61:GLN:O	4:D:4430:HOH:O	2.11	0.69
1:E:80:ASP:OD1	4:E:5326:HOH:O	2.10	0.69
1:E:253:LEU:N	4:E:5364:HOH:O	2.25	0.69
1:E:262:CYS:CB	4:E:5342:HOH:O	2.37	0.69
4:A:1315:HOH:O	1:E:228:LYS:HE2	1.92	0.68
1:C:203:VAL:CA	4:C:3355:HOH:O	2.34	0.68
1:D:67:PHE:N	4:D:4327:HOH:O	2.26	0.68
1:E:133:THR:CG2	4:E:5385:HOH:O	2.40	0.68
1:A:183:THR:C	4:A:1354:HOH:O	2.32	0.68
1:A:230:ASN:CB	4:A:1317:HOH:O	2.40	0.68
1:B:229:ASP:OD1	4:B:2386:HOH:O	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ILE:CG1	4:C:3394:HOH:O	2.32	0.68
1:D:3:VAL:HB	1:D:30:ILE:CD1	2.22	0.68
1:E:11:LEU:O	1:E:15:LEU:HD12	1.93	0.68
1:E:175:GLY:O	4:E:5397:HOH:O	2.10	0.68
1:E:251:ARG:CD	4:E:5330:HOH:O	2.40	0.68
1:C:129:ARG:CD	2:C:3300:NAI:O7N	2.41	0.68
1:C:257:ALA:O	4:C:3378:HOH:O	2.11	0.68
1:C:266:ARG:HG2	4:C:3340:HOH:O	1.92	0.68
1:D:133:THR:HG21	1:D:153:LEU:HD12	1.75	0.68
1:E:2:SER:HB3	4:E:5387:HOH:O	1.93	0.68
1:A:-1:ARG:HG2	4:A:1332:HOH:O	1.87	0.68
1:D:175:GLY:O	4:D:4309:HOH:O	2.10	0.68
1:E:251:ARG:N	4:E:5317:HOH:O	2.26	0.68
1:A:150:GLU:OE2	4:A:1383:HOH:O	2.11	0.68
1:B:6:ILE:CD1	1:B:59:THR:HB	2.24	0.68
1:A:194:LYS:HE2	1:E:240:HIS:CE1	2.29	0.68
1:C:124:THR:N	1:C:125:PRO:HD2	2.08	0.68
1:D:88:ASP:HA	4:D:4432:HOH:O	1.91	0.68
1:D:251:ARG:HD3	4:D:4427:HOH:O	1.94	0.68
1:A:130:GLU:CD	2:A:1300:NAI:H2D	2.13	0.68
1:E:48:MET:HG2	1:E:48:MET:O	1.94	0.68
1:B:6:ILE:HD13	1:B:59:THR:HB	1.75	0.68
1:C:252:SER:OG	4:C:3308:HOH:O	2.07	0.68
1:E:225:GLY:HA2	4:E:5353:HOH:O	1.86	0.68
1:E:251:ARG:HD2	4:E:5330:HOH:O	1.94	0.68
1:C:185:LEU:CD2	4:C:3324:HOH:O	2.42	0.68
1:B:124:THR:N	1:B:125:PRO:HD2	2.09	0.68
1:C:180:TYR:HD2	4:C:3302:HOH:O	1.76	0.68
1:C:203:VAL:HG13	4:C:3355:HOH:O	1.92	0.68
1:D:150:GLU:HB2	4:D:4443:HOH:O	1.94	0.68
1:E:114:ALA:O	4:E:5436:HOH:O	2.11	0.68
1:A:22:ALA:CB	4:A:1425:HOH:O	2.41	0.67
1:D:181:ALA:O	4:D:4330:HOH:O	2.11	0.67
1:E:190:ASP:OD1	4:E:5381:HOH:O	2.12	0.67
1:A:266:ARG:NE	4:A:1331:HOH:O	2.21	0.67
1:B:50:VAL:HA	4:B:2378:HOH:O	1.95	0.67
1:B:124:THR:O	1:B:127:VAL:HG23	1.94	0.67
1:D:148:LEU:HB2	4:D:4348:HOH:O	1.93	0.67
1:E:147:ARG:O	1:E:151:GLN:HB2	1.94	0.67
1:B:101:ILE:O	1:B:105:GLU:HB2	1.93	0.67
1:C:29:LYS:HB3	4:C:3306:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:ASP:N	4:D:4310:HOH:O	2.25	0.67
1:C:150:GLU:O	4:C:3319:HOH:O	2.13	0.67
1:E:199:ARG:NH2	4:E:5316:HOH:O	2.28	0.67
1:A:76:PRO:O	4:A:1356:HOH:O	2.12	0.67
1:B:61:GLN:HA	4:B:2325:HOH:O	1.94	0.67
1:B:71:LYS:HB3	1:B:72:PRO:CD	2.22	0.67
1:D:30:ILE:CB	4:D:4425:HOH:O	2.28	0.67
1:E:123:ASN:HB3	4:E:5397:HOH:O	1.94	0.67
1:C:66:LEU:HD23	1:C:67:PHE:N	2.10	0.67
1:C:223:HIS:N	4:C:3304:HOH:O	2.21	0.67
1:A:158:PHE:CZ	2:A:1300:NAI:O3B	2.48	0.67
1:A:165:ASP:O	4:A:1393:HOH:O	2.12	0.67
1:B:129:ARG:C	4:B:2372:HOH:O	2.33	0.67
1:E:122:THR:CB	1:E:133:THR:HG22	2.23	0.67
1:A:124:THR:OG1	4:A:1325:HOH:O	2.13	0.66
1:B:178:PRO:O	4:B:2373:HOH:O	2.13	0.66
1:C:29:LYS:CE	4:C:3404:HOH:O	2.33	0.66
1:C:231:VAL:O	1:C:231:VAL:HG12	1.95	0.66
1:C:260:ALA:HB3	4:C:3378:HOH:O	1.94	0.66
1:C:273:ASP:C	4:C:3393:HOH:O	2.33	0.66
1:C:275:GLU:N	4:C:3393:HOH:O	2.23	0.66
1:E:75:ILE:HG21	1:E:104:ILE:HD11	1.78	0.66
1:E:179:ALA:O	4:E:5322:HOH:O	2.14	0.66
1:C:75:ILE:HA	4:C:3407:HOH:O	1.94	0.66
1:D:62:HIS:ND1	1:D:62:HIS:O	2.27	0.66
1:D:161:GLU:CD	4:D:4398:HOH:O	2.33	0.66
1:A:120:CYS:CB	4:A:1368:HOH:O	2.42	0.66
1:A:187:ALA:C	4:A:1303:HOH:O	2.34	0.66
1:B:255:ILE:HG12	4:B:2303:HOH:O	1.96	0.66
1:E:185:LEU:HD21	1:E:210:LEU:HD12	1.76	0.66
1:A:79:LEU:HD11	1:A:104:ILE:CD1	2.24	0.66
1:C:251:ARG:O	1:C:252:SER:O	2.13	0.66
1:D:32:ALA:HB3	1:D:52:LEU:CD2	2.25	0.66
1:D:266:ARG:NE	4:D:4378:HOH:O	2.27	0.66
1:C:198:PRO:CD	4:C:3361:HOH:O	2.42	0.66
1:C:265:THR:HG22	4:C:3340:HOH:O	1.94	0.66
1:D:61:GLN:O	4:D:4415:HOH:O	2.13	0.66
1:D:151:GLN:HB3	4:D:4444:HOH:O	1.94	0.66
1:A:26:ALA:HB1	4:A:1382:HOH:O	1.96	0.66
1:A:253:LEU:HD23	4:A:1405:HOH:O	1.95	0.66
1:B:129:ARG:CA	4:B:2372:HOH:O	2.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:PHE:CD1	4:B:2373:HOH:O	2.47	0.66
1:B:219:HIS:HE1	2:B:2300:NAI:O5D	1.73	0.66
1:D:232:SER:HB3	1:D:239:ILE:HG12	1.78	0.66
1:A:124:THR:N	1:A:125:PRO:HD2	2.10	0.66
1:C:101:ILE:HD11	1:C:117:VAL:O	1.95	0.66
1:A:193:VAL:HG23	4:A:1369:HOH:O	1.96	0.66
1:B:129:ARG:HH21	3:B:2301:GLU:HB2	1.59	0.66
1:D:251:ARG:CZ	4:D:4427:HOH:O	2.42	0.66
1:E:220:SER:O	1:E:221:GLU:HB2	1.95	0.66
1:B:168:ASP:CB	4:B:2357:HOH:O	2.43	0.66
1:D:93:VAL:HA	4:D:4408:HOH:O	1.95	0.66
1:E:193:VAL:O	4:E:5303:HOH:O	2.12	0.66
1:D:3:VAL:HB	1:D:30:ILE:HD12	1.78	0.66
1:D:256:ASN:O	4:D:4318:HOH:O	2.13	0.66
1:E:55:HIS:HB3	1:E:57:LYS:HE2	1.78	0.66
1:A:120:CYS:C	4:A:1327:HOH:O	2.35	0.65
1:A:206:GLY:O	4:A:1421:HOH:O	2.14	0.65
1:A:1:MET:CB	4:A:1427:HOH:O	2.25	0.65
1:B:189:ALA:CA	4:B:2302:HOH:O	2.35	0.65
1:C:118:ILE:HG22	1:C:137:THR:HA	1.76	0.65
1:E:114:ALA:HB1	1:E:140:HIS:CG	2.31	0.65
1:B:94:SER:HB2	4:B:2306:HOH:O	1.95	0.65
1:C:50:VAL:N	4:C:3363:HOH:O	2.27	0.65
1:C:192:GLY:HA3	4:C:3367:HOH:O	1.88	0.65
1:B:195:MET:HA	1:B:195:MET:CE	2.26	0.65
1:D:3:VAL:HG22	1:D:65:VAL:CG1	2.27	0.65
1:D:90:HIS:O	4:D:4455:HOH:O	2.14	0.65
1:D:264:ARG:NH2	4:D:4380:HOH:O	2.15	0.65
1:C:29:LYS:C	1:C:30:ILE:HD12	2.17	0.65
2:D:4300:NAI:N1N	3:D:4301:GLU:CA	2.55	0.65
1:E:118:ILE:O	4:E:5325:HOH:O	2.13	0.65
1:A:85:ASP:HB2	4:A:1437:HOH:O	1.95	0.65
1:A:240:HIS:HA	4:A:1352:HOH:O	1.97	0.65
1:B:160:THR:N	4:B:2311:HOH:O	2.23	0.65
1:B:172:GLY:HA2	1:B:261:SER:OG	1.96	0.65
1:C:29:LYS:CG	4:C:3404:HOH:O	2.39	0.65
1:C:29:LYS:N	4:C:3404:HOH:O	2.29	0.65
1:A:182:PHE:O	4:A:1354:HOH:O	2.13	0.65
1:A:187:ALA:HB1	4:A:1303:HOH:O	1.97	0.65
1:A:198:PRO:HG2	1:A:201:LEU:HB3	1.77	0.65
1:B:3:VAL:H	1:B:30:ILE:HG23	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:LYS:NZ	4:D:4438:HOH:O	2.28	0.65
1:E:178:PRO:CD	4:E:5315:HOH:O	2.44	0.65
1:A:238:THR:OG1	4:A:1320:HOH:O	2.14	0.65
1:B:218:LEU:CD1	2:B:2300:NAI:H52N	2.25	0.65
1:C:171:THR:OG1	4:C:3380:HOH:O	2.15	0.65
1:A:142:GLN:N	4:A:1390:HOH:O	2.05	0.65
1:A:240:HIS:NE2	4:A:1375:HOH:O	2.22	0.65
1:C:251:ARG:CA	4:C:3359:HOH:O	2.40	0.65
1:A:198:PRO:HD2	1:A:201:LEU:HD23	1.77	0.65
1:D:53:THR:HG22	1:D:55:HIS:N	2.11	0.65
1:D:222:GLN:O	1:D:223:HIS:CB	2.44	0.65
1:E:83:GLY:HA2	1:E:86:ILE:HD12	1.79	0.65
1:E:163:GLU:OE2	4:E:5399:HOH:O	2.14	0.65
2:E:5300:NAI:O2A	2:E:5300:NAI:C4B	2.45	0.65
1:A:135:TYR:OH	1:A:150:GLU:HG3	1.97	0.64
1:B:9:GLY:H	1:B:12:ALA:CB	2.05	0.64
1:B:63:SER:HB2	1:B:89:ARG:NH1	2.13	0.64
1:B:73:HIS:ND1	4:B:2390:HOH:O	2.26	0.64
1:B:74:ILE:HG23	1:B:78:ILE:HG21	1.79	0.64
1:B:133:THR:O	4:B:2311:HOH:O	2.15	0.64
1:A:126:VAL:HG22	1:A:156:VAL:CG1	2.26	0.64
1:B:126:VAL:HA	4:B:2372:HOH:O	1.98	0.64
1:B:185:LEU:O	1:B:187:ALA:N	2.30	0.64
1:D:224:PRO:N	4:D:4372:HOH:O	2.29	0.64
1:E:220:SER:HB2	1:E:222:GLN:HG2	1.79	0.64
1:A:138:GLY:CA	4:A:1310:HOH:O	2.39	0.64
1:B:128:VAL:O	1:B:129:ARG:HB2	1.97	0.64
1:D:223:HIS:CE1	4:D:4355:HOH:O	2.51	0.64
2:D:4300:NAI:C6N	3:D:4301:GLU:C	2.65	0.64
1:A:181:ALA:O	4:A:1419:HOH:O	2.12	0.64
1:B:134:VAL:HA	4:B:2311:HOH:O	1.98	0.64
1:C:43:SER:O	1:C:46:ARG:HB2	1.97	0.64
1:C:131:GLY:CA	4:C:3307:HOH:O	2.41	0.64
1:D:125:PRO:HB2	1:D:131:GLY:HA2	1.80	0.64
1:A:128:VAL:O	1:A:129:ARG:HB2	1.97	0.64
1:B:95:CYS:HA	1:B:120:CYS:O	1.97	0.64
1:C:24:VAL:N	4:C:3369:HOH:O	2.09	0.64
1:C:124:THR:O	1:C:127:VAL:HG23	1.97	0.64
1:C:169:ALA:HB2	4:C:3320:HOH:O	1.97	0.64
1:E:178:PRO:HB2	4:E:5393:HOH:O	1.96	0.64
1:A:11:LEU:HD12	4:A:1399:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:SER:CA	4:A:1321:HOH:O	2.45	0.64
1:E:0:GLY:O	4:E:5371:HOH:O	2.13	0.64
1:E:124:THR:O	1:E:127:VAL:HG23	1.96	0.64
1:E:151:GLN:HB3	4:E:5428:HOH:O	1.98	0.64
1:A:111:PHE:O	4:A:1365:HOH:O	2.14	0.64
1:A:194:LYS:O	1:A:195:MET:SD	2.55	0.64
1:C:185:LEU:N	4:C:3352:HOH:O	2.31	0.64
1:C:198:PRO:HD3	4:C:3361:HOH:O	1.98	0.64
1:A:26:ALA:HB3	1:A:29:LYS:HB2	1.78	0.64
3:A:1301:GLU:HG2	4:A:1408:HOH:O	1.97	0.64
1:C:62:HIS:CE1	4:C:3362:HOH:O	2.50	0.64
1:C:178:PRO:CA	4:C:3396:HOH:O	2.46	0.64
1:D:99:VAL:O	4:D:4317:HOH:O	2.15	0.64
1:A:135:TYR:CE2	1:A:150:GLU:HG2	2.33	0.64
4:B:2308:HOH:O	1:D:239:ILE:HG21	1.92	0.64
1:E:13:PHE:CE1	4:E:5306:HOH:O	2.51	0.64
1:E:56:ASN:O	1:E:60:VAL:HG23	1.98	0.64
1:E:130:GLU:OE2	2:E:5300:NAI:C2D	2.46	0.64
1:E:232:SER:HB2	4:E:5345:HOH:O	1.97	0.64
1:A:156:VAL:HG12	1:A:156:VAL:O	1.98	0.64
1:C:223:HIS:ND1	1:C:224:PRO:HD2	2.13	0.64
1:D:22:ALA:HB3	1:D:24:VAL:HG23	1.80	0.64
1:D:115:PRO:HA	4:D:4307:HOH:O	1.98	0.64
1:E:63:SER:CA	4:E:5417:HOH:O	2.43	0.64
1:E:203:VAL:HG23	4:E:5320:HOH:O	1.98	0.64
1:E:218:LEU:HD22	2:E:5300:NAI:H52A	1.79	0.64
1:A:119:ARG:HG2	4:A:1372:HOH:O	1.90	0.63
1:C:112:ARG:HH11	1:C:112:ARG:HG3	1.63	0.63
1:A:33:SER:OG	1:A:56:ASN:HB3	1.98	0.63
1:A:36:ASP:O	1:A:37:MET:HB2	1.98	0.63
1:A:269:GLN:C	1:A:271:MET:H	2.02	0.63
1:B:4:GLY:HA2	1:B:59:THR:HG22	1.79	0.63
1:B:73:HIS:O	1:B:78:ILE:HD13	1.98	0.63
1:C:117:VAL:HG23	4:C:3315:HOH:O	1.98	0.63
1:C:213:ALA:CB	4:C:3386:HOH:O	2.24	0.63
1:A:129:ARG:HD2	4:A:1371:HOH:O	1.98	0.63
1:B:182:PHE:CE1	4:B:2373:HOH:O	2.51	0.63
1:B:259:GLU:CA	4:B:2382:HOH:O	2.43	0.63
1:C:29:LYS:HG2	4:C:3404:HOH:O	1.98	0.63
1:C:155:SER:HA	2:C:3300:NAI:N7N	2.09	0.63
1:C:160:THR:HG22	1:C:161:GLU:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:LEU:HB3	4:D:4323:HOH:O	1.98	0.63
1:A:164:GLU:HA	1:A:167:ILE:HG12	1.80	0.63
1:A:271:MET:HG2	1:A:271:MET:O	1.98	0.63
1:B:155:SER:C	2:B:2300:NAI:H72N	2.02	0.63
1:C:123:ASN:N	4:C:3331:HOH:O	2.17	0.63
1:C:172:GLY:HA2	1:C:261:SER:OG	1.98	0.63
1:A:17:LYS:HA	1:A:48:MET:HE3	1.81	0.63
1:E:198:PRO:HG2	1:E:201:LEU:HB3	1.81	0.63
1:B:94:SER:C	4:B:2349:HOH:O	2.36	0.63
1:D:87:GLU:CB	4:D:4322:HOH:O	2.34	0.63
1:E:190:ASP:CG	4:E:5381:HOH:O	2.35	0.63
1:A:89:ARG:HG3	1:A:90:HIS:N	2.14	0.63
1:B:158:PHE:CZ	2:B:2300:NAI:C3B	2.82	0.63
1:D:168:ASP:CG	4:D:4337:HOH:O	2.37	0.63
1:E:158:PHE:CE2	2:E:5300:NAI:O3B	2.52	0.63
1:E:177:GLY:HA2	1:E:180:TYR:CD1	2.34	0.63
1:E:211:LEU:CD1	4:E:5314:HOH:O	2.46	0.63
1:E:229:ASP:CA	4:E:5337:HOH:O	2.20	0.63
1:A:55:HIS:HB3	1:A:57:LYS:HD2	1.80	0.63
1:B:256:ASN:CB	4:B:2369:HOH:O	2.42	0.63
1:A:100:THR:HG22	1:A:102:SER:H	1.64	0.63
1:C:114:ALA:HB1	1:C:140:HIS:ND1	2.14	0.63
1:E:30:ILE:HB	1:E:50:VAL:HG22	1.79	0.63
1:E:94:SER:N	4:E:5325:HOH:O	2.05	0.63
1:A:123:ASN:HB2	4:A:1325:HOH:O	1.98	0.62
1:B:160:THR:HG22	1:B:161:GLU:H	1.62	0.62
1:C:172:GLY:O	1:C:258:VAL:HG22	1.99	0.62
1:C:266:ARG:HG2	1:C:266:ARG:NH1	2.14	0.62
1:E:225:GLY:O	4:E:5353:HOH:O	2.16	0.62
1:A:139:THR:N	4:A:1310:HOH:O	2.31	0.62
1:C:3:VAL:O	1:C:30:ILE:HA	1.98	0.62
1:E:169:ALA:C	1:E:171:THR:H	2.01	0.62
1:A:174:SER:CB	4:A:1339:HOH:O	2.46	0.62
1:C:218:LEU:CB	2:C:3300:NAI:H52N	2.28	0.62
1:E:17:LYS:HB3	4:E:5306:HOH:O	1.90	0.62
1:E:153:LEU:C	4:E:5432:HOH:O	2.37	0.62
1:B:109:SER:OG	1:B:115:PRO:HD2	1.98	0.62
1:B:129:ARG:N	4:B:2372:HOH:O	2.32	0.62
1:C:19:PHE:O	4:C:3369:HOH:O	2.15	0.62
1:C:155:SER:CA	2:C:3300:NAI:H72N	2.10	0.62
1:C:218:LEU:HB3	2:C:3300:NAI:C5D	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ILE:HG12	1:A:119:ARG:HB2	1.81	0.62
1:B:259:GLU:N	4:B:2382:HOH:O	2.33	0.62
1:D:103:SER:CA	4:D:4449:HOH:O	2.45	0.62
1:A:121:MET:N	4:A:1327:HOH:O	2.33	0.62
1:D:266:ARG:C	1:D:268:LEU:H	2.03	0.62
1:D:176:SER:O	1:D:179:ALA:HB3	1.99	0.62
1:A:78:ILE:N	4:A:1356:HOH:O	2.31	0.62
1:B:162:VAL:HG12	1:B:163:GLU:HG2	1.82	0.62
1:B:264:ARG:O	1:B:268:LEU:HG	2.00	0.62
1:C:25:LEU:HD11	1:C:30:ILE:HD11	1.81	0.62
1:D:71:LYS:O	1:D:75:ILE:HD12	1.99	0.62
2:D:4300:NAI:H3D	4:D:4423:HOH:O	2.00	0.62
1:E:193:VAL:C	4:E:5303:HOH:O	2.37	0.62
1:B:141:ALA:HB1	1:B:145:ASP:OD2	2.00	0.62
1:B:225:GLY:O	1:B:228:LYS:HB3	1.99	0.62
1:C:258:VAL:O	1:C:258:VAL:CG1	2.47	0.62
1:A:118:ILE:HD12	1:A:149:MET:SD	2.39	0.61
1:A:172:GLY:HA2	1:A:261:SER:HB3	1.82	0.61
1:B:122:THR:HG22	1:B:133:THR:OG1	1.99	0.61
1:B:200:ARG:NH1	1:B:204:ARG:HH21	1.98	0.61
1:C:71:LYS:HB2	1:C:73:HIS:CE1	2.35	0.61
1:C:185:LEU:HD23	4:C:3324:HOH:O	1.99	0.61
1:D:30:ILE:CA	4:D:4365:HOH:O	2.41	0.61
1:A:13:PHE:CA	4:A:1379:HOH:O	2.47	0.61
1:A:123:ASN:HD21	1:A:132:ALA:N	1.97	0.61
1:A:193:VAL:C	1:A:195:MET:H	2.04	0.61
1:B:125:PRO:HG2	1:B:131:GLY:HA2	1.82	0.61
1:E:122:THR:HG22	1:E:133:THR:CB	2.28	0.61
1:A:258:VAL:HG23	4:A:1302:HOH:O	1.94	0.61
1:C:68:LEU:HD11	1:C:78:ILE:HG21	1.82	0.61
1:C:250:PHE:N	4:C:3312:HOH:O	2.33	0.61
1:D:53:THR:HG21	1:D:58:GLU:OE1	2.00	0.61
1:D:58:GLU:HB3	4:D:4358:HOH:O	1.99	0.61
1:E:209:ALA:C	4:E:5360:HOH:O	2.37	0.61
1:A:2:SER:CB	4:A:1403:HOH:O	2.47	0.61
1:C:3:VAL:HB	1:C:30:ILE:HG12	1.82	0.61
1:A:93:VAL:HG13	1:A:118:ILE:HG13	1.82	0.61
1:B:119:ARG:HD2	1:B:164:GLU:OE2	2.00	0.61
1:C:37:MET:HA	1:C:42:VAL:HG11	1.82	0.61
1:C:208:GLN:OE1	4:C:3395:HOH:O	2.16	0.61
1:E:86:ILE:HD12	1:E:108:LEU:HD22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ILE:CD1	1:A:263:ILE:H	2.14	0.61
1:B:129:ARG:CZ	2:B:2300:NAI:C3N	2.78	0.61
1:B:231:VAL:HG13	4:B:2363:HOH:O	1.99	0.61
1:C:119:ARG:NH2	4:C:3310:HOH:O	2.31	0.61
1:D:229:ASP:HA	4:D:4316:HOH:O	2.01	0.61
1:A:241:ALA:O	1:A:244:VAL:HG22	2.01	0.61
1:B:14:ALA:CA	1:B:127:VAL:HG22	2.28	0.61
2:B:2300:NAI:N1N	3:B:2301:GLU:OXT	2.33	0.61
1:C:122:THR:CB	4:C:3331:HOH:O	2.15	0.61
2:C:3300:NAI:N1N	3:C:3301:GLU:OXT	2.33	0.61
1:A:68:LEU:HD12	1:A:94:SER:HB2	1.82	0.61
1:C:133:THR:HG22	4:C:3331:HOH:O	2.00	0.61
1:E:106:LYS:CB	4:E:5384:HOH:O	2.47	0.61
1:B:64:ASP:O	1:B:90:HIS:HA	1.99	0.61
1:B:70:VAL:HG23	4:B:2368:HOH:O	2.01	0.61
1:B:129:ARG:NH2	3:B:2301:GLU:HG3	2.14	0.61
1:D:220:SER:HB2	1:D:222:GLN:HG2	1.82	0.61
1:E:113:PRO:HD2	4:E:5367:HOH:O	2.01	0.61
1:A:220:SER:HB2	4:A:1441:HOH:O	2.00	0.61
1:A:259:GLU:N	4:A:1366:HOH:O	2.29	0.61
1:B:133:THR:HG22	4:B:2387:HOH:O	2.01	0.61
1:B:256:ASN:C	4:B:2381:HOH:O	2.38	0.61
1:A:115:PRO:HD2	1:A:140:HIS:CD2	2.36	0.60
1:B:266:ARG:O	1:B:269:GLN:HG2	2.01	0.60
1:C:48:MET:HB3	4:C:3371:HOH:O	1.89	0.60
1:D:30:ILE:CG1	4:D:4425:HOH:O	2.48	0.60
1:D:38:ASP:OD2	1:D:40:ALA:HB3	2.01	0.60
1:E:135:TYR:CE1	1:E:161:GLU:HB3	2.36	0.60
1:E:251:ARG:NE	4:E:5348:HOH:O	2.34	0.60
1:A:79:LEU:HD11	1:A:104:ILE:HG23	1.83	0.60
1:B:245:LEU:CA	4:B:2353:HOH:O	2.40	0.60
1:C:49:GLY:CA	4:C:3363:HOH:O	2.47	0.60
1:E:77:PHE:HD1	1:E:77:PHE:H	1.47	0.60
1:B:178:PRO:HG2	4:B:2345:HOH:O	2.02	0.60
1:C:264:ARG:NH2	4:C:3353:HOH:O	2.23	0.60
1:D:168:ASP:HA	4:D:4337:HOH:O	2.01	0.60
1:D:266:ARG:CZ	4:D:4378:HOH:O	2.46	0.60
1:A:45:LEU:HD21	4:A:1379:HOH:O	2.01	0.60
1:B:218:LEU:HD22	2:B:2300:NAI:O5B	2.00	0.60
1:C:93:VAL:CG1	1:C:118:ILE:HD11	2.30	0.60
1:C:45:LEU:O	1:C:48:MET:HB3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:VAL:HG13	1:D:156:VAL:CG1	2.30	0.60
1:D:246:GLU:CG	4:D:4383:HOH:O	2.44	0.60
1:D:266:ARG:CD	4:D:4311:HOH:O	2.49	0.60
1:A:123:ASN:C	1:A:125:PRO:HD2	2.22	0.60
1:A:222:GLN:O	1:A:223:HIS:CB	2.49	0.60
1:B:70:VAL:HG12	1:B:71:LYS:H	1.66	0.60
2:B:2300:NAI:H2N	3:B:2301:GLU:HB3	1.78	0.60
1:D:78:ILE:HG23	1:D:82:ILE:HD13	1.83	0.60
1:D:185:LEU:CG	4:D:4330:HOH:O	2.28	0.60
1:D:203:VAL:HG12	1:D:204:ARG:N	2.17	0.60
1:A:186:ASP:CB	4:A:1354:HOH:O	2.45	0.60
1:B:188:LEU:C	1:B:190:ASP:H	2.05	0.60
1:D:265:THR:CB	4:D:4360:HOH:O	2.06	0.60
1:E:128:VAL:O	1:E:129:ARG:C	2.39	0.60
1:E:133:THR:HG21	4:E:5385:HOH:O	2.01	0.60
1:A:95:CYS:N	4:A:1321:HOH:O	2.33	0.60
1:A:106:LYS:HG3	4:A:1344:HOH:O	2.02	0.60
1:B:102:SER:HA	1:B:105:GLU:HB2	1.82	0.60
1:B:223:HIS:ND1	1:B:224:PRO:HD2	2.16	0.60
1:C:249:GLY:O	1:C:252:SER:HB3	2.02	0.60
1:E:86:ILE:CD1	1:E:108:LEU:HD22	2.32	0.60
1:B:258:VAL:HG22	4:B:2382:HOH:O	2.02	0.60
1:C:3:VAL:HB	1:C:30:ILE:HG13	1.84	0.60
1:C:105:GLU:CG	4:C:3315:HOH:O	2.41	0.60
1:E:22:ALA:HA	1:E:129:ARG:NH2	2.17	0.60
1:E:133:THR:HG22	4:E:5385:HOH:O	2.01	0.60
1:B:129:ARG:NH2	3:B:2301:GLU:CG	2.56	0.60
1:A:55:HIS:C	1:A:57:LYS:H	2.05	0.59
1:C:51:LYS:HB2	1:C:51:LYS:NZ	2.17	0.59
1:C:115:PRO:HG3	4:C:3358:HOH:O	2.01	0.59
1:C:169:ALA:CA	4:C:3320:HOH:O	2.49	0.59
1:D:116:ARG:O	4:D:4455:HOH:O	2.16	0.59
1:D:151:GLN:C	4:D:4444:HOH:O	2.41	0.59
1:D:174:SER:HA	4:D:4315:HOH:O	1.98	0.59
1:D:211:LEU:CD1	4:D:4406:HOH:O	2.42	0.59
1:A:123:ASN:ND2	1:A:132:ALA:H	2.00	0.59
1:A:182:PHE:CD1	4:A:1324:HOH:O	2.45	0.59
1:B:82:ILE:HG22	1:B:86:ILE:CD1	2.31	0.59
1:C:125:PRO:HB2	1:C:130:GLU:O	2.02	0.59
1:C:238:THR:O	1:C:241:ALA:N	2.35	0.59
1:D:222:GLN:N	4:D:4384:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:VAL:CB	4:E:5413:HOH:O	2.47	0.59
1:A:26:ALA:C	4:A:1382:HOH:O	2.40	0.59
1:A:28:HIS:CD2	4:A:1329:HOH:O	2.56	0.59
1:A:239:ILE:N	4:A:1391:HOH:O	2.34	0.59
1:B:235:GLY:O	4:B:2318:HOH:O	2.17	0.59
1:E:64:ASP:N	4:E:5417:HOH:O	2.31	0.59
1:E:70:VAL:O	1:E:71:LYS:HB2	2.02	0.59
1:B:94:SER:O	1:B:96:ALA:N	2.35	0.59
1:C:266:ARG:NH2	4:C:3311:HOH:O	2.15	0.59
1:A:94:SER:OG	4:A:1321:HOH:O	2.15	0.59
1:B:41:THR:O	1:B:45:LEU:HG	2.02	0.59
1:B:129:ARG:HH12	2:B:2300:NAI:C2N	2.06	0.59
1:B:251:ARG:O	1:B:254:LEU:N	2.31	0.59
1:B:269:GLN:C	1:B:271:MET:H	2.06	0.59
1:C:35:PRO:O	1:C:36:ASP:HB2	2.02	0.59
1:E:136:ALA:HB3	4:E:5434:HOH:O	2.01	0.59
1:A:122:THR:HG22	1:A:123:ASN:H	1.64	0.59
1:B:11:LEU:CD2	4:B:2343:HOH:O	2.43	0.59
1:B:101:ILE:HG13	1:B:102:SER:N	2.17	0.59
1:B:231:VAL:O	4:B:2363:HOH:O	2.17	0.59
1:D:123:ASN:CB	4:D:4309:HOH:O	2.43	0.59
1:E:185:LEU:CG	4:E:5383:HOH:O	2.11	0.59
1:B:168:ASP:HB3	4:B:2357:HOH:O	2.00	0.59
1:D:116:ARG:HB2	4:D:4455:HOH:O	2.03	0.59
1:E:176:SER:CA	4:E:5333:HOH:O	2.20	0.59
1:A:223:HIS:ND1	1:A:224:PRO:HD2	2.16	0.59
2:A:1300:NAI:C5D	4:A:1431:HOH:O	2.44	0.59
1:B:189:ALA:HA	4:B:2302:HOH:O	1.99	0.59
1:E:168:ASP:OD2	1:E:266:ARG:HG3	2.03	0.59
1:E:223:HIS:ND1	1:E:224:PRO:HD2	2.18	0.59
1:A:112:ARG:HD3	4:A:1365:HOH:O	2.02	0.59
1:B:240:HIS:C	4:B:2329:HOH:O	2.40	0.59
1:C:156:VAL:O	1:C:156:VAL:HG12	2.02	0.59
1:D:13:PHE:HA	1:D:16:ALA:HB3	1.85	0.59
1:D:197:LEU:HD22	1:D:201:LEU:HD23	1.85	0.59
1:A:68:LEU:HB2	4:A:1321:HOH:O	2.02	0.59
1:A:133:THR:HG21	1:A:153:LEU:CD1	2.25	0.59
1:C:177:GLY:HA2	1:C:180:TYR:CD1	2.37	0.59
1:D:6:ILE:CD1	1:D:66:LEU:HD21	2.32	0.59
1:A:60:VAL:HG21	1:A:82:ILE:HD12	1.85	0.58
1:A:268:LEU:HD21	4:A:1322:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:THR:HG23	1:B:58:GLU:OE2	2.03	0.58
1:B:215:LYS:NZ	4:B:2394:HOH:O	2.29	0.58
1:A:22:ALA:HB2	4:A:1425:HOH:O	2.02	0.58
1:B:176:SER:HB3	1:B:180:TYR:CE2	2.37	0.58
1:C:246:GLU:O	4:C:3402:HOH:O	2.17	0.58
1:A:190:ASP:N	1:A:199:ARG:HH12	2.00	0.58
1:C:266:ARG:CG	4:C:3340:HOH:O	2.50	0.58
1:D:117:VAL:O	1:D:138:GLY:HA3	2.02	0.58
1:D:264:ARG:O	1:D:268:LEU:HB2	2.03	0.58
1:D:266:ARG:O	1:D:268:LEU:N	2.36	0.58
1:E:37:MET:O	4:E:5392:HOH:O	2.16	0.58
1:E:89:ARG:NH2	4:E:5324:HOH:O	2.36	0.58
1:E:122:THR:CG2	1:E:133:THR:HB	2.30	0.58
1:B:123:ASN:HB2	1:B:125:PRO:HD2	1.84	0.58
1:D:88:ASP:C	4:D:4432:HOH:O	2.37	0.58
1:D:275:GLU:C	4:D:4456:HOH:O	2.41	0.58
1:E:222:GLN:O	1:E:223:HIS:CB	2.51	0.58
1:B:215:LYS:HG3	4:B:2377:HOH:O	2.03	0.58
1:C:250:PHE:O	4:C:3359:HOH:O	2.17	0.58
1:D:97:ALA:CA	4:D:4333:HOH:O	2.50	0.58
1:E:123:ASN:HB2	4:E:5310:HOH:O	2.04	0.58
1:E:274:GLN:HG3	1:E:275:GLU:N	2.17	0.58
1:B:13:PHE:HB2	1:B:41:THR:HG21	1.86	0.58
1:D:75:ILE:HG21	1:D:104:ILE:HD11	1.86	0.58
1:D:113:PRO:CD	4:D:4329:HOH:O	2.49	0.58
1:E:75:ILE:HG13	1:E:99:VAL:HG21	1.85	0.58
1:E:188:LEU:HB3	4:E:5396:HOH:O	2.02	0.58
1:A:138:GLY:C	4:A:1310:HOH:O	2.42	0.58
1:A:267:GLU:O	1:A:271:MET:HB3	2.03	0.58
1:B:8:ALA:HB1	1:B:45:LEU:CD1	2.34	0.58
1:C:194:LYS:N	4:C:3309:HOH:O	2.35	0.58
1:D:258:VAL:HG12	1:D:259:GLU:N	2.18	0.58
1:D:264:ARG:NE	4:D:4380:HOH:O	2.26	0.58
1:E:62:HIS:ND1	4:E:5372:HOH:O	2.31	0.58
1:A:175:GLY:O	4:A:1436:HOH:O	2.16	0.58
1:B:221:GLU:O	1:B:223:HIS:N	2.37	0.58
1:C:79:LEU:HD22	1:C:108:LEU:HD11	1.85	0.58
1:C:131:GLY:N	4:C:3307:HOH:O	2.37	0.58
1:A:136:ALA:HA	4:A:1404:HOH:O	2.02	0.58
1:D:98:GLY:HA3	1:D:269:GLN:HB2	1.86	0.58
1:D:57:LYS:HD3	4:D:4438:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:THR:HG22	1:E:101:ILE:N	2.19	0.57
1:E:125:PRO:CG	4:E:5302:HOH:O	2.52	0.57
1:E:251:ARG:CZ	4:E:5366:HOH:O	2.52	0.57
1:B:71:LYS:HB2	1:B:73:HIS:CE1	2.39	0.57
1:E:117:VAL:O	1:E:138:GLY:HA3	2.03	0.57
1:A:264:ARG:NE	4:A:1322:HOH:O	2.12	0.57
1:B:159:CYS:HA	4:B:2311:HOH:O	2.03	0.57
1:C:101:ILE:CD1	4:C:3394:HOH:O	2.52	0.57
1:A:68:LEU:HB2	1:A:94:SER:HA	1.87	0.57
1:B:192:GLY:N	4:B:2355:HOH:O	2.37	0.57
1:D:169:ALA:C	1:D:171:THR:H	2.07	0.57
1:E:106:LYS:HA	4:E:5398:HOH:O	2.04	0.57
1:E:159:CYS:N	4:E:5425:HOH:O	2.35	0.57
1:A:231:VAL:O	1:A:231:VAL:HG12	2.04	0.57
1:B:160:THR:CG2	1:B:161:GLU:H	2.17	0.57
1:C:124:THR:C	1:C:126:VAL:H	2.07	0.57
1:D:177:GLY:HA2	1:D:180:TYR:CD1	2.40	0.57
1:E:195:MET:HA	1:E:195:MET:CE	2.35	0.57
1:A:259:GLU:OE1	4:A:1330:HOH:O	2.18	0.57
1:C:185:LEU:CA	4:C:3352:HOH:O	2.53	0.57
1:C:221:GLU:HA	1:C:221:GLU:OE2	2.02	0.57
1:D:130:GLU:OE2	2:D:4300:NAI:H2D	2.05	0.57
1:C:121:MET:HG3	4:C:3351:HOH:O	2.04	0.57
1:B:1:MET:HB2	1:B:64:ASP:HB2	1.85	0.57
1:B:70:VAL:HG12	1:B:71:LYS:N	2.18	0.57
1:C:45:LEU:O	1:C:45:LEU:HD23	2.05	0.57
1:C:55:HIS:C	1:C:57:LYS:H	2.09	0.57
1:E:73:HIS:CD2	4:E:5429:HOH:O	2.56	0.57
1:E:169:ALA:O	1:E:171:THR:N	2.38	0.57
1:C:185:LEU:HA	4:C:3352:HOH:O	2.04	0.57
1:E:141:ALA:CB	4:E:5388:HOH:O	2.52	0.57
1:E:172:GLY:HA2	1:E:261:SER:HG	1.69	0.57
1:A:29:LYS:CG	4:A:1329:HOH:O	2.52	0.57
1:A:187:ALA:CB	4:A:1303:HOH:O	2.52	0.57
1:B:101:ILE:HG23	1:B:164:GLU:OE2	2.05	0.57
1:D:1:MET:CE	1:D:25:LEU:HD21	2.33	0.57
1:E:47:LYS:CE	4:E:5338:HOH:O	2.37	0.57
1:A:89:ARG:HG3	1:A:90:HIS:H	1.69	0.56
1:B:160:THR:CG2	1:B:161:GLU:N	2.67	0.56
1:C:264:ARG:O	1:C:268:LEU:HG	2.05	0.56
1:E:229:ASP:HA	4:E:5340:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLU:N	4:A:1355:HOH:O	2.32	0.56
1:A:264:ARG:NH2	4:A:1322:HOH:O	2.36	0.56
1:B:74:ILE:O	1:B:79:LEU:HG	2.06	0.56
1:B:82:ILE:CA	4:B:2376:HOH:O	2.44	0.56
1:B:219:HIS:CE1	2:B:2300:NAI:PN	2.99	0.56
1:C:203:VAL:CG1	4:C:3355:HOH:O	2.49	0.56
1:A:249:GLY:HA2	4:A:1318:HOH:O	2.04	0.56
2:A:1300:NAI:C1D	2:A:1300:NAI:C6N	2.78	0.56
1:B:153:LEU:C	1:B:155:SER:H	2.07	0.56
1:B:176:SER:HA	4:B:2327:HOH:O	2.05	0.56
1:B:220:SER:C	4:B:2322:HOH:O	2.42	0.56
2:B:2300:NAI:C5N	3:B:2301:GLU:OXT	2.53	0.56
1:C:169:ALA:HA	4:C:3320:HOH:O	2.05	0.56
1:C:197:LEU:HD12	4:C:3367:HOH:O	2.04	0.56
1:D:80:ASP:CG	4:D:4370:HOH:O	2.43	0.56
1:E:22:ALA:HA	1:E:129:ARG:HH21	1.69	0.56
1:E:119:ARG:HA	4:E:5325:HOH:O	2.04	0.56
1:E:179:ALA:C	4:E:5369:HOH:O	2.39	0.56
1:E:222:GLN:HG3	1:E:227:LEU:HD21	1.87	0.56
1:B:74:ILE:O	1:B:78:ILE:HB	2.05	0.56
1:D:62:HIS:HA	4:D:4415:HOH:O	2.05	0.56
1:D:229:ASP:CA	4:D:4310:HOH:O	2.54	0.56
1:A:70:VAL:HG22	1:A:75:ILE:HD12	1.86	0.56
1:B:115:PRO:HB3	4:B:2328:HOH:O	2.05	0.56
1:B:231:VAL:HG12	4:B:2363:HOH:O	2.02	0.56
1:B:259:GLU:OE1	4:B:2334:HOH:O	2.17	0.56
1:C:236:GLY:HA2	4:C:3398:HOH:O	1.98	0.56
1:C:269:GLN:C	1:C:271:MET:H	2.08	0.56
1:E:163:GLU:CD	4:E:5399:HOH:O	2.36	0.56
1:B:94:SER:OG	1:B:119:ARG:HA	2.06	0.56
1:B:222:GLN:O	1:B:223:HIS:CB	2.52	0.56
1:B:236:GLY:HA2	1:B:239:ILE:CG2	2.30	0.56
1:C:163:GLU:CG	4:C:3397:HOH:O	2.45	0.56
1:C:194:LYS:CA	4:C:3309:HOH:O	2.44	0.56
1:C:260:ALA:N	4:C:3381:HOH:O	2.39	0.56
1:D:103:SER:N	4:D:4449:HOH:O	2.38	0.56
1:E:170:VAL:O	1:E:170:VAL:HG12	2.06	0.56
1:E:228:LYS:C	4:E:5337:HOH:O	2.44	0.56
1:B:184:ALA:O	1:B:188:LEU:HG	2.06	0.56
1:C:114:ALA:HB1	1:C:140:HIS:CE1	2.41	0.56
1:C:181:ALA:N	4:C:3336:HOH:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ILE:HD12	1:D:82:ILE:N	2.20	0.56
1:D:169:ALA:O	1:D:171:THR:N	2.39	0.56
1:E:33:SER:O	1:E:35:PRO:HD3	2.06	0.56
1:E:63:SER:HB3	4:E:5372:HOH:O	2.06	0.56
1:C:75:ILE:HB	1:C:76:PRO:HD3	1.88	0.56
1:D:141:ALA:CA	4:D:4386:HOH:O	2.38	0.56
1:D:269:GLN:C	1:D:271:MET:H	2.10	0.56
1:E:162:VAL:CG1	1:E:166:LEU:HB2	2.35	0.56
1:B:198:PRO:HD2	1:B:201:LEU:HD23	1.87	0.56
1:B:241:ALA:CA	4:B:2329:HOH:O	2.44	0.56
1:E:151:GLN:N	4:E:5327:HOH:O	2.30	0.56
1:C:75:ILE:HG13	1:C:99:VAL:HG21	1.87	0.56
1:C:141:ALA:HA	1:C:145:ASP:OD1	2.05	0.56
1:D:113:PRO:HD2	4:D:4329:HOH:O	2.06	0.56
1:D:164:GLU:HA	1:D:167:ILE:HG12	1.87	0.56
1:E:105:GLU:HB2	4:E:5437:HOH:O	2.06	0.56
1:A:2:SER:HB2	4:A:1403:HOH:O	2.04	0.55
1:A:135:TYR:HE2	1:A:150:GLU:HG2	1.70	0.55
1:B:200:ARG:O	1:B:204:ARG:HG2	2.06	0.55
1:C:118:ILE:HD13	1:C:118:ILE:N	2.19	0.55
1:C:249:GLY:O	1:C:253:LEU:HD13	2.06	0.55
1:D:136:ALA:HB3	4:D:4367:HOH:O	2.05	0.55
1:D:269:GLN:O	1:D:271:MET:N	2.39	0.55
1:A:172:GLY:HA2	1:A:261:SER:CB	2.35	0.55
1:A:116:ARG:NH2	1:A:145:ASP:OD1	2.38	0.55
1:B:35:PRO:HG2	1:B:71:LYS:NZ	2.21	0.55
1:B:251:ARG:C	4:B:2303:HOH:O	2.44	0.55
1:C:86:ILE:HG22	1:C:87:GLU:N	2.21	0.55
1:E:218:LEU:CD2	4:E:5424:HOH:O	2.54	0.55
1:B:198:PRO:HG2	1:B:201:LEU:HB3	1.88	0.55
1:C:45:LEU:HD21	1:C:50:VAL:HB	1.87	0.55
1:C:124:THR:O	1:C:126:VAL:N	2.39	0.55
1:C:218:LEU:CB	2:C:3300:NAI:C5D	2.84	0.55
1:D:57:LYS:HE3	4:D:4376:HOH:O	1.97	0.55
1:D:81:GLU:HB3	1:D:82:ILE:HD12	1.89	0.55
1:D:180:TYR:HD2	4:D:4308:HOH:O	1.88	0.55
1:E:91:ILE:O	4:E:5344:HOH:O	2.18	0.55
1:B:231:VAL:HB	4:B:2364:HOH:O	2.05	0.55
1:C:53:THR:CG2	1:C:58:GLU:HB2	2.35	0.55
1:D:252:SER:N	4:D:4342:HOH:O	2.39	0.55
1:A:230:ASN:ND2	4:A:1317:HOH:O	2.11	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ARG:NH2	4:A:1440:HOH:O	2.36	0.55
1:B:68:LEU:HB3	4:B:2368:HOH:O	2.05	0.55
1:B:102:SER:HA	1:B:105:GLU:CB	2.37	0.55
1:B:220:SER:O	1:B:221:GLU:CB	2.55	0.55
1:C:258:VAL:C	4:C:3391:HOH:O	2.38	0.55
1:C:275:GLU:C	4:C:3401:HOH:O	2.45	0.55
1:E:75:ILE:O	1:E:79:LEU:HG	2.05	0.55
1:E:125:PRO:O	1:E:129:ARG:O	2.25	0.55
1:A:120:CYS:N	4:A:1372:HOH:O	2.40	0.55
1:C:29:LYS:NZ	4:C:3344:HOH:O	2.25	0.55
1:C:185:LEU:HD21	1:C:210:LEU:HD12	1.88	0.55
1:C:236:GLY:O	1:C:237:ALA:HB3	2.06	0.55
1:C:253:LEU:H	1:C:253:LEU:HD12	1.71	0.55
2:C:3300:NAI:H2N	3:C:3301:GLU:HB3	1.79	0.55
1:D:101:ILE:HD11	1:D:117:VAL:O	2.07	0.55
1:D:128:VAL:O	1:D:129:ARG:CB	2.55	0.55
1:D:170:VAL:O	1:D:170:VAL:HG12	2.07	0.55
1:E:106:LYS:HB2	4:E:5384:HOH:O	2.06	0.55
1:A:182:PHE:CZ	4:A:1324:HOH:O	2.48	0.55
1:A:219:HIS:O	1:A:220:SER:HB3	2.06	0.55
1:B:235:GLY:C	4:B:2318:HOH:O	2.44	0.55
2:C:3300:NAI:C5N	3:C:3301:GLU:OXT	2.53	0.55
1:D:62:HIS:CA	4:D:4448:HOH:O	2.53	0.55
1:D:183:THR:HG21	4:D:4428:HOH:O	2.07	0.55
1:D:211:LEU:HD12	1:D:211:LEU:C	2.27	0.55
1:D:231:VAL:CG1	4:D:4401:HOH:O	2.16	0.55
1:A:221:GLU:N	4:A:1441:HOH:O	2.11	0.55
1:E:101:ILE:O	1:E:105:GLU:HG3	2.06	0.55
1:E:225:GLY:C	4:E:5353:HOH:O	2.40	0.55
1:D:167:ILE:HG23	4:D:4324:HOH:O	2.06	0.54
1:D:229:ASP:HA	4:D:4310:HOH:O	2.07	0.54
1:E:16:ALA:O	1:E:20:THR:HG23	2.07	0.54
1:E:60:VAL:CG2	1:E:82:ILE:HD12	2.34	0.54
1:E:179:ALA:C	4:E:5322:HOH:O	2.44	0.54
1:B:186:ASP:HB3	4:B:2305:HOH:O	2.06	0.54
1:C:4:GLY:C	1:C:66:LEU:HG	2.27	0.54
1:D:78:ILE:O	1:D:82:ILE:HD13	2.07	0.54
2:D:4300:NAI:N1N	3:D:4301:GLU:C	2.60	0.54
1:A:178:PRO:C	4:A:1324:HOH:O	2.42	0.54
1:B:82:ILE:O	1:B:86:ILE:HG13	2.08	0.54
1:B:129:ARG:O	1:B:157:GLY:HA2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:ALA:HB2	4:C:3411:HOH:O	1.93	0.54
1:E:126:VAL:HG13	1:E:156:VAL:HG11	1.89	0.54
1:A:129:ARG:HA	1:A:156:VAL:O	2.08	0.54
1:A:230:ASN:HB3	4:A:1317:HOH:O	2.05	0.54
1:B:60:VAL:O	1:B:89:ARG:NH2	2.39	0.54
1:B:77:PHE:C	1:B:78:ILE:HD12	2.27	0.54
1:B:178:PRO:CG	4:B:2345:HOH:O	2.56	0.54
1:C:87:GLU:N	1:C:90:HIS:HE1	2.06	0.54
1:C:266:ARG:NH2	4:C:3320:HOH:O	2.40	0.54
1:A:133:THR:O	1:A:159:CYS:HA	2.07	0.54
1:B:27:ALA:O	4:B:2378:HOH:O	2.19	0.54
1:C:51:LYS:HD3	1:C:51:LYS:H	1.72	0.54
1:E:9:GLY:O	1:E:12:ALA:HB3	2.06	0.54
1:E:45:LEU:HD23	1:E:48:MET:HE1	1.89	0.54
1:E:169:ALA:C	1:E:171:THR:N	2.61	0.54
1:B:101:ILE:HD12	1:B:138:GLY:HA2	1.89	0.54
1:C:7:GLY:CA	1:C:70:VAL:HG22	2.38	0.54
1:E:45:LEU:HA	1:E:48:MET:HE3	1.90	0.54
1:E:68:LEU:HB2	1:E:94:SER:HA	1.90	0.54
1:E:181:ALA:O	1:E:184:ALA:N	2.39	0.54
1:A:99:VAL:HG11	1:A:104:ILE:HD11	1.90	0.54
1:A:266:ARG:NE	4:A:1440:HOH:O	2.35	0.54
1:B:158:PHE:O	4:B:2387:HOH:O	2.18	0.54
1:C:89:ARG:HE	1:C:90:HIS:CD2	2.26	0.54
1:C:93:VAL:HG13	1:C:118:ILE:HD11	1.89	0.54
1:D:39:LEU:HA	4:D:4405:HOH:O	2.06	0.54
1:A:-1:ARG:N	4:A:1427:HOH:O	2.08	0.54
1:A:91:ILE:H	1:A:91:ILE:HD12	1.72	0.54
1:B:99:VAL:CG2	4:B:2309:HOH:O	2.15	0.54
1:B:238:THR:O	1:B:240:HIS:N	2.41	0.54
1:B:259:GLU:CA	4:B:2307:HOH:O	2.34	0.54
1:C:87:GLU:H	1:C:90:HIS:HE1	1.55	0.54
1:C:91:ILE:N	1:C:91:ILE:HD12	2.23	0.54
1:C:122:THR:CG2	1:C:133:THR:HG22	2.37	0.54
2:C:3300:NAI:C3N	3:C:3301:GLU:CB	2.81	0.54
1:E:105:GLU:CB	4:E:5437:HOH:O	2.56	0.54
1:E:185:LEU:CD1	4:E:5383:HOH:O	2.51	0.54
1:A:178:PRO:CD	4:A:1436:HOH:O	2.32	0.54
1:A:255:ILE:C	4:A:1335:HOH:O	2.42	0.54
1:B:258:VAL:HG13	1:B:259:GLU:H	1.72	0.54
1:D:93:VAL:HG13	4:D:4408:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:ALA:HA	1:E:127:VAL:HG22	1.89	0.54
1:E:82:ILE:O	1:E:85:ASP:N	2.37	0.54
1:E:125:PRO:HG3	4:E:5302:HOH:O	2.07	0.54
1:E:211:LEU:HD12	4:E:5314:HOH:O	2.05	0.54
1:E:218:LEU:HA	4:E:5424:HOH:O	2.08	0.54
1:B:78:ILE:HD12	1:B:78:ILE:N	2.23	0.54
1:B:137:THR:HG21	4:B:2339:HOH:O	2.07	0.54
1:B:162:VAL:HB	1:B:166:LEU:HD12	1.90	0.54
1:B:218:LEU:CD1	2:B:2300:NAI:C5D	2.81	0.54
1:C:49:GLY:N	4:C:3363:HOH:O	2.40	0.54
1:C:164:GLU:HG2	4:C:3372:HOH:O	2.07	0.54
1:D:3:VAL:HG22	1:D:65:VAL:HG13	1.90	0.54
1:E:130:GLU:OE2	2:E:5300:NAI:C1D	2.55	0.54
1:E:169:ALA:N	4:E:5375:HOH:O	2.37	0.54
1:A:100:THR:HG22	1:A:102:SER:N	2.22	0.53
1:B:82:ILE:CG2	1:B:86:ILE:HD11	2.36	0.53
1:B:93:VAL:HG12	1:B:95:CYS:SG	2.48	0.53
1:B:153:LEU:O	1:B:155:SER:N	2.41	0.53
1:C:129:ARG:NH2	2:C:3300:NAI:H2N	2.23	0.53
1:D:77:PHE:HD1	1:D:77:PHE:H	1.56	0.53
1:D:183:THR:CG2	4:D:4428:HOH:O	2.55	0.53
1:A:101:ILE:HG13	1:A:164:GLU:OE1	2.09	0.53
1:B:91:ILE:HD12	1:B:91:ILE:N	2.24	0.53
1:C:112:ARG:HH11	1:C:113:PRO:CD	2.09	0.53
1:C:116:ARG:HA	1:C:140:HIS:HB2	1.90	0.53
1:C:122:THR:HG22	1:C:133:THR:HB	1.90	0.53
1:C:134:VAL:CG1	1:C:162:VAL:HG22	2.38	0.53
1:A:26:ALA:CB	1:A:29:LYS:HE3	2.38	0.53
1:B:45:LEU:HB3	4:B:2385:HOH:O	2.08	0.53
1:B:158:PHE:CE1	2:B:2300:NAI:C4B	2.82	0.53
1:B:169:ALA:O	1:B:171:THR:N	2.42	0.53
1:C:50:VAL:CG2	4:C:3363:HOH:O	2.55	0.53
1:C:82:ILE:HG22	1:C:86:ILE:CD1	2.36	0.53
1:C:123:ASN:ND2	1:C:132:ALA:HB3	2.20	0.53
1:D:72:PRO:HA	1:D:75:ILE:HD13	1.90	0.53
1:D:134:VAL:CG2	1:D:162:VAL:HB	2.37	0.53
1:A:50:VAL:HG12	1:A:51:LYS:N	2.23	0.53
1:A:255:ILE:CG2	4:A:1335:HOH:O	2.47	0.53
1:C:19:PHE:O	1:C:22:ALA:HB3	2.09	0.53
1:D:57:LYS:CD	4:D:4438:HOH:O	2.55	0.53
1:E:60:VAL:HG21	1:E:82:ILE:CG2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:HG22	1:A:118:ILE:HD11	1.91	0.53
1:A:115:PRO:O	1:A:140:HIS:HB2	2.08	0.53
1:B:139:THR:O	1:B:139:THR:HG22	2.09	0.53
1:B:190:ASP:OD2	1:D:228:LYS:NZ	2.41	0.53
1:B:196:GLY:O	1:D:234:PRO:HB3	2.09	0.53
1:C:180:TYR:CA	4:C:3302:HOH:O	2.20	0.53
1:E:98:GLY:O	4:E:5400:HOH:O	2.19	0.53
1:E:178:PRO:HD3	4:E:5315:HOH:O	2.06	0.53
1:E:269:GLN:OE1	4:E:5400:HOH:O	2.19	0.53
1:C:6:ILE:H	1:C:66:LEU:HD21	1.74	0.53
1:D:79:LEU:HD22	1:D:104:ILE:HD13	1.89	0.53
1:E:231:VAL:HG12	1:E:231:VAL:O	2.08	0.53
1:C:3:VAL:HA	1:C:65:VAL:O	2.08	0.53
1:C:104:ILE:HG22	1:C:117:VAL:HG21	1.90	0.53
1:C:236:GLY:HA2	1:C:239:ILE:HG22	1.91	0.53
1:C:261:SER:CA	4:C:3354:HOH:O	2.21	0.53
1:D:119:ARG:CD	4:D:4422:HOH:O	2.24	0.53
2:D:4300:NAI:C3D	4:D:4410:HOH:O	2.47	0.53
1:E:3:VAL:O	1:E:30:ILE:HA	2.09	0.53
1:A:29:LYS:N	4:A:1329:HOH:O	2.41	0.53
1:A:106:LYS:HB3	4:A:1432:HOH:O	2.09	0.53
1:A:258:VAL:C	4:A:1366:HOH:O	2.46	0.53
1:B:188:LEU:O	1:B:190:ASP:N	2.42	0.53
1:D:31:MET:N	4:D:4365:HOH:O	2.42	0.53
1:A:178:PRO:CG	4:A:1436:HOH:O	2.55	0.53
1:B:45:LEU:HD23	1:B:48:MET:SD	2.48	0.53
1:B:75:ILE:HD12	1:B:75:ILE:N	2.22	0.53
1:B:199:ARG:HD3	4:B:2340:HOH:O	2.08	0.53
1:C:39:LEU:HA	1:C:43:SER:CB	2.39	0.53
1:C:115:PRO:CB	4:C:3358:HOH:O	2.51	0.53
1:C:257:ALA:CA	4:C:3378:HOH:O	2.17	0.53
1:E:7:GLY:H	1:E:33:SER:HB2	1.73	0.53
1:E:75:ILE:CG2	1:E:104:ILE:HD11	2.39	0.53
1:E:124:THR:N	1:E:125:PRO:HD2	2.24	0.53
1:A:135:TYR:OH	1:A:161:GLU:HG3	2.09	0.53
1:B:185:LEU:O	1:B:186:ASP:C	2.47	0.53
1:C:261:SER:N	4:C:3391:HOH:O	2.41	0.53
1:D:31:MET:CE	4:D:4358:HOH:O	2.55	0.53
1:E:150:GLU:O	1:E:152:LEU:N	2.41	0.53
1:E:228:LYS:HE3	1:E:242:LEU:HD13	1.91	0.53
1:A:6:ILE:HD11	1:A:66:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:O	1:A:143:VAL:HG12	2.09	0.52
1:A:192:GLY:O	1:A:195:MET:HB2	2.09	0.52
1:B:157:GLY:O	2:B:2300:NAI:C4N	2.56	0.52
2:B:2300:NAI:C3N	3:B:2301:GLU:CB	2.81	0.52
1:C:25:LEU:HD11	1:C:30:ILE:CD1	2.38	0.52
1:E:55:HIS:CB	1:E:57:LYS:HE2	2.38	0.52
1:A:236:GLY:HA2	1:A:239:ILE:HG22	1.91	0.52
1:B:8:ALA:HA	1:B:12:ALA:HB2	1.90	0.52
1:B:94:SER:OG	4:B:2333:HOH:O	2.03	0.52
1:B:130:GLU:OE2	2:B:2300:NAI:H2D	2.09	0.52
1:E:45:LEU:HA	1:E:48:MET:CE	2.39	0.52
1:E:177:GLY:O	1:E:180:TYR:N	2.42	0.52
1:A:-1:ARG:CB	4:A:1342:HOH:O	2.52	0.52
1:A:149:MET:CE	1:A:153:LEU:HG	2.39	0.52
1:A:198:PRO:HG2	1:A:201:LEU:CB	2.40	0.52
1:B:176:SER:O	1:B:177:GLY:C	2.46	0.52
1:C:24:VAL:O	1:C:24:VAL:HG12	2.09	0.52
2:C:3300:NAI:O2B	4:C:3408:HOH:O	2.18	0.52
1:D:266:ARG:C	1:D:268:LEU:N	2.62	0.52
1:E:112:ARG:NE	4:E:5328:HOH:O	2.41	0.52
1:A:218:LEU:CD2	2:A:1300:NAI:H52A	2.22	0.52
1:B:5:PHE:HZ	1:B:15:LEU:CB	2.15	0.52
1:B:12:ALA:O	1:B:16:ALA:HB2	2.08	0.52
1:B:73:HIS:HB2	4:B:2320:HOH:O	2.09	0.52
1:C:199:ARG:O	1:C:203:VAL:HG23	2.09	0.52
1:E:185:LEU:HD22	4:E:5408:HOH:O	2.09	0.52
1:A:62:HIS:ND1	1:A:62:HIS:O	2.43	0.52
1:A:251:ARG:HG3	4:A:1314:HOH:O	2.08	0.52
1:C:147:ARG:O	1:C:151:GLN:HG3	2.10	0.52
1:D:123:ASN:HB2	1:D:125:PRO:HD2	1.91	0.52
1:D:232:SER:HA	4:D:4343:HOH:O	2.08	0.52
1:E:97:ALA:CB	4:E:5358:HOH:O	2.58	0.52
1:E:221:GLU:HG3	4:E:5350:HOH:O	2.09	0.52
1:A:70:VAL:CG2	1:A:75:ILE:HD12	2.40	0.52
1:A:91:ILE:HD12	1:A:91:ILE:N	2.24	0.52
1:B:18:GLY:O	1:B:20:THR:N	2.43	0.52
1:C:33:SER:OG	1:C:56:ASN:HA	2.09	0.52
1:D:252:SER:OG	1:D:253:LEU:N	2.43	0.52
1:E:3:VAL:HG12	1:E:4:GLY:N	2.23	0.52
1:A:249:GLY:C	4:A:1314:HOH:O	2.41	0.52
1:B:34:SER:C	1:B:36:ASP:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:LEU:O	1:B:247:SER:N	2.43	0.52
1:C:158:PHE:CD1	2:C:3300:NAI:H4B	2.44	0.52
1:A:36:ASP:O	1:A:37:MET:CB	2.56	0.52
1:A:256:ASN:HA	4:A:1335:HOH:O	2.10	0.52
2:A:1300:NAI:C4D	4:A:1435:HOH:O	2.58	0.52
1:B:68:LEU:C	4:B:2368:HOH:O	2.48	0.52
1:C:56:ASN:C	4:C:3383:HOH:O	2.48	0.52
1:D:224:PRO:HB2	4:D:4355:HOH:O	2.10	0.52
1:A:32:ALA:O	1:A:52:LEU:HA	2.10	0.52
1:B:13:PHE:HB2	1:B:41:THR:CG2	2.40	0.52
1:E:242:LEU:HD11	4:E:5345:HOH:O	2.09	0.52
1:A:6:ILE:CD1	1:A:66:LEU:HD11	2.39	0.52
1:C:51:LYS:H	1:C:51:LYS:HZ2	1.56	0.52
1:C:169:ALA:CB	4:C:3320:HOH:O	2.55	0.52
1:D:169:ALA:C	1:D:171:THR:N	2.63	0.52
1:B:75:ILE:CB	1:B:76:PRO:HD3	2.26	0.51
1:C:218:LEU:HD13	2:C:3300:NAI:C4D	2.39	0.51
1:C:242:LEU:O	1:C:245:LEU:N	2.40	0.51
1:D:60:VAL:O	1:D:90:HIS:NE2	2.39	0.51
1:D:73:HIS:O	1:D:76:PRO:HD2	2.10	0.51
1:D:181:ALA:C	4:D:4330:HOH:O	2.48	0.51
1:E:121:MET:HE2	1:E:122:THR:O	2.10	0.51
1:E:183:THR:C	4:E:5370:HOH:O	2.48	0.51
1:E:206:GLY:O	1:E:209:ALA:HB3	2.10	0.51
1:A:94:SER:CB	4:A:1321:HOH:O	2.58	0.51
1:A:121:MET:HG3	4:A:1402:HOH:O	2.09	0.51
1:A:191:GLY:CA	4:A:1420:HOH:O	2.24	0.51
1:B:118:ILE:HG21	1:B:149:MET:SD	2.50	0.51
1:B:156:VAL:O	1:B:156:VAL:HG12	2.11	0.51
1:B:195:MET:CE	1:B:195:MET:CA	2.88	0.51
1:C:122:THR:CG2	4:C:3317:HOH:O	2.50	0.51
1:C:266:ARG:N	4:C:3340:HOH:O	2.42	0.51
1:D:141:ALA:CB	4:D:4386:HOH:O	2.57	0.51
1:A:79:LEU:CD1	1:A:104:ILE:HG23	2.40	0.51
1:B:158:PHE:CE1	2:B:2300:NAI:O1A	2.64	0.51
1:B:159:CYS:CA	4:B:2311:HOH:O	2.56	0.51
1:C:15:LEU:HD12	4:C:3348:HOH:O	2.01	0.51
1:C:29:LYS:HG3	4:C:3306:HOH:O	2.11	0.51
1:C:100:THR:HG22	1:C:101:ILE:N	2.25	0.51
1:C:251:ARG:HD2	4:C:3376:HOH:O	2.09	0.51
1:D:166:LEU:O	1:D:168:ASP:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:LEU:CA	4:E:5424:HOH:O	2.57	0.51
1:A:11:LEU:O	1:A:11:LEU:HD23	2.10	0.51
1:B:2:SER:OG	1:B:30:ILE:HA	2.10	0.51
1:E:34:SER:HB3	1:E:54:PRO:HA	1.91	0.51
1:E:136:ALA:CB	4:E:5434:HOH:O	2.58	0.51
1:B:168:ASP:HB2	4:B:2357:HOH:O	2.06	0.51
1:C:51:LYS:HB2	1:C:51:LYS:HZ2	1.74	0.51
1:D:228:LYS:HB2	4:D:4397:HOH:O	2.11	0.51
1:E:39:LEU:HA	1:E:43:SER:HB2	1.93	0.51
1:E:94:SER:HB3	4:E:5325:HOH:O	2.09	0.51
1:E:136:ALA:HB2	1:E:167:ILE:HD11	1.93	0.51
1:E:262:CYS:HB3	4:E:5342:HOH:O	2.06	0.51
1:A:215:LYS:O	1:A:216:MET:C	2.49	0.51
2:B:2300:NAI:H2A	4:B:2380:HOH:O	2.09	0.51
1:E:89:ARG:HG2	1:E:89:ARG:HH11	1.76	0.51
1:E:225:GLY:HA3	4:E:5353:HOH:O	1.98	0.51
1:A:30:ILE:HG22	1:A:31:MET:N	2.26	0.51
1:A:141:ALA:CA	4:A:1390:HOH:O	2.04	0.51
1:B:9:GLY:O	1:B:41:THR:HG21	2.11	0.51
1:B:140:HIS:O	1:B:141:ALA:HB2	2.11	0.51
1:E:118:ILE:N	1:E:118:ILE:HD12	2.26	0.51
1:E:168:ASP:HB2	4:E:5349:HOH:O	2.10	0.51
1:A:163:GLU:O	1:A:165:ASP:N	2.43	0.51
1:B:188:LEU:O	4:B:2302:HOH:O	2.19	0.51
1:C:86:ILE:HB	1:C:112:ARG:HB2	1.93	0.51
1:C:122:THR:CA	4:C:3331:HOH:O	2.51	0.51
1:E:114:ALA:N	4:E:5367:HOH:O	2.39	0.51
1:A:38:ASP:O	1:A:39:LEU:C	2.49	0.51
1:A:236:GLY:O	1:A:237:ALA:HB3	2.10	0.51
1:C:11:LEU:HD12	1:C:14:ALA:HB3	1.92	0.51
1:C:218:LEU:CD1	2:C:3300:NAI:H51N	2.40	0.51
1:C:237:ALA:HB3	4:C:3406:HOH:O	2.11	0.51
1:D:75:ILE:HB	1:D:76:PRO:HD3	1.92	0.51
1:D:224:PRO:CB	4:D:4355:HOH:O	2.58	0.51
1:D:266:ARG:NH1	4:D:4442:HOH:O	2.01	0.51
1:A:219:HIS:NE2	2:A:1300:NAI:H51N	2.25	0.51
1:C:269:GLN:HG3	1:C:270:SER:H	1.76	0.51
1:A:121:MET:CG	1:A:171:THR:HG23	2.41	0.50
1:A:156:VAL:CG1	1:A:156:VAL:O	2.59	0.50
1:C:255:ILE:CA	4:C:3332:HOH:O	2.53	0.50
1:C:270:SER:O	1:C:274:GLN:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:LYS:HG3	1:D:219:HIS:CE1	2.46	0.50
1:E:74:ILE:C	1:E:76:PRO:HD2	2.31	0.50
1:A:60:VAL:HG21	1:A:82:ILE:HG23	1.92	0.50
1:C:185:LEU:HD22	4:C:3324:HOH:O	2.07	0.50
1:E:102:SER:CB	4:E:5347:HOH:O	2.52	0.50
1:E:121:MET:CE	1:E:122:THR:H	2.21	0.50
1:E:158:PHE:CD2	2:E:5300:NAI:O3B	2.64	0.50
1:A:76:PRO:C	1:A:78:ILE:H	2.14	0.50
1:B:215:LYS:HE3	4:B:2377:HOH:O	2.12	0.50
1:A:6:ILE:HD11	1:A:60:VAL:HG22	1.93	0.50
1:C:218:LEU:CG	2:C:3300:NAI:H52N	2.40	0.50
1:D:123:ASN:HB2	4:D:4312:HOH:O	2.11	0.50
1:D:194:LYS:NZ	4:D:4319:HOH:O	2.06	0.50
1:E:112:ARG:CG	4:E:5328:HOH:O	2.36	0.50
1:E:132:ALA:CB	4:E:5391:HOH:O	2.41	0.50
1:A:11:LEU:CB	4:A:1389:HOH:O	2.15	0.50
1:C:26:ALA:C	1:C:28:HIS:H	2.15	0.50
1:C:274:GLN:O	1:C:274:GLN:HG2	2.12	0.50
1:D:73:HIS:CE1	1:D:74:ILE:HG12	2.46	0.50
1:D:251:ARG:HG2	1:D:251:ARG:HH11	1.77	0.50
1:A:112:ARG:CD	4:A:1365:HOH:O	2.57	0.50
1:A:194:LYS:C	4:E:5309:HOH:O	2.50	0.50
1:B:180:TYR:O	1:B:183:THR:HB	2.11	0.50
1:B:251:ARG:O	1:B:252:SER:C	2.50	0.50
1:D:101:ILE:HG22	1:D:102:SER:N	2.26	0.50
1:D:143:VAL:C	1:D:145:ASP:H	2.13	0.50
1:D:229:ASP:CG	4:D:4393:HOH:O	2.49	0.50
1:A:174:SER:HB2	4:A:1339:HOH:O	2.08	0.50
1:B:123:ASN:O	1:B:126:VAL:HG23	2.12	0.50
1:C:160:THR:CG2	1:C:161:GLU:N	2.74	0.50
1:D:135:TYR:CE1	4:D:4398:HOH:O	2.27	0.50
1:A:115:PRO:HD2	1:A:140:HIS:HD2	1.75	0.50
1:A:134:VAL:HG13	1:A:162:VAL:CG2	2.42	0.50
1:B:79:LEU:HD12	1:B:107:LYS:HD3	1.94	0.50
1:D:30:ILE:HG12	4:D:4425:HOH:O	2.11	0.50
1:D:121:MET:HE3	1:D:171:THR:HG23	1.92	0.50
1:E:25:LEU:N	1:E:25:LEU:HD23	2.26	0.50
1:A:130:GLU:OE2	2:A:1300:NAI:C2D	2.60	0.50
1:C:187:ALA:O	1:C:190:ASP:HB2	2.12	0.50
1:E:45:LEU:HD23	1:E:48:MET:CE	2.42	0.50
1:E:177:GLY:C	4:E:5315:HOH:O	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:PRO:HD2	1:E:201:LEU:HD23	1.93	0.50
1:A:45:LEU:HD21	4:A:1387:HOH:O	2.10	0.49
1:A:123:ASN:HB2	4:A:1436:HOH:O	2.12	0.49
1:A:238:THR:C	4:A:1391:HOH:O	2.50	0.49
1:A:253:LEU:CD2	4:A:1405:HOH:O	2.54	0.49
1:B:25:LEU:HD22	1:B:30:ILE:HD11	1.93	0.49
1:B:264:ARG:O	1:B:264:ARG:HD2	2.11	0.49
1:C:82:ILE:HA	1:C:85:ASP:HB2	1.93	0.49
1:C:211:LEU:C	1:C:211:LEU:HD13	2.32	0.49
1:D:124:THR:O	1:D:126:VAL:N	2.45	0.49
1:E:19:PHE:CE2	1:E:152:LEU:HG	2.47	0.49
1:A:13:PHE:N	4:A:1379:HOH:O	2.45	0.49
1:A:29:LYS:HG3	4:A:1329:HOH:O	2.11	0.49
1:B:91:ILE:HD12	1:B:91:ILE:H	1.77	0.49
1:B:100:THR:CG2	1:B:101:ILE:N	2.76	0.49
1:C:108:LEU:C	4:C:3358:HOH:O	2.51	0.49
1:D:97:ALA:HA	4:D:4435:HOH:O	2.11	0.49
1:E:70:VAL:CA	4:E:5305:HOH:O	2.56	0.49
1:B:58:GLU:O	1:B:61:GLN:HG3	2.12	0.49
1:B:135:TYR:O	1:B:161:GLU:HB2	2.13	0.49
1:C:79:LEU:O	4:C:3329:HOH:O	2.20	0.49
1:E:98:GLY:HA2	4:E:5400:HOH:O	2.10	0.49
1:E:232:SER:OG	1:E:239:ILE:HB	2.12	0.49
2:A:1300:NAI:H52N	4:A:1435:HOH:O	2.12	0.49
1:B:147:ARG:HG3	1:B:147:ARG:O	2.11	0.49
1:C:74:ILE:O	1:C:74:ILE:HG22	2.12	0.49
1:C:115:PRO:CG	4:C:3358:HOH:O	2.57	0.49
1:C:197:LEU:CG	4:C:3367:HOH:O	2.60	0.49
1:E:13:PHE:CZ	4:E:5306:HOH:O	2.66	0.49
1:E:95:CYS:N	4:E:5423:HOH:O	2.42	0.49
1:E:134:VAL:CG1	1:E:162:VAL:HB	2.42	0.49
1:E:228:LYS:O	4:E:5337:HOH:O	2.19	0.49
1:B:74:ILE:HD11	1:B:96:ALA:HB3	1.94	0.49
1:B:100:THR:CG2	1:B:101:ILE:H	2.24	0.49
1:A:6:ILE:HD13	1:A:59:THR:CG2	2.43	0.49
1:A:31:MET:HA	1:A:51:LYS:O	2.12	0.49
1:A:94:SER:C	4:A:1321:HOH:O	2.50	0.49
1:B:152:LEU:C	4:B:2392:HOH:O	2.47	0.49
1:C:9:GLY:O	1:C:12:ALA:HB3	2.13	0.49
1:C:45:LEU:CD2	1:C:50:VAL:HB	2.42	0.49
1:C:104:ILE:HG21	1:C:117:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:GLN:O	1:D:223:HIS:HB3	2.12	0.49
1:A:117:VAL:HG12	4:A:1343:HOH:O	2.11	0.49
1:A:178:PRO:CB	4:A:1324:HOH:O	2.61	0.49
1:D:58:GLU:CB	4:D:4358:HOH:O	2.57	0.49
1:D:70:VAL:HG12	1:D:74:ILE:HB	1.95	0.49
1:E:70:VAL:O	1:E:70:VAL:HG12	2.13	0.49
1:E:190:ASP:HB2	4:E:5381:HOH:O	2.12	0.49
1:B:160:THR:HA	4:B:2312:HOH:O	2.12	0.49
1:E:36:ASP:OD1	1:E:37:MET:N	2.46	0.49
1:E:222:GLN:O	1:E:223:HIS:HB2	2.12	0.49
1:E:236:GLY:HA2	1:E:239:ILE:HG22	1.93	0.49
1:B:71:LYS:H	1:B:71:LYS:HD2	1.76	0.49
1:C:72:PRO:HG2	1:C:97:ALA:O	2.13	0.49
1:C:75:ILE:N	1:C:76:PRO:CD	2.75	0.49
1:E:124:THR:O	1:E:126:VAL:N	2.45	0.49
1:A:41:THR:O	1:A:44:ALA:HB3	2.12	0.49
1:B:105:GLU:OE1	1:B:105:GLU:HA	2.13	0.49
1:C:119:ARG:NE	4:C:3345:HOH:O	2.46	0.49
1:C:240:HIS:N	4:C:3398:HOH:O	2.34	0.49
1:D:68:LEU:HD12	1:D:94:SER:HB2	1.94	0.49
1:D:121:MET:CE	1:D:171:THR:HG23	2.42	0.49
1:D:242:LEU:O	1:D:243:HIS:C	2.51	0.49
1:A:101:ILE:CG1	1:A:119:ARG:HB2	2.43	0.48
1:B:79:LEU:HD22	1:B:104:ILE:HG23	1.95	0.48
1:B:137:THR:CG2	4:B:2339:HOH:O	2.59	0.48
1:B:155:SER:C	2:B:2300:NAI:N7N	2.66	0.48
1:C:26:ALA:O	1:C:28:HIS:N	2.46	0.48
2:D:4300:NAI:C3N	4:D:4413:HOH:O	2.61	0.48
2:D:4300:NAI:H2N	4:D:4436:HOH:O	2.11	0.48
1:E:113:PRO:HD2	4:E:5328:HOH:O	2.12	0.48
1:E:251:ARG:NH2	4:E:5366:HOH:O	2.45	0.48
1:A:45:LEU:CD2	4:A:1387:HOH:O	2.60	0.48
1:A:171:THR:N	4:A:1402:HOH:O	2.34	0.48
1:B:75:ILE:HB	1:B:76:PRO:CD	2.27	0.48
1:B:134:VAL:HG13	1:B:160:THR:O	2.12	0.48
1:C:61:GLN:C	1:C:63:SER:N	2.66	0.48
1:D:231:VAL:HG12	1:D:231:VAL:O	2.13	0.48
2:E:5300:NAI:N1N	3:E:5301:GLU:N	2.61	0.48
1:A:178:PRO:HG2	4:A:1436:HOH:O	2.13	0.48
1:B:74:ILE:HD11	1:B:96:ALA:CB	2.43	0.48
1:B:122:THR:CG2	1:B:133:THR:HB	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:THR:C	1:B:240:HIS:N	2.66	0.48
1:C:3:VAL:O	1:C:30:ILE:HG13	2.12	0.48
1:C:140:HIS:CB	4:C:3385:HOH:O	2.56	0.48
1:C:147:ARG:HG2	1:C:151:GLN:OE1	2.13	0.48
1:D:22:ALA:HA	1:D:129:ARG:CZ	2.44	0.48
1:D:80:ASP:OD2	1:D:107:LYS:NZ	2.45	0.48
1:E:221:GLU:N	4:E:5350:HOH:O	2.47	0.48
1:A:14:ALA:HA	1:A:127:VAL:HG22	1.94	0.48
1:C:122:THR:HG22	1:C:133:THR:CB	2.43	0.48
1:C:257:ALA:C	1:C:259:GLU:H	2.17	0.48
1:D:118:ILE:CG1	4:D:4408:HOH:O	2.57	0.48
1:D:231:VAL:CG2	4:D:4402:HOH:O	2.61	0.48
1:A:42:VAL:CG2	4:A:1349:HOH:O	2.05	0.48
1:C:222:GLN:CA	4:C:3304:HOH:O	2.56	0.48
1:E:68:LEU:HD12	1:E:94:SER:HB2	1.96	0.48
1:A:6:ILE:HG22	1:A:6:ILE:O	2.13	0.48
1:B:180:TYR:CD2	1:B:180:TYR:N	2.77	0.48
1:B:221:GLU:HB2	4:B:2322:HOH:O	2.13	0.48
1:B:231:VAL:O	1:B:231:VAL:HG12	2.12	0.48
1:C:7:GLY:HA3	1:C:69:ALA:O	2.12	0.48
1:C:72:PRO:HA	1:C:75:ILE:HG13	1.95	0.48
1:C:112:ARG:CG	1:C:113:PRO:HD2	2.34	0.48
1:D:60:VAL:HG21	1:D:82:ILE:CG2	2.39	0.48
1:D:223:HIS:ND1	1:D:224:PRO:HD2	2.29	0.48
1:E:46:ARG:HG3	1:E:46:ARG:NH1	2.28	0.48
1:E:187:ALA:CB	4:E:5363:HOH:O	2.34	0.48
1:A:194:LYS:HA	4:E:5309:HOH:O	2.13	0.48
1:A:222:GLN:O	1:A:223:HIS:HB3	2.13	0.48
1:B:178:PRO:HD2	4:B:2345:HOH:O	2.13	0.48
1:C:27:ALA:CB	4:C:3363:HOH:O	2.58	0.48
1:C:33:SER:HA	1:C:53:THR:O	2.14	0.48
1:D:15:LEU:HA	1:D:126:VAL:HG11	1.96	0.48
1:E:106:LYS:CG	4:E:5398:HOH:O	2.62	0.48
1:E:112:ARG:CD	4:E:5328:HOH:O	2.62	0.48
1:E:123:ASN:CB	4:E:5310:HOH:O	2.59	0.48
1:E:134:VAL:HG21	1:E:170:VAL:HG11	1.96	0.48
1:E:199:ARG:NE	4:E:5346:HOH:O	2.26	0.48
1:A:28:HIS:N	4:A:1382:HOH:O	2.47	0.48
1:A:112:ARG:HG2	4:A:1392:HOH:O	2.13	0.48
1:C:83:GLY:CA	4:C:3329:HOH:O	2.60	0.48
1:C:126:VAL:C	1:C:128:VAL:N	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ALA:HB1	1:D:48:MET:HE1	1.96	0.48
1:D:37:MET:HA	1:D:37:MET:HE3	1.96	0.48
1:D:161:GLU:HG3	4:D:4394:HOH:O	2.14	0.48
1:E:55:HIS:HB3	1:E:57:LYS:HG2	1.95	0.48
1:E:179:ALA:CB	4:E:5322:HOH:O	2.51	0.48
1:A:149:MET:HE2	1:A:153:LEU:HG	1.96	0.48
1:A:240:HIS:HD2	4:A:1352:HOH:O	1.95	0.48
1:B:112:ARG:HG3	1:B:113:PRO:HD2	1.95	0.48
1:B:124:THR:O	1:B:126:VAL:N	2.47	0.48
1:C:29:LYS:HB2	1:C:30:ILE:HD12	1.96	0.48
1:C:39:LEU:HA	1:C:43:SER:HB3	1.96	0.48
1:E:91:ILE:CG2	1:E:118:ILE:HD13	2.44	0.48
1:E:193:VAL:HG21	1:E:199:ARG:HD2	1.96	0.48
1:B:84:ALA:H	1:B:111:PHE:HD2	1.62	0.47
1:B:101:ILE:HG12	1:B:164:GLU:OE1	2.14	0.47
1:B:147:ARG:HG3	1:B:151:GLN:HE21	1.79	0.47
1:C:25:LEU:HD21	1:C:30:ILE:CD1	2.44	0.47
1:C:134:VAL:HG11	1:C:162:VAL:HG22	1.95	0.47
1:C:240:HIS:CE1	1:D:194:LYS:HE2	2.49	0.47
1:D:119:ARG:NH1	4:D:4422:HOH:O	2.46	0.47
1:D:228:LYS:HG2	4:D:4310:HOH:O	2.13	0.47
1:D:262:CYS:O	4:D:4360:HOH:O	2.20	0.47
1:E:91:ILE:C	4:E:5344:HOH:O	2.50	0.47
1:E:123:ASN:HB2	1:E:125:PRO:HD2	1.96	0.47
1:A:64:ASP:O	1:A:90:HIS:CB	2.62	0.47
1:C:82:ILE:O	1:C:86:ILE:HG12	2.14	0.47
1:E:118:ILE:HG21	1:E:149:MET:HG2	1.96	0.47
1:A:123:ASN:H	1:A:123:ASN:HD22	1.62	0.47
1:A:242:LEU:O	1:A:243:HIS:C	2.51	0.47
1:B:115:PRO:CG	4:B:2328:HOH:O	2.61	0.47
1:D:79:LEU:HD21	1:D:104:ILE:HA	1.95	0.47
1:D:184:ALA:CA	4:D:4340:HOH:O	2.63	0.47
1:E:46:ARG:HG3	1:E:46:ARG:HH11	1.79	0.47
1:E:226:GLN:HA	1:E:226:GLN:NE2	2.29	0.47
1:C:8:ALA:HB3	1:C:34:SER:HB2	1.96	0.47
1:C:199:ARG:HD2	4:C:3392:HOH:O	2.05	0.47
1:D:70:VAL:O	1:D:75:ILE:HD11	2.15	0.47
1:D:143:VAL:C	1:D:145:ASP:N	2.67	0.47
1:D:146:GLY:O	1:D:149:MET:HB3	2.14	0.47
1:E:15:LEU:HB3	1:E:19:PHE:CE1	2.50	0.47
1:E:109:SER:C	1:E:111:PHE:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ILE:CA	4:A:1437:HOH:O	2.14	0.47
1:A:134:VAL:HG12	1:A:167:ILE:CD1	2.44	0.47
1:C:89:ARG:NE	1:C:90:HIS:CD2	2.82	0.47
1:D:172:GLY:HA2	1:D:261:SER:OG	2.14	0.47
1:E:67:PHE:HA	1:E:93:VAL:O	2.14	0.47
1:E:112:ARG:N	4:E:5422:HOH:O	2.47	0.47
1:E:184:ALA:N	4:E:5370:HOH:O	2.47	0.47
1:A:13:PHE:CB	4:A:1379:HOH:O	2.53	0.47
1:A:82:ILE:O	1:A:85:ASP:N	2.48	0.47
1:D:88:ASP:CB	4:D:4432:HOH:O	2.60	0.47
1:E:123:ASN:O	1:E:126:VAL:HB	2.15	0.47
1:A:4:GLY:HA2	1:A:31:MET:O	2.15	0.47
1:A:75:ILE:HG22	1:A:76:PRO:N	2.29	0.47
1:A:193:VAL:C	1:A:195:MET:N	2.68	0.47
1:B:2:SER:O	1:B:3:VAL:HG23	2.15	0.47
1:B:172:GLY:O	1:B:258:VAL:HA	2.13	0.47
1:B:236:GLY:CA	4:B:2318:HOH:O	2.48	0.47
1:B:245:LEU:C	1:B:247:SER:H	2.16	0.47
1:C:3:VAL:HG12	1:C:4:GLY:N	2.30	0.47
1:C:101:ILE:HD11	4:C:3394:HOH:O	2.14	0.47
1:C:218:LEU:CD2	2:C:3300:NAI:H52A	2.45	0.47
1:D:34:SER:HB2	1:D:36:ASP:O	2.14	0.47
1:D:115:PRO:CA	4:D:4374:HOH:O	2.52	0.47
1:D:217:LEU:CD1	4:D:4372:HOH:O	2.26	0.47
1:D:251:ARG:CB	4:D:4342:HOH:O	2.28	0.47
1:E:82:ILE:HG22	1:E:86:ILE:HG13	1.97	0.47
1:E:124:THR:C	1:E:126:VAL:H	2.16	0.47
1:E:124:THR:C	1:E:126:VAL:N	2.68	0.47
2:E:5300:NAI:O1N	3:E:5301:GLU:C	2.53	0.47
1:A:11:LEU:N	4:A:1389:HOH:O	2.35	0.47
1:B:241:ALA:N	4:B:2329:HOH:O	2.47	0.47
1:B:245:LEU:C	1:B:247:SER:N	2.67	0.47
1:C:50:VAL:HG23	4:C:3363:HOH:O	2.14	0.47
1:C:168:ASP:HB2	1:C:266:ARG:NH1	2.30	0.47
1:C:251:ARG:C	1:C:252:SER:O	2.53	0.47
1:D:88:ASP:HB3	4:D:4432:HOH:O	2.14	0.47
1:D:238:THR:HG22	1:D:239:ILE:N	2.30	0.47
1:E:158:PHE:CA	4:E:5425:HOH:O	2.23	0.47
1:A:55:HIS:O	1:A:57:LYS:N	2.40	0.47
1:A:239:ILE:C	4:A:1352:HOH:O	2.52	0.47
1:B:158:PHE:CE2	2:B:2300:NAI:H4B	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:ASP:HB2	1:C:266:ARG:HH12	1.80	0.47
1:C:231:VAL:O	1:C:231:VAL:CG1	2.62	0.47
1:D:156:VAL:HG12	4:D:4331:HOH:O	2.15	0.47
1:D:193:VAL:C	1:D:195:MET:H	2.17	0.47
1:E:95:CYS:CA	4:E:5423:HOH:O	2.63	0.47
1:E:123:ASN:CA	4:E:5310:HOH:O	2.63	0.47
1:A:45:LEU:HB2	1:A:52:LEU:HD11	1.96	0.47
1:A:264:ARG:CZ	4:A:1322:HOH:O	2.59	0.47
1:C:128:VAL:CG1	1:C:129:ARG:N	2.78	0.47
1:D:179:ALA:C	4:D:4308:HOH:O	2.49	0.47
1:D:185:LEU:HD21	1:D:210:LEU:CD1	2.42	0.47
1:E:46:ARG:C	1:E:48:MET:H	2.17	0.47
1:E:162:VAL:HG11	1:E:166:LEU:HB2	1.95	0.47
1:E:243:HIS:ND1	4:E:5357:HOH:O	2.35	0.47
1:A:128:VAL:HG12	1:A:129:ARG:N	2.30	0.46
1:A:238:THR:C	1:A:240:HIS:N	2.65	0.46
1:B:29:LYS:C	1:B:30:ILE:HG13	2.35	0.46
1:B:115:PRO:HD3	4:B:2328:HOH:O	2.13	0.46
1:B:129:ARG:NH1	2:B:2300:NAI:C2D	2.77	0.46
1:B:153:LEU:C	1:B:155:SER:N	2.69	0.46
1:C:53:THR:HG23	1:C:58:GLU:OE2	2.15	0.46
1:D:191:GLY:O	1:D:192:GLY:C	2.53	0.46
1:B:73:HIS:C	1:B:75:ILE:H	2.19	0.46
1:B:195:MET:N	1:B:195:MET:HE3	2.31	0.46
1:C:143:VAL:O	1:C:143:VAL:HG12	2.15	0.46
1:D:266:ARG:HD2	4:D:4311:HOH:O	2.13	0.46
1:E:79:LEU:HD21	1:E:104:ILE:HG12	1.96	0.46
1:E:87:GLU:O	1:E:89:ARG:N	2.49	0.46
1:A:111:PHE:N	1:A:111:PHE:CD1	2.84	0.46
1:B:112:ARG:CD	1:B:113:PRO:HD2	2.45	0.46
1:B:143:VAL:HG12	1:B:144:GLU:N	2.30	0.46
1:C:28:HIS:HB2	4:C:3404:HOH:O	2.15	0.46
1:C:169:ALA:O	1:C:172:GLY:N	2.38	0.46
1:C:233:SER:N	4:C:3374:HOH:O	2.47	0.46
1:C:269:GLN:HG3	1:C:270:SER:N	2.30	0.46
1:D:39:LEU:O	1:D:40:ALA:O	2.34	0.46
1:E:113:PRO:CD	4:E:5367:HOH:O	2.60	0.46
1:B:105:GLU:OE2	1:B:139:THR:HB	2.15	0.46
1:B:119:ARG:HD3	1:B:167:ILE:HD13	1.98	0.46
2:B:2300:NAI:O4D	2:B:2300:NAI:O3	2.34	0.46
1:E:73:HIS:HB3	4:E:5415:HOH:O	2.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ILE:N	1:E:76:PRO:CD	2.79	0.46
1:A:26:ALA:HB3	1:A:29:LYS:HE3	1.97	0.46
1:B:7:GLY:HA3	1:B:69:ALA:C	2.35	0.46
1:B:36:ASP:O	1:B:37:MET:HB2	2.15	0.46
1:B:105:GLU:HG2	1:B:139:THR:OG1	2.15	0.46
1:C:6:ILE:HG21	1:C:78:ILE:HG21	1.96	0.46
1:C:52:LEU:C	1:C:52:LEU:HD23	2.35	0.46
1:D:265:THR:CG2	4:D:4360:HOH:O	2.51	0.46
1:E:206:GLY:C	4:E:5408:HOH:O	2.48	0.46
1:B:70:VAL:CB	4:B:2368:HOH:O	2.63	0.46
1:C:240:HIS:CB	4:C:3398:HOH:O	2.52	0.46
1:D:17:LYS:HD2	1:D:127:VAL:CG1	2.45	0.46
1:D:70:VAL:HG12	1:D:71:LYS:N	2.31	0.46
1:D:112:ARG:HB3	4:D:4347:HOH:O	2.14	0.46
1:E:97:ALA:N	4:E:5358:HOH:O	2.23	0.46
1:E:129:ARG:C	4:E:5401:HOH:O	2.49	0.46
1:E:218:LEU:HD23	4:E:5424:HOH:O	2.15	0.46
1:A:62:HIS:HE1	4:A:1334:HOH:O	1.98	0.46
1:A:160:THR:HG22	1:A:161:GLU:O	2.15	0.46
1:C:109:SER:OG	1:C:115:PRO:HD2	2.16	0.46
1:C:112:ARG:HG3	1:C:112:ARG:NH1	2.30	0.46
1:D:97:ALA:C	4:D:4333:HOH:O	2.43	0.46
1:D:114:ALA:HB1	1:D:140:HIS:CG	2.51	0.46
1:E:229:ASP:N	4:E:5337:HOH:O	2.43	0.46
2:E:5300:NAI:C6N	4:E:5402:HOH:O	2.64	0.46
1:A:55:HIS:C	1:A:57:LYS:N	2.69	0.46
1:A:62:HIS:CE1	4:A:1334:HOH:O	2.69	0.46
1:B:52:LEU:O	1:B:54:PRO:HD3	2.16	0.46
1:B:218:LEU:CD2	2:B:2300:NAI:C5B	2.93	0.46
1:C:7:GLY:HA3	1:C:69:ALA:C	2.35	0.46
1:C:45:LEU:HD23	1:C:45:LEU:C	2.36	0.46
1:C:121:MET:CB	4:C:3327:HOH:O	2.64	0.46
1:C:193:VAL:C	4:C:3309:HOH:O	2.54	0.46
1:E:62:HIS:C	4:E:5372:HOH:O	2.43	0.46
1:E:106:LYS:HG2	4:E:5398:HOH:O	2.15	0.46
1:E:115:PRO:O	1:E:140:HIS:HB2	2.16	0.46
1:A:189:ALA:O	1:A:190:ASP:C	2.54	0.46
1:A:263:ILE:CD1	1:A:263:ILE:N	2.78	0.46
1:B:233:SER:O	1:B:234:PRO:C	2.54	0.46
1:C:149:MET:C	1:C:151:GLN:H	2.18	0.46
1:C:223:HIS:C	4:C:3417:HOH:O	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:LEU:HD12	1:C:253:LEU:N	2.30	0.46
1:E:33:SER:O	1:E:35:PRO:CD	2.64	0.46
1:E:62:HIS:CE1	4:E:5387:HOH:O	2.69	0.46
1:A:79:LEU:HD22	1:A:108:LEU:HD13	1.96	0.46
1:B:6:ILE:CD1	1:B:56:ASN:O	2.60	0.46
1:C:163:GLU:HB2	1:C:165:ASP:OD2	2.16	0.46
1:D:16:ALA:HB1	1:D:48:MET:CE	2.46	0.46
1:E:135:TYR:CZ	1:E:161:GLU:HB3	2.51	0.46
1:E:194:LYS:N	4:E:5303:HOH:O	2.41	0.46
1:E:215:LYS:O	1:E:219:HIS:HD2	1.99	0.46
1:A:132:ALA:HB3	4:A:1339:HOH:O	2.16	0.45
1:A:178:PRO:HB3	4:A:1324:HOH:O	2.14	0.45
1:C:178:PRO:N	4:C:3396:HOH:O	2.49	0.45
1:C:218:LEU:HD22	2:C:3300:NAI:O5B	2.16	0.45
1:D:29:LYS:O	1:D:30:ILE:HD13	2.16	0.45
2:D:4300:NAI:O4D	2:D:4300:NAI:O3	2.34	0.45
1:E:126:VAL:O	1:E:156:VAL:CG1	2.65	0.45
1:E:143:VAL:HG12	1:E:143:VAL:O	2.16	0.45
1:A:33:SER:HA	1:A:53:THR:O	2.16	0.45
1:C:61:GLN:C	1:C:63:SER:H	2.19	0.45
2:C:3300:NAI:O4D	2:C:3300:NAI:O3	2.34	0.45
1:E:89:ARG:HG3	1:E:90:HIS:N	2.30	0.45
1:A:27:ALA:HB1	1:A:49:GLY:HA3	1.99	0.45
1:A:136:ALA:CA	4:A:1404:HOH:O	2.63	0.45
1:B:15:LEU:O	1:B:19:PHE:CE1	2.69	0.45
1:B:238:THR:HG22	1:B:239:ILE:N	2.30	0.45
1:C:9:GLY:O	1:C:10:GLN:C	2.55	0.45
1:C:14:ALA:HB1	1:C:126:VAL:HG23	1.98	0.45
1:C:237:ALA:CB	4:C:3406:HOH:O	2.64	0.45
1:D:232:SER:HB3	1:D:239:ILE:CG1	2.44	0.45
1:B:35:PRO:HG2	1:B:71:LYS:HZ2	1.82	0.45
1:B:101:ILE:CD1	1:B:138:GLY:HA2	2.46	0.45
1:B:239:ILE:N	4:B:2352:HOH:O	2.49	0.45
2:B:2300:NAI:H1D	2:B:2300:NAI:O1N	2.17	0.45
1:C:73:HIS:CE1	1:C:74:ILE:HG12	2.51	0.45
1:C:118:ILE:O	1:C:118:ILE:HG12	2.17	0.45
2:C:3300:NAI:O1N	2:C:3300:NAI:H1D	2.17	0.45
1:B:124:THR:C	1:B:126:VAL:H	2.20	0.45
1:C:176:SER:O	1:C:177:GLY:C	2.53	0.45
2:D:4300:NAI:H1D	2:D:4300:NAI:O1N	2.16	0.45
1:E:28:HIS:C	1:E:28:HIS:CD2	2.88	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:LEU:HD23	1:E:39:LEU:H	1.81	0.45
1:A:9:GLY:CA	1:A:41:THR:HG21	2.46	0.45
1:C:187:ALA:O	1:C:188:LEU:C	2.55	0.45
1:D:100:THR:HG22	1:D:101:ILE:N	2.31	0.45
1:D:237:ALA:O	1:D:240:HIS:HB2	2.17	0.45
1:D:257:ALA:O	1:D:258:VAL:C	2.55	0.45
1:E:154:SER:O	2:E:5300:NAI:H42N	2.17	0.45
1:E:175:GLY:C	4:E:5333:HOH:O	2.54	0.45
1:B:83:GLY:C	1:B:85:ASP:H	2.19	0.45
1:B:84:ALA:N	1:B:111:PHE:HD2	2.15	0.45
1:C:45:LEU:CA	4:C:3371:HOH:O	2.44	0.45
1:C:171:THR:HA	4:C:3351:HOH:O	2.00	0.45
1:C:255:ILE:HG23	4:C:3332:HOH:O	2.16	0.45
1:D:242:LEU:O	1:D:244:VAL:N	2.50	0.45
1:E:1:MET:HG2	1:E:2:SER:N	2.31	0.45
1:E:74:ILE:CG2	1:E:78:ILE:HD11	2.46	0.45
1:E:106:LYS:HB3	4:E:5384:HOH:O	2.14	0.45
1:E:190:ASP:CB	4:E:5381:HOH:O	2.65	0.45
1:E:254:LEU:O	1:E:257:ALA:HB3	2.17	0.45
1:A:95:CYS:SG	4:A:1337:HOH:O	2.61	0.45
2:A:1300:NAI:C3N	3:A:1301:GLU:CB	2.91	0.45
1:B:18:GLY:O	1:B:19:PHE:C	2.55	0.45
1:B:222:GLN:OE1	1:B:226:GLN:HG2	2.15	0.45
1:C:189:ALA:HB2	1:C:203:VAL:HA	1.97	0.45
1:D:77:PHE:N	1:D:77:PHE:CD1	2.83	0.45
2:D:4300:NAI:C5N	3:D:4301:GLU:OXT	2.64	0.45
1:E:70:VAL:O	1:E:71:LYS:CB	2.65	0.45
1:E:137:THR:HG23	1:E:137:THR:O	2.17	0.45
1:A:124:THR:O	1:A:126:VAL:N	2.50	0.45
1:B:190:ASP:O	4:B:2308:HOH:O	2.21	0.45
1:B:245:LEU:O	4:B:2353:HOH:O	2.21	0.45
1:B:258:VAL:HG13	1:B:259:GLU:N	2.31	0.45
1:D:37:MET:HE3	1:D:42:VAL:HB	1.99	0.45
1:D:133:THR:HG21	1:D:153:LEU:CD1	2.45	0.45
1:D:184:ALA:N	4:D:4340:HOH:O	2.50	0.45
2:D:4300:NAI:C3N	3:D:4301:GLU:CA	2.91	0.45
2:D:4300:NAI:H2N	3:D:4301:GLU:HA	1.89	0.45
1:E:46:ARG:C	1:E:48:MET:N	2.70	0.45
1:E:262:CYS:O	1:E:263:ILE:C	2.54	0.45
1:A:225:GLY:O	1:A:228:LYS:HB3	2.17	0.45
1:B:66:LEU:N	1:B:91:ILE:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:TYR:HE1	1:B:161:GLU:OE1	1.99	0.45
1:B:236:GLY:C	1:B:238:THR:H	2.20	0.45
1:C:60:VAL:N	4:C:3383:HOH:O	2.47	0.45
1:C:206:GLY:O	1:C:209:ALA:HB3	2.17	0.45
1:D:14:ALA:HA	1:D:127:VAL:HG22	1.98	0.45
1:E:47:LYS:NZ	4:E:5338:HOH:O	2.47	0.45
1:E:53:THR:HG21	1:E:58:GLU:CB	2.47	0.45
1:E:177:GLY:HA2	1:E:180:TYR:HD1	1.81	0.45
1:E:211:LEU:HD13	4:E:5314:HOH:O	2.13	0.45
1:E:251:ARG:CG	4:E:5304:HOH:O	2.64	0.45
1:A:233:SER:O	1:A:235:GLY:N	2.50	0.44
1:A:236:GLY:C	4:A:1391:HOH:O	2.54	0.44
1:A:258:VAL:HG13	4:A:1366:HOH:O	2.16	0.44
1:B:199:ARG:NH1	4:B:2340:HOH:O	2.22	0.44
1:C:19:PHE:HE2	1:C:153:LEU:HD23	1.82	0.44
1:C:126:VAL:CG1	4:C:3307:HOH:O	2.57	0.44
1:C:160:THR:CG2	1:C:161:GLU:H	2.30	0.44
1:D:64:ASP:CG	4:D:4353:HOH:O	2.34	0.44
1:D:227:LEU:HD12	4:D:4363:HOH:O	2.16	0.44
1:D:269:GLN:C	1:D:271:MET:N	2.70	0.44
1:E:43:SER:O	1:E:46:ARG:HB2	2.17	0.44
1:E:177:GLY:O	1:E:180:TYR:HB2	2.17	0.44
1:A:6:ILE:HD13	1:A:59:THR:HG21	2.00	0.44
1:A:120:CYS:HB2	4:A:1368:HOH:O	2.12	0.44
1:A:219:HIS:CE1	4:A:1431:HOH:O	2.69	0.44
1:B:129:ARG:HH12	2:B:2300:NAI:C2D	2.29	0.44
1:C:61:GLN:O	1:C:89:ARG:NH2	2.49	0.44
1:C:275:GLU:C	4:C:3393:HOH:O	2.56	0.44
1:D:195:MET:HG2	4:D:4366:HOH:O	2.16	0.44
1:A:123:ASN:N	1:A:123:ASN:HD22	2.16	0.44
1:A:135:TYR:OH	1:A:150:GLU:CG	2.64	0.44
1:A:195:MET:N	4:E:5309:HOH:O	2.50	0.44
1:A:252:SER:HA	1:A:255:ILE:HD12	1.99	0.44
1:A:269:GLN:C	1:A:271:MET:N	2.70	0.44
1:B:47:LYS:NZ	1:B:47:LYS:HB3	2.33	0.44
1:C:9:GLY:H	1:C:12:ALA:HB3	1.81	0.44
1:C:93:VAL:HG12	1:C:118:ILE:HD11	1.99	0.44
1:C:101:ILE:HB	1:C:164:GLU:OE1	2.17	0.44
1:C:124:THR:C	1:C:126:VAL:N	2.71	0.44
1:D:10:GLN:N	4:D:4387:HOH:O	2.50	0.44
2:D:4300:NAI:C3N	3:D:4301:GLU:HA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:ASP:H	1:E:42:VAL:CG2	2.29	0.44
1:E:62:HIS:HE1	4:E:5387:HOH:O	2.00	0.44
1:E:104:ILE:HG22	1:E:117:VAL:HG21	1.99	0.44
1:E:150:GLU:O	1:E:151:GLN:C	2.56	0.44
1:E:172:GLY:HA2	1:E:261:SER:CB	2.47	0.44
1:A:200:ARG:O	1:A:204:ARG:HG2	2.17	0.44
1:A:256:ASN:CA	4:A:1335:HOH:O	2.53	0.44
1:B:169:ALA:C	1:B:171:THR:N	2.70	0.44
1:B:251:ARG:HD2	4:B:2330:HOH:O	2.11	0.44
1:D:30:ILE:C	4:D:4365:HOH:O	2.56	0.44
1:D:92:VAL:HB	1:D:117:VAL:HG22	1.99	0.44
1:A:255:ILE:O	1:A:258:VAL:N	2.48	0.44
1:B:221:GLU:N	4:B:2322:HOH:O	2.50	0.44
1:C:8:ALA:HB3	1:C:34:SER:CB	2.48	0.44
1:C:61:GLN:O	1:C:63:SER:N	2.51	0.44
1:C:124:THR:N	1:C:125:PRO:CD	2.79	0.44
1:C:167:ILE:HG22	4:C:3345:HOH:O	2.03	0.44
1:E:184:ALA:O	1:E:187:ALA:HB3	2.17	0.44
1:A:11:LEU:CD1	4:A:1399:HOH:O	2.59	0.44
1:A:266:ARG:NH1	1:A:266:ARG:HG2	2.24	0.44
1:C:199:ARG:NH1	4:C:3392:HOH:O	2.48	0.44
1:A:1:MET:HG2	1:A:2:SER:N	2.33	0.44
1:A:28:HIS:C	4:A:1329:HOH:O	2.56	0.44
1:A:211:LEU:CD1	1:A:211:LEU:C	2.86	0.44
1:C:3:VAL:C	4:C:3356:HOH:O	2.49	0.44
1:E:220:SER:O	4:E:5362:HOH:O	2.21	0.44
1:E:251:ARG:HG2	4:E:5304:HOH:O	2.17	0.44
1:E:264:ARG:O	1:E:265:THR:C	2.55	0.44
1:A:172:GLY:C	4:A:1302:HOH:O	2.55	0.44
1:C:71:LYS:HB2	1:C:73:HIS:HE1	1.80	0.44
1:C:261:SER:HB3	4:C:3391:HOH:O	2.18	0.44
1:D:100:THR:HG22	1:D:102:SER:N	2.30	0.44
1:D:219:HIS:CE1	2:D:4300:NAI:H51N	2.37	0.44
1:D:249:GLY:O	1:D:250:PHE:C	2.56	0.44
1:A:101:ILE:HG21	1:A:138:GLY:HA2	2.00	0.44
1:A:121:MET:N	4:A:1368:HOH:O	2.49	0.44
1:A:190:ASP:N	1:A:199:ARG:NH1	2.65	0.44
1:B:60:VAL:O	1:B:89:ARG:NH1	2.51	0.44
1:B:218:LEU:HB3	2:B:2300:NAI:H52N	2.00	0.44
1:C:13:PHE:O	1:C:16:ALA:HB3	2.18	0.44
1:C:26:ALA:HB3	1:C:29:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:ILE:HD12	1:C:30:ILE:N	2.32	0.44
1:C:75:ILE:CA	4:C:3407:HOH:O	2.60	0.44
1:C:266:ARG:O	1:C:269:GLN:HG2	2.18	0.44
1:D:115:PRO:CB	4:D:4374:HOH:O	2.65	0.44
1:D:222:GLN:O	1:D:223:HIS:HB2	2.18	0.44
1:D:266:ARG:HD3	4:D:4311:HOH:O	2.13	0.44
1:E:211:LEU:C	4:E:5314:HOH:O	2.55	0.44
1:E:228:LYS:CE	1:E:242:LEU:HD13	2.48	0.44
1:A:3:VAL:HG11	1:A:67:PHE:HE1	1.82	0.43
1:A:169:ALA:O	1:A:170:VAL:C	2.57	0.43
1:A:176:SER:HB3	1:A:180:TYR:CE2	2.54	0.43
1:A:194:LYS:CB	4:A:1420:HOH:O	2.65	0.43
1:A:238:THR:CG2	4:A:1320:HOH:O	2.66	0.43
1:A:258:VAL:HG22	4:A:1302:HOH:O	2.09	0.43
1:B:142:GLN:CG	1:B:143:VAL:N	2.64	0.43
1:B:236:GLY:O	1:B:237:ALA:HB3	2.17	0.43
1:C:39:LEU:HA	1:C:43:SER:HB2	2.00	0.43
1:C:91:ILE:HG23	1:C:116:ARG:CB	2.43	0.43
1:C:140:HIS:N	4:C:3385:HOH:O	2.51	0.43
1:C:262:CYS:O	1:C:265:THR:HB	2.18	0.43
1:C:269:GLN:O	1:C:271:MET:N	2.45	0.43
1:D:92:VAL:N	4:D:4455:HOH:O	2.51	0.43
1:D:124:THR:N	4:D:4375:HOH:O	2.50	0.43
1:E:242:LEU:O	1:E:244:VAL:N	2.50	0.43
1:E:259:GLU:O	1:E:262:CYS:N	2.50	0.43
1:A:218:LEU:CD1	4:A:1435:HOH:O	2.65	0.43
1:A:231:VAL:O	1:A:231:VAL:CG1	2.65	0.43
1:B:74:ILE:O	1:B:74:ILE:HG22	2.18	0.43
1:B:163:GLU:HG3	1:B:165:ASP:OD1	2.18	0.43
1:B:214:ALA:O	1:B:217:LEU:N	2.50	0.43
1:C:29:LYS:CG	4:C:3306:HOH:O	2.65	0.43
1:C:123:ASN:O	1:C:126:VAL:HG22	2.17	0.43
1:C:138:GLY:HA3	4:C:3394:HOH:O	2.18	0.43
1:C:233:SER:O	1:C:234:PRO:C	2.56	0.43
1:D:121:MET:O	1:D:133:THR:HA	2.19	0.43
1:D:124:THR:N	1:D:125:PRO:CD	2.80	0.43
1:D:135:TYR:HE2	1:D:150:GLU:HG3	1.83	0.43
1:D:224:PRO:HG2	4:D:4355:HOH:O	2.12	0.43
1:E:238:THR:CG2	4:E:5321:HOH:O	2.25	0.43
1:A:64:ASP:O	1:A:90:HIS:HB3	2.18	0.43
1:A:123:ASN:N	1:A:123:ASN:ND2	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ASN:CB	4:A:1436:HOH:O	2.67	0.43
1:A:211:LEU:C	1:A:211:LEU:HD12	2.39	0.43
1:C:150:GLU:C	1:C:154:SER:HB2	2.38	0.43
1:D:193:VAL:C	1:D:195:MET:N	2.71	0.43
1:E:53:THR:HG22	1:E:55:HIS:N	2.19	0.43
1:E:94:SER:O	4:E:5423:HOH:O	2.19	0.43
1:E:126:VAL:HG22	1:E:156:VAL:HG12	2.01	0.43
1:A:139:THR:HG23	4:A:1430:HOH:O	2.18	0.43
1:A:193:VAL:O	1:A:195:MET:N	2.48	0.43
1:B:164:GLU:O	1:B:167:ILE:HB	2.18	0.43
1:C:15:LEU:O	1:C:19:PHE:CD1	2.71	0.43
1:C:93:VAL:HG12	1:C:118:ILE:CG1	2.48	0.43
1:C:240:HIS:CE1	4:C:3365:HOH:O	2.71	0.43
1:D:245:LEU:HD23	1:D:245:LEU:HA	1.87	0.43
1:E:41:THR:O	1:E:42:VAL:C	2.57	0.43
1:E:233:SER:O	1:E:235:GLY:N	2.52	0.43
1:A:60:VAL:HG21	1:A:82:ILE:CG2	2.49	0.43
1:A:86:ILE:O	1:A:86:ILE:HG22	2.19	0.43
1:A:119:ARG:HA	4:A:1372:HOH:O	2.18	0.43
1:A:221:GLU:O	1:A:222:GLN:HB2	2.18	0.43
1:B:185:LEU:CD2	1:B:210:LEU:HD12	2.40	0.43
1:C:60:VAL:O	1:C:60:VAL:HG12	2.18	0.43
1:C:83:GLY:O	1:C:86:ILE:HG12	2.18	0.43
1:D:112:ARG:C	4:D:4329:HOH:O	2.54	0.43
1:D:185:LEU:O	4:D:4361:HOH:O	2.21	0.43
1:E:107:LYS:HG3	4:E:5384:HOH:O	2.18	0.43
1:E:212:GLY:O	1:E:213:ALA:C	2.56	0.43
2:E:5300:NAI:O2D	3:E:5301:GLU:N	2.51	0.43
1:B:79:LEU:CD2	1:B:104:ILE:HG23	2.48	0.43
1:B:83:GLY:HA3	1:B:111:PHE:CD2	2.54	0.43
1:C:51:LYS:HD3	1:C:51:LYS:N	2.32	0.43
1:C:89:ARG:CD	1:C:90:HIS:N	2.68	0.43
1:C:112:ARG:NH1	1:C:113:PRO:HD2	2.11	0.43
1:D:42:VAL:HA	1:D:45:LEU:HD12	2.00	0.43
1:E:136:ALA:C	4:E:5434:HOH:O	2.55	0.43
1:E:191:GLY:O	1:E:192:GLY:C	2.56	0.43
1:A:34:SER:HB2	1:A:37:MET:HG2	2.01	0.43
1:A:262:CYS:O	1:A:265:THR:N	2.52	0.43
1:B:32:ALA:O	1:B:53:THR:HB	2.18	0.43
1:C:38:ASP:H	1:C:42:VAL:HB	1.84	0.43
1:D:128:VAL:HG13	1:D:129:ARG:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:VAL:CG1	1:D:166:LEU:HB2	2.48	0.43
1:E:223:HIS:O	1:E:224:PRO:C	2.57	0.43
1:A:194:LYS:HE2	1:E:240:HIS:ND1	2.34	0.43
1:B:128:VAL:O	1:B:129:ARG:CB	2.66	0.43
1:B:256:ASN:O	4:B:2381:HOH:O	2.21	0.43
1:D:73:HIS:ND1	1:D:74:ILE:HG12	2.34	0.43
1:E:106:LYS:CA	4:E:5398:HOH:O	2.66	0.43
1:E:129:ARG:HA	1:E:156:VAL:HG13	2.01	0.43
1:A:56:ASN:O	1:A:82:ILE:HD11	2.19	0.43
1:B:26:ALA:HB3	1:B:29:LYS:HB2	2.00	0.43
1:B:260:ALA:N	4:B:2381:HOH:O	2.50	0.43
1:C:35:PRO:O	1:C:36:ASP:CB	2.66	0.43
1:C:75:ILE:HG21	1:C:99:VAL:HG11	2.01	0.43
1:A:73:HIS:O	1:A:76:PRO:HD2	2.19	0.43
1:B:133:THR:N	4:B:2387:HOH:O	2.51	0.43
1:B:147:ARG:NH1	1:B:150:GLU:OE2	2.52	0.43
1:C:112:ARG:HG3	1:C:113:PRO:CD	2.39	0.43
1:E:125:PRO:HB2	1:E:130:GLU:O	2.19	0.43
1:E:131:GLY:O	1:E:157:GLY:HA3	2.19	0.43
1:A:6:ILE:HG23	1:A:56:ASN:HB2	2.00	0.42
1:B:111:PHE:N	1:B:111:PHE:CD1	2.87	0.42
1:B:238:THR:O	1:B:241:ALA:N	2.51	0.42
1:B:269:GLN:O	1:B:271:MET:N	2.47	0.42
1:C:24:VAL:O	1:C:25:LEU:HB2	2.16	0.42
1:C:46:ARG:O	1:C:48:MET:N	2.52	0.42
1:C:79:LEU:HD11	1:C:104:ILE:CG1	2.48	0.42
1:C:252:SER:HA	4:C:3364:HOH:O	2.19	0.42
1:D:89:ARG:CZ	1:D:90:HIS:CE1	3.02	0.42
1:D:121:MET:HE3	1:D:171:THR:HA	2.00	0.42
1:B:105:GLU:O	1:B:109:SER:HB2	2.18	0.42
1:B:154:SER:C	2:B:2300:NAI:N7N	2.66	0.42
1:C:123:ASN:HD21	1:C:132:ALA:CB	2.22	0.42
1:D:134:VAL:HG23	1:D:160:THR:O	2.19	0.42
1:D:142:GLN:C	1:D:145:ASP:HB2	2.40	0.42
1:D:203:VAL:CG1	1:D:204:ARG:N	2.82	0.42
1:E:115:PRO:CA	4:E:5436:HOH:O	2.52	0.42
1:E:136:ALA:HB2	1:E:167:ILE:CD1	2.49	0.42
1:E:195:MET:HA	1:E:195:MET:HE2	2.01	0.42
1:E:243:HIS:O	1:E:247:SER:OG	2.35	0.42
1:B:124:THR:N	1:B:125:PRO:CD	2.80	0.42
1:B:204:ARG:HD3	1:B:204:ARG:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:PRO:HG3	4:C:3346:HOH:O	2.19	0.42
1:C:185:LEU:HG	4:C:3352:HOH:O	2.19	0.42
1:D:39:LEU:O	1:D:43:SER:HB3	2.19	0.42
1:D:57:LYS:O	1:D:61:GLN:HG3	2.19	0.42
1:D:109:SER:C	1:D:111:PHE:H	2.22	0.42
1:E:238:THR:CB	4:E:5321:HOH:O	2.60	0.42
1:A:92:VAL:O	1:A:117:VAL:HG23	2.20	0.42
1:A:119:ARG:O	1:A:135:TYR:HA	2.19	0.42
1:B:39:LEU:HA	1:B:43:SER:HB2	2.01	0.42
1:B:165:ASP:OD1	1:B:166:LEU:N	2.53	0.42
1:B:218:LEU:CB	2:B:2300:NAI:H52N	2.50	0.42
1:C:129:ARG:NH1	3:C:3301:GLU:HG2	2.32	0.42
1:E:31:MET:HE3	1:E:51:LYS:HD3	2.01	0.42
1:E:259:GLU:O	1:E:260:ALA:C	2.57	0.42
1:A:169:ALA:O	1:A:172:GLY:N	2.51	0.42
1:A:258:VAL:HG12	1:A:259:GLU:N	2.34	0.42
1:A:269:GLN:O	1:A:271:MET:N	2.52	0.42
1:B:172:GLY:HA2	1:B:261:SER:CB	2.49	0.42
1:B:188:LEU:C	1:B:190:ASP:N	2.71	0.42
1:D:111:PHE:O	1:D:112:ARG:C	2.57	0.42
1:E:132:ALA:CA	4:E:5351:HOH:O	2.52	0.42
1:E:246:GLU:CA	4:E:5312:HOH:O	2.66	0.42
1:A:105:GLU:O	1:A:107:LYS:N	2.45	0.42
1:A:119:ARG:CA	4:A:1372:HOH:O	2.68	0.42
1:A:149:MET:O	1:A:151:GLN:N	2.52	0.42
1:A:219:HIS:NE2	2:A:1300:NAI:C5D	2.82	0.42
1:A:249:GLY:O	1:A:252:SER:HB3	2.20	0.42
1:B:75:ILE:H	1:B:75:ILE:CD1	2.27	0.42
1:C:11:LEU:O	1:C:15:LEU:HG	2.20	0.42
1:C:22:ALA:CB	4:C:3369:HOH:O	2.40	0.42
1:E:89:ARG:NH2	1:E:90:HIS:HE1	2.17	0.42
1:E:111:PHE:O	1:E:112:ARG:C	2.56	0.42
1:E:199:ARG:NH2	4:E:5346:HOH:O	2.49	0.42
1:E:211:LEU:O	1:E:211:LEU:HD13	2.19	0.42
1:A:50:VAL:CG1	1:A:51:LYS:N	2.83	0.42
1:A:173:LEU:HB3	1:A:174:SER:H	1.55	0.42
1:B:274:GLN:HG2	1:B:275:GLU:HG3	2.01	0.42
1:D:28:HIS:CD2	1:D:28:HIS:C	2.93	0.42
1:D:133:THR:HG22	1:D:158:PHE:O	2.19	0.42
1:E:62:HIS:O	4:E:5417:HOH:O	2.22	0.42
1:E:260:ALA:HA	4:E:5329:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:SER:O	1:A:104:ILE:N	2.53	0.42
1:A:109:SER:C	1:A:111:PHE:H	2.23	0.42
1:A:166:LEU:O	1:A:168:ASP:N	2.52	0.42
1:A:194:LYS:CA	4:E:5309:HOH:O	2.66	0.42
1:A:249:GLY:CA	4:A:1318:HOH:O	2.66	0.42
1:B:158:PHE:HE2	2:B:2300:NAI:O3B	1.85	0.42
1:C:177:GLY:O	1:C:180:TYR:N	2.45	0.42
1:C:185:LEU:HD23	1:C:185:LEU:HA	1.90	0.42
1:D:30:ILE:CB	1:D:50:VAL:HG22	2.40	0.42
1:D:70:VAL:CG1	1:D:74:ILE:HB	2.50	0.42
1:A:80:ASP:OD2	1:A:107:LYS:NZ	2.42	0.42
1:A:162:VAL:CG1	1:A:166:LEU:HD12	2.45	0.42
1:A:267:GLU:O	1:A:268:LEU:C	2.57	0.42
1:B:176:SER:HB2	1:B:180:TYR:OH	2.20	0.42
1:B:191:GLY:O	1:B:194:LYS:HB3	2.20	0.42
1:C:57:LYS:C	4:C:3383:HOH:O	2.58	0.42
1:C:86:ILE:HG22	1:C:87:GLU:H	1.84	0.42
1:D:62:HIS:HA	4:D:4448:HOH:O	2.16	0.42
1:D:251:ARG:NH1	1:D:251:ARG:HG2	2.35	0.42
1:E:39:LEU:HA	1:E:43:SER:CB	2.50	0.42
1:A:106:LYS:CB	4:A:1432:HOH:O	2.67	0.42
1:B:89:ARG:O	1:B:89:ARG:HD2	2.20	0.42
1:B:164:GLU:HA	1:B:167:ILE:CD1	2.49	0.42
1:D:119:ARG:CZ	4:D:4422:HOH:O	2.68	0.42
1:E:78:ILE:O	1:E:81:GLU:HB2	2.19	0.42
1:A:119:ARG:HH11	1:A:164:GLU:HG2	1.85	0.41
1:B:57:LYS:HG3	1:B:58:GLU:N	2.35	0.41
1:B:250:PHE:N	4:B:2361:HOH:O	2.53	0.41
1:C:133:THR:O	1:C:159:CYS:HA	2.19	0.41
1:C:197:LEU:CD1	4:C:3367:HOH:O	2.66	0.41
1:D:219:HIS:NE2	2:D:4300:NAI:O5D	2.52	0.41
1:E:116:ARG:HA	4:E:5388:HOH:O	2.20	0.41
1:E:121:MET:HE3	1:E:121:MET:HA	2.02	0.41
1:E:218:LEU:CB	4:E:5424:HOH:O	2.68	0.41
1:A:146:GLY:O	1:A:150:GLU:HB2	2.20	0.41
1:A:187:ALA:O	1:A:190:ASP:HB2	2.20	0.41
1:B:5:PHE:CE1	1:B:12:ALA:HA	2.55	0.41
1:B:45:LEU:CA	4:B:2385:HOH:O	2.69	0.41
1:B:228:LYS:NZ	4:E:5316:HOH:O	2.32	0.41
1:C:240:HIS:HE1	4:C:3365:HOH:O	2.03	0.41
1:D:17:LYS:HD2	1:D:127:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:GLY:O	1:D:99:VAL:C	2.58	0.41
1:D:172:GLY:HA2	1:D:261:SER:CB	2.50	0.41
1:E:180:TYR:CE2	1:E:257:ALA:HB1	2.55	0.41
1:E:229:ASP:O	1:E:231:VAL:N	2.52	0.41
1:A:223:HIS:ND1	1:A:224:PRO:CD	2.83	0.41
1:B:101:ILE:HG23	1:B:164:GLU:CD	2.41	0.41
1:C:87:GLU:HB2	1:C:90:HIS:CE1	2.55	0.41
1:D:43:SER:CB	4:D:4405:HOH:O	2.56	0.41
1:D:227:LEU:HA	1:D:230:ASN:HB2	2.02	0.41
1:E:6:ILE:HG12	1:E:66:LEU:HD11	2.02	0.41
1:A:73:HIS:HE1	4:E:5334:HOH:O	2.03	0.41
1:A:123:ASN:HD21	1:A:131:GLY:CA	2.34	0.41
1:B:86:ILE:HD12	1:B:108:LEU:HD22	2.03	0.41
1:C:12:ALA:HA	1:C:15:LEU:HD12	2.02	0.41
1:C:133:THR:HG21	4:C:3317:HOH:O	2.04	0.41
1:C:173:LEU:HD12	1:C:173:LEU:HA	1.85	0.41
1:C:213:ALA:O	1:C:216:MET:HB2	2.19	0.41
1:E:94:SER:CA	4:E:5325:HOH:O	2.60	0.41
1:A:171:THR:O	1:A:175:GLY:HA3	2.21	0.41
1:A:263:ILE:HD13	1:A:263:ILE:H	1.81	0.41
1:B:70:VAL:HB	4:B:2368:HOH:O	2.19	0.41
1:C:15:LEU:HB3	1:C:19:PHE:CE1	2.55	0.41
1:C:16:ALA:O	1:C:18:GLY:N	2.53	0.41
1:D:166:LEU:O	1:D:167:ILE:C	2.59	0.41
1:D:229:ASP:O	4:D:4316:HOH:O	2.22	0.41
1:E:69:ALA:CB	4:E:5379:HOH:O	2.48	0.41
1:A:149:MET:CE	1:A:149:MET:HA	2.51	0.41
1:B:42:VAL:C	1:B:44:ALA:H	2.23	0.41
1:B:218:LEU:HD21	2:B:2300:NAI:H52A	2.02	0.41
1:B:233:SER:O	1:B:235:GLY:N	2.53	0.41
1:C:4:GLY:CA	1:C:66:LEU:HG	2.51	0.41
1:C:74:ILE:HG22	1:C:78:ILE:HG12	2.03	0.41
1:C:123:ASN:OD1	1:C:132:ALA:N	2.53	0.41
1:C:134:VAL:O	4:C:3327:HOH:O	2.22	0.41
1:D:89:ARG:CZ	1:D:90:HIS:HE1	2.34	0.41
1:E:57:LYS:N	1:E:57:LYS:CD	2.74	0.41
1:A:22:ALA:HB1	4:A:1425:HOH:O	2.15	0.41
1:A:38:ASP:O	1:A:40:ALA:N	2.54	0.41
1:A:41:THR:HG22	1:A:42:VAL:N	2.36	0.41
1:A:149:MET:HE1	1:A:153:LEU:HG	2.03	0.41
1:A:167:ILE:O	1:A:167:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:THR:HG21	1:B:58:GLU:HB2	2.03	0.41
1:B:89:ARG:NH1	1:B:90:HIS:HD1	2.18	0.41
1:B:140:HIS:O	1:B:141:ALA:CB	2.68	0.41
1:B:229:ASP:C	1:B:231:VAL:H	2.23	0.41
1:C:19:PHE:CE2	1:C:153:LEU:HD23	2.55	0.41
1:D:164:GLU:OE2	4:D:4422:HOH:O	2.21	0.41
1:D:210:LEU:O	1:D:211:LEU:C	2.58	0.41
1:D:220:SER:C	1:D:222:GLN:H	2.24	0.41
1:D:236:GLY:O	1:D:237:ALA:HB3	2.21	0.41
1:E:129:ARG:CB	4:E:5401:HOH:O	2.56	0.41
1:A:116:ARG:HG3	4:A:1416:HOH:O	2.19	0.41
1:C:6:ILE:HD12	1:C:56:ASN:CB	2.46	0.41
1:C:119:ARG:NH1	4:C:3372:HOH:O	2.53	0.41
1:C:252:SER:O	1:C:253:LEU:C	2.58	0.41
1:D:67:PHE:O	4:D:4327:HOH:O	2.21	0.41
1:D:80:ASP:O	1:D:82:ILE:N	2.54	0.41
1:D:161:GLU:O	1:D:162:VAL:HG23	2.21	0.41
1:E:117:VAL:O	1:E:138:GLY:CA	2.67	0.41
1:E:134:VAL:CG2	1:E:170:VAL:HG11	2.51	0.41
1:A:7:GLY:CA	4:A:1305:HOH:O	2.59	0.41
1:A:11:LEU:HD11	4:A:1346:HOH:O	2.20	0.41
1:A:13:PHE:HA	1:A:45:LEU:HD21	2.03	0.41
1:A:240:HIS:CD2	1:C:194:LYS:HE3	2.56	0.41
1:B:8:ALA:HB1	1:B:45:LEU:HD12	2.03	0.41
1:B:28:HIS:CD2	1:B:49:GLY:O	2.73	0.41
1:B:164:GLU:CG	1:B:167:ILE:HD12	2.42	0.41
1:B:241:ALA:O	1:B:242:LEU:C	2.57	0.41
1:C:137:THR:O	4:C:3414:HOH:O	2.22	0.41
1:C:158:PHE:HZ	2:C:3300:NAI:HO2A	1.66	0.41
1:C:222:GLN:HG3	1:C:227:LEU:HD21	2.02	0.41
1:D:24:VAL:HG11	1:D:152:LEU:CD2	2.51	0.41
1:D:46:ARG:HG3	1:D:52:LEU:HD12	2.02	0.41
1:D:121:MET:CE	1:D:171:THR:HA	2.50	0.41
1:D:165:ASP:O	4:D:4368:HOH:O	2.22	0.41
1:D:187:ALA:O	1:D:190:ASP:HB2	2.20	0.41
1:D:269:GLN:NE2	4:D:4445:HOH:O	2.52	0.41
1:E:75:ILE:HG21	1:E:99:VAL:HG11	2.02	0.41
1:E:100:THR:HG22	1:E:101:ILE:H	1.86	0.41
1:E:242:LEU:O	1:E:245:LEU:N	2.54	0.41
1:A:98:GLY:CA	4:A:1328:HOH:O	2.39	0.41
1:A:185:LEU:HG	4:A:1419:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ALA:C	1:B:18:GLY:N	2.72	0.41
1:B:91:ILE:HG23	1:B:116:ARG:HB3	2.03	0.41
1:B:107:LYS:HE2	1:B:107:LYS:HB3	1.91	0.41
1:B:134:VAL:HG12	1:B:135:TYR:N	2.36	0.41
1:C:104:ILE:CG2	1:C:117:VAL:HG11	2.51	0.41
1:C:119:ARG:NH2	4:C:3345:HOH:O	2.53	0.41
1:D:89:ARG:NH1	1:D:90:HIS:CE1	2.89	0.41
1:D:193:VAL:HA	1:D:197:LEU:O	2.21	0.41
1:E:3:VAL:HG22	1:E:65:VAL:HB	2.03	0.41
1:A:77:PHE:N	1:A:77:PHE:CD1	2.89	0.40
1:A:242:LEU:O	1:A:244:VAL:N	2.53	0.40
1:B:228:LYS:HE2	1:B:229:ASP:OD1	2.21	0.40
1:C:129:ARG:O	1:C:157:GLY:HA2	2.21	0.40
1:C:160:THR:HG22	1:C:161:GLU:H	1.81	0.40
1:C:233:SER:N	4:C:3313:HOH:O	2.45	0.40
1:E:215:LYS:O	1:E:219:HIS:CD2	2.74	0.40
1:E:255:ILE:O	1:E:256:ASN:C	2.59	0.40
1:A:26:ALA:HB2	1:A:29:LYS:HE3	2.03	0.40
1:B:12:ALA:O	1:B:16:ALA:CB	2.69	0.40
1:B:12:ALA:HB1	4:B:2314:HOH:O	2.13	0.40
1:B:76:PRO:HB2	1:B:77:PHE:CD1	2.56	0.40
1:B:194:LYS:HG2	1:B:195:MET:HE3	2.02	0.40
1:C:82:ILE:HG22	1:C:82:ILE:O	2.21	0.40
1:D:156:VAL:O	1:D:156:VAL:CG1	2.56	0.40
1:D:206:GLY:O	1:D:209:ALA:HB3	2.22	0.40
1:D:251:ARG:CD	4:D:4427:HOH:O	2.59	0.40
1:E:133:THR:O	1:E:159:CYS:HA	2.21	0.40
2:E:5300:NAI:C2D	3:E:5301:GLU:N	2.85	0.40
1:A:62:HIS:O	1:A:62:HIS:CG	2.74	0.40
1:A:124:THR:C	1:A:126:VAL:H	2.24	0.40
1:A:240:HIS:HD2	1:C:194:LYS:HG3	1.86	0.40
1:B:160:THR:HG22	4:B:2360:HOH:O	2.07	0.40
1:B:269:GLN:C	1:B:271:MET:N	2.74	0.40
1:C:50:VAL:HG22	4:C:3363:HOH:O	2.18	0.40
1:C:128:VAL:CG1	1:C:129:ARG:H	2.26	0.40
1:D:129:ARG:HD3	1:D:155:SER:O	2.21	0.40
1:E:63:SER:CB	4:E:5372:HOH:O	2.67	0.40
1:E:77:PHE:CD1	1:E:77:PHE:N	2.86	0.40
1:E:113:PRO:N	4:E:5367:HOH:O	2.55	0.40
1:A:26:ALA:O	1:A:27:ALA:C	2.60	0.40
1:A:40:ALA:O	1:A:44:ALA:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:THR:HG22	1:A:101:ILE:N	2.37	0.40
1:B:73:HIS:C	1:B:75:ILE:N	2.74	0.40
1:B:77:PHE:CD1	1:B:77:PHE:N	2.85	0.40
1:B:89:ARG:HD2	1:B:89:ARG:C	2.41	0.40
1:B:216:MET:CE	4:B:2315:HOH:O	2.69	0.40
1:C:79:LEU:HD11	1:C:104:ILE:HG12	2.04	0.40
1:C:176:SER:HB2	1:C:180:TYR:CZ	2.56	0.40
1:C:228:LYS:NZ	1:C:229:ASP:OD1	2.55	0.40
1:D:251:ARG:NH1	4:D:4447:HOH:O	2.28	0.40
1:E:181:ALA:C	4:E:5383:HOH:O	2.58	0.40
1:A:5:PHE:C	1:A:7:GLY:N	2.74	0.40
1:E:135:TYR:N	4:E:5413:HOH:O	2.54	0.40

All (22) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ARG:NH1	2:B:2300:NAI:N7A[2_555]	1.66	0.54
1:A:204:ARG:CB	2:C:3300:NAI:C3B[2_555]	1.75	0.45
1:B:204:ARG:CB	2:B:2300:NAI:C3B[2_555]	1.76	0.44
2:B:2300:NAI:O5B	4:B:2359:HOH:O[2_555]	1.88	0.32
1:D:204:ARG:CB	2:E:5300:NAI:C2B[2_555]	1.94	0.26
1:B:204:ARG:CG	2:B:2300:NAI:C2B[2_555]	2.01	0.19
1:B:204:ARG:NE	2:B:2300:NAI:C8A[2_555]	2.03	0.17
1:E:250:PHE:CE2	4:D:4340:HOH:O[2_555]	2.03	0.17
4:A:1320:HOH:O	4:C:3330:HOH:O[2_555]	2.04	0.16
1:A:243:HIS:NE2	4:A:1335:HOH:O[2_555]	2.07	0.13
1:A:251:ARG:NH1	1:A:251:ARG:NH1[2_555]	2.09	0.11
4:A:1398:HOH:O	4:C:3376:HOH:O[2_555]	2.09	0.11
4:B:2337:HOH:O	4:B:2363:HOH:O[2_555]	2.09	0.11
1:C:231:VAL:CG1	4:A:1347:HOH:O[2_555]	2.10	0.10
4:A:1380:HOH:O	4:C:3336:HOH:O[2_555]	2.11	0.09
1:C:255:ILE:CG2	4:E:5357:HOH:O[2_555]	2.11	0.09
1:A:204:ARG:CG	2:C:3300:NAI:C2B[2_555]	2.15	0.05
1:A:204:ARG:CG	2:C:3300:NAI:O4B[2_555]	2.16	0.04
1:D:29:LYS:CE	4:D:4430:HOH:O[2_556]	2.16	0.04
4:A:1442:HOH:O	4:C:3379:HOH:O[2_555]	2.17	0.03
1:B:258:VAL:CG2	4:B:2355:HOH:O[2_555]	2.17	0.03
1:A:204:ARG:CB	2:C:3300:NAI:O4B[2_555]	2.18	0.02

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 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	275/277 (99%)	189 (69%)	54 (20%)	32 (12%)	0	2
1	B	272/277 (98%)	168 (62%)	62 (23%)	42 (15%)	0	0
1	C	275/277 (99%)	198 (72%)	49 (18%)	28 (10%)	0	3
1	D	275/277 (99%)	190 (69%)	64 (23%)	21 (8%)	1	5
1	E	275/277 (99%)	178 (65%)	64 (23%)	33 (12%)	0	1
All	All	1372/1385 (99%)	923 (67%)	293 (21%)	156 (11%)	0	2

All (156) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	36	ASP
1	A	39	LEU
1	A	107	LYS
1	A	129	ARG
1	A	164	GLU
1	A	173	LEU
1	B	10	GLN
1	B	19	PHE
1	B	36	ASP
1	B	37	MET
1	B	76	PRO
1	B	95	CYS
1	B	97	ALA
1	B	129	ARG
1	B	137	THR
1	B	140	HIS
1	B	141	ALA
1	B	142	GLN
1	B	221	GLU
1	B	222	GLN

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Mol	Chain	Res	Type
1	B	223	HIS
1	C	10	GLN
1	C	27	ALA
1	C	63	SER
1	C	65	VAL
1	C	113	PRO
1	C	252	SER
1	C	253	LEU
1	D	40	ALA
1	D	99	VAL
1	D	129	ARG
1	D	164	GLU
1	D	223	HIS
1	E	88	ASP
1	E	164	GLU
1	E	222	GLN
1	E	223	HIS
1	E	274	GLN
1	A	41	THR
1	A	42	VAL
1	A	235	GLY
1	B	61	GLN
1	B	77	PHE
1	B	113	PRO
1	B	154	SER
1	B	160	THR
1	B	170	VAL
1	B	177	GLY
1	B	186	ASP
1	B	189	ALA
1	C	16	ALA
1	C	36	ASP
1	C	64	ASP
1	C	107	LYS
1	D	8	ALA
1	D	167	ILE
1	D	267	GLU
1	D	270	SER
1	E	41	THR
1	E	42	VAL
1	E	50	VAL
1	E	78	ILE

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Mol	Chain	Res	Type
1	E	90	HIS
1	E	151	GLN
1	E	170	VAL
1	E	230	ASN
1	E	235	GLY
1	E	260	ALA
1	A	37	MET
1	A	77	PHE
1	A	103	SER
1	A	106	LYS
1	A	167	ILE
1	A	223	HIS
1	A	243	HIS
1	A	256	ASN
1	A	270	SER
1	B	38	ASP
1	B	94	SER
1	B	143	VAL
1	B	163	GLU
1	B	199	ARG
1	B	220	SER
1	B	230	ASN
1	B	270	SER
1	C	17	LYS
1	C	20	THR
1	C	47	LYS
1	C	56	ASN
1	C	125	PRO
1	C	139	THR
1	C	197	LEU
1	C	258	VAL
1	D	10	GLN
1	D	41	THR
1	D	81	GLU
1	D	170	VAL
1	D	258	VAL
1	E	243	HIS
1	E	250	PHE
1	A	40	ALA
1	A	87	GLU
1	A	102	SER
1	A	150	GLU

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Mol	Chain	Res	Type
1	A	163	GLU
1	A	187	ALA
1	A	220	SER
1	B	16	ALA
1	B	20	THR
1	B	125	PRO
1	B	246	GLU
1	C	46	ARG
1	C	72	PRO
1	C	173	LEU
1	D	235	GLY
1	D	257	ALA
1	E	36	ASP
1	E	77	PHE
1	E	130	GLU
1	E	163	GLU
1	E	221	GLU
1	E	237	ALA
1	E	259	GLU
1	A	177	GLY
1	A	234	PRO
1	B	71	LYS
1	C	11	LEU
1	C	40	ALA
1	C	62	HIS
1	C	150	GLU
1	C	270	SER
1	D	77	PHE
1	D	125	PRO
1	D	238	THR
1	E	113	PRO
1	E	143	VAL
1	A	56	ASN
1	A	263	ILE
1	C	177	GLY
1	D	42	VAL
1	D	111	PHE
1	E	81	GLU
1	A	125	PRO
1	B	239	ILE
1	E	74	ILE
1	E	125	PRO

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Mol	Chain	Res	Type
1	A	34	SER
1	B	24	VAL
1	B	235	GLY
1	E	234	PRO
1	B	234	PRO
1	B	127	VAL
1	E	34	SER
1	E	71	LYS
1	E	167	ILE

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 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	215/215 (100%)	188 (87%)	27 (13%)	4 18
1	B	213/215 (99%)	197 (92%)	16 (8%)	13 42
1	C	214/215 (100%)	197 (92%)	17 (8%)	12 40
1	D	215/215 (100%)	195 (91%)	20 (9%)	9 32
1	E	215/215 (100%)	200 (93%)	15 (7%)	15 45
All	All	1072/1075 (100%)	977 (91%)	95 (9%)	9 34

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	20	THR
1	A	25	LEU
1	A	36	ASP
1	A	38	ASP
1	A	73	HIS
1	A	75	ILE
1	A	90	HIS
1	A	111	PHE
1	A	120	CYS

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Mol	Chain	Res	Type
1	A	121	MET
1	A	123	ASN
1	A	124	THR
1	A	126	VAL
1	A	148	LEU
1	A	150	GLU
1	A	171	THR
1	A	183	THR
1	A	211	LEU
1	A	228	LYS
1	A	234	PRO
1	A	247	SER
1	A	258	VAL
1	A	263	ILE
1	A	265	THR
1	A	269	GLN
1	A	271	MET
1	B	5	PHE
1	B	10	GLN
1	B	13	PHE
1	B	19	PHE
1	B	47	LYS
1	B	90	HIS
1	B	105	GLU
1	B	111	PHE
1	B	120	CYS
1	B	124	THR
1	B	140	HIS
1	B	211	LEU
1	B	234	PRO
1	B	244	VAL
1	B	247	SER
1	B	265	THR
1	C	13	PHE
1	C	51	LYS
1	C	61	GLN
1	C	72	PRO
1	C	89	ARG
1	C	90	HIS
1	C	118	ILE
1	C	120	CYS
1	C	121	MET

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Mol	Chain	Res	Type
1	C	123	ASN
1	C	124	THR
1	C	190	ASP
1	C	195	MET
1	C	216	MET
1	C	244	VAL
1	C	265	THR
1	C	273	ASP
1	D	10	GLN
1	D	28	HIS
1	D	31	MET
1	D	37	MET
1	D	77	PHE
1	D	101	ILE
1	D	118	ILE
1	D	120	CYS
1	D	122	THR
1	D	124	THR
1	D	137	THR
1	D	144	GLU
1	D	145	ASP
1	D	153	LEU
1	D	168	ASP
1	D	203	VAL
1	D	211	LEU
1	D	244	VAL
1	D	258	VAL
1	D	259	GLU
1	E	28	HIS
1	E	57	LYS
1	E	77	PHE
1	E	90	HIS
1	E	101	ILE
1	E	120	CYS
1	E	124	THR
1	E	160	THR
1	E	168	ASP
1	E	176	SER
1	E	178	PRO
1	E	195	MET
1	E	211	LEU
1	E	216	MET

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Mol	Chain	Res	Type
1	E	233	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	90	HIS
1	A	123	ASN
1	A	140	HIS
1	A	226	GLN
1	A	240	HIS
1	B	151	GLN
1	C	73	HIS
1	C	90	HIS
1	C	240	HIS
1	C	243	HIS
1	D	28	HIS
1	D	55	HIS
1	D	140	HIS
1	D	219	HIS
1	E	28	HIS
1	E	142	GLN
1	E	219	HIS
1	E	226	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)

10 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	$\#\|Z\| > 2$
3	GLU	B	2301	-	8,9,9	1.86	2 (25%)	10,11,11	5.43	2 (20%)
2	NAI	D	4300	-	40,47,48	5.42	23 (57%)	43,71,73	4.67	21 (48%)
2	NAI	E	5300	-	40,47,48	5.83	25 (62%)	43,71,73	6.29	31 (72%)
3	GLU	D	4301	-	8,9,9	1.38	1 (12%)	10,11,11	1.91	2 (20%)
3	GLU	A	1301	-	8,9,9	1.57	1 (12%)	10,11,11	5.34	1 (10%)
2	NAI	C	3300	-	40,47,48	5.41	22 (55%)	43,71,73	4.67	21 (48%)
3	GLU	C	3301	-	8,9,9	1.86	2 (25%)	10,11,11	5.43	2 (20%)
3	GLU	E	5301	-	8,9,9	1.39	1 (12%)	10,11,11	1.65	2 (20%)
2	NAI	A	1300	-	40,47,48	6.28	27 (67%)	43,71,73	5.94	24 (55%)
2	NAI	B	2300	-	40,47,48	5.41	23 (57%)	43,71,73	4.66	21 (48%)

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
3	GLU	B	2301	-	-	5/9/9/9	-
2	NAI	D	4300	-	1/1/13/16	12/25/72/72	0/5/5/5
2	NAI	E	5300	-	3/3/13/16	11/25/72/72	0/5/5/5
3	GLU	D	4301	-	-	1/9/9/9	-
3	GLU	A	1301	-	-	5/9/9/9	-
2	NAI	C	3300	-	1/1/13/16	12/25/72/72	0/5/5/5
3	GLU	C	3301	-	-	5/9/9/9	-
3	GLU	E	5301	-	-	1/9/9/9	-
2	NAI	A	1300	-	2/2/13/16	14/25/72/72	0/5/5/5
2	NAI	B	2300	-	1/1/13/16	12/25/72/72	0/5/5/5

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3300	NAI	C8A-N7A	16.62	1.64	1.34
2	B	2300	NAI	C8A-N7A	16.61	1.64	1.34
2	D	4300	NAI	C8A-N7A	16.58	1.64	1.34
2	E	5300	NAI	C8A-N7A	16.55	1.64	1.34
2	A	1300	NAI	O7N-C7N	15.71	1.61	1.24
2	A	1300	NAI	O4D-C4D	-14.41	1.12	1.45
2	D	4300	NAI	O4D-C4D	-14.40	1.12	1.45
2	C	3300	NAI	O4D-C4D	-14.40	1.12	1.45
2	B	2300	NAI	O4D-C4D	-14.39	1.12	1.45
2	A	1300	NAI	O4B-C1B	14.05	1.60	1.41
2	A	1300	NAI	C2B-C1B	-13.33	1.33	1.53
2	E	5300	NAI	C3D-C4D	-12.48	1.21	1.53
2	E	5300	NAI	C1D-N1N	12.24	1.81	1.46
2	D	4300	NAI	O4B-C1B	12.14	1.58	1.41
2	C	3300	NAI	O4B-C1B	12.11	1.58	1.41
2	E	5300	NAI	O4B-C1B	12.08	1.57	1.41
2	B	2300	NAI	O4B-C1B	12.08	1.57	1.41
2	E	5300	NAI	O7N-C7N	10.88	1.50	1.24
2	A	1300	NAI	C7N-C3N	-9.74	1.27	1.48
2	A	1300	NAI	C4A-N3A	9.14	1.48	1.35
2	D	4300	NAI	C3D-C4D	-9.09	1.29	1.53
2	A	1300	NAI	O4D-C1D	-9.07	1.20	1.42
2	D	4300	NAI	O4D-C1D	-9.07	1.20	1.42
2	C	3300	NAI	O4D-C1D	-9.06	1.20	1.42
2	C	3300	NAI	C3D-C4D	-9.06	1.29	1.53
2	A	1300	NAI	C3D-C4D	-9.05	1.29	1.53
2	B	2300	NAI	C3D-C4D	-9.04	1.29	1.53
2	B	2300	NAI	O4D-C1D	-9.03	1.20	1.42
2	C	3300	NAI	PA-O1A	8.99	1.82	1.50
2	D	4300	NAI	PA-O1A	8.98	1.82	1.50
2	A	1300	NAI	PA-O1A	8.97	1.82	1.50
2	B	2300	NAI	PA-O1A	8.96	1.82	1.50
2	E	5300	NAI	C2A-N3A	8.93	1.46	1.32
2	A	1300	NAI	C1D-N1N	7.86	1.68	1.46
2	E	5300	NAI	O3D-C3D	-7.81	1.24	1.43
2	C	3300	NAI	C7N-N7N	7.55	1.53	1.33
2	B	2300	NAI	C7N-N7N	7.55	1.53	1.33
2	E	5300	NAI	C7N-N7N	7.54	1.53	1.33
2	D	4300	NAI	C7N-N7N	7.50	1.53	1.33
2	E	5300	NAI	O5B-C5B	6.95	1.71	1.44
2	A	1300	NAI	PN-O2N	6.81	1.75	1.50
2	E	5300	NAI	PA-O1A	-6.33	1.28	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3300	NAI	C1D-N1N	6.32	1.64	1.46
2	D	4300	NAI	C1D-N1N	6.28	1.64	1.46
2	B	2300	NAI	C1D-N1N	6.27	1.64	1.46
2	E	5300	NAI	C2D-C1D	-6.23	1.33	1.53
2	B	2300	NAI	PA-O2A	5.72	1.82	1.55
2	D	4300	NAI	PA-O2A	5.71	1.82	1.55
2	A	1300	NAI	PA-O2A	5.71	1.82	1.55
2	C	3300	NAI	PA-O2A	5.70	1.82	1.55
2	E	5300	NAI	PN-O5D	-5.51	1.37	1.59
2	E	5300	NAI	PN-O2N	5.03	1.68	1.50
2	A	1300	NAI	C8A-N7A	5.01	1.43	1.34
2	C	3300	NAI	PN-O5D	-4.85	1.39	1.59
2	D	4300	NAI	PN-O5D	-4.84	1.39	1.59
2	B	2300	NAI	PN-O5D	-4.83	1.39	1.59
2	A	1300	NAI	PN-O1N	4.74	1.77	1.55
2	C	3300	NAI	C4A-N3A	-4.49	1.29	1.35
2	A	1300	NAI	C6N-C5N	4.48	1.41	1.33
2	E	5300	NAI	C4A-N3A	-4.48	1.29	1.35
2	B	2300	NAI	C4A-N3A	-4.45	1.29	1.35
2	D	4300	NAI	C4A-N3A	-4.43	1.29	1.35
2	D	4300	NAI	O5B-C5B	4.36	1.61	1.44
2	B	2300	NAI	O5B-C5B	4.35	1.61	1.44
2	C	3300	NAI	O5B-C5B	4.33	1.61	1.44
2	E	5300	NAI	O2D-C2D	-4.30	1.32	1.43
2	C	3300	NAI	O7N-C7N	-4.16	1.14	1.24
2	B	2300	NAI	O7N-C7N	-4.14	1.14	1.24
2	D	4300	NAI	O7N-C7N	-4.14	1.14	1.24
2	A	1300	NAI	C4N-C5N	-4.06	1.38	1.48
2	E	5300	NAI	C5D-C4D	-4.04	1.39	1.51
2	A	1300	NAI	C5A-C4A	-3.84	1.30	1.40
2	B	2300	NAI	C6N-N1N	3.77	1.46	1.37
2	C	3300	NAI	C6N-N1N	3.77	1.46	1.37
2	D	4300	NAI	C6N-N1N	3.76	1.46	1.37
2	E	5300	NAI	C6N-N1N	3.71	1.46	1.37
2	D	4300	NAI	PA-O5B	-3.59	1.44	1.59
2	B	2300	NAI	PA-O5B	-3.58	1.44	1.59
2	C	3300	NAI	PA-O5B	-3.57	1.44	1.59
2	A	1300	NAI	PA-O5B	-3.47	1.45	1.59
3	C	3301	GLU	CB-CG	3.46	1.63	1.52
3	B	2301	GLU	CB-CG	3.46	1.63	1.52
3	A	1301	GLU	CB-CG	3.46	1.63	1.52
2	A	1300	NAI	C6N-N1N	3.40	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5301	GLU	OXT-C	-3.28	1.19	1.30
3	D	4301	GLU	OXT-C	-3.25	1.19	1.30
3	C	3301	GLU	OXT-C	-3.22	1.20	1.30
2	A	1300	NAI	C7N-N7N	3.21	1.41	1.33
3	B	2301	GLU	OXT-C	-3.20	1.20	1.30
2	A	1300	NAI	C4N-C3N	-2.86	1.44	1.49
2	E	5300	NAI	C5A-N7A	2.80	1.47	1.38
2	C	3300	NAI	C5A-N7A	2.80	1.47	1.38
2	D	4300	NAI	C5A-N7A	2.78	1.47	1.38
2	B	2300	NAI	C5A-N7A	2.76	1.47	1.38
2	D	4300	NAI	C2N-C3N	2.73	1.42	1.34
2	C	3300	NAI	C2N-C3N	2.73	1.42	1.34
2	E	5300	NAI	O4D-C4D	-2.73	1.38	1.45
2	B	2300	NAI	C2N-C3N	2.72	1.42	1.34
2	E	5300	NAI	C2N-C3N	2.71	1.42	1.34
2	E	5300	NAI	PA-O5B	2.70	1.70	1.59
2	D	4300	NAI	C2A-N3A	2.65	1.36	1.32
2	B	2300	NAI	C2A-N3A	2.64	1.36	1.32
2	A	1300	NAI	C2A-N3A	2.61	1.36	1.32
2	C	3300	NAI	C2A-N3A	2.61	1.36	1.32
2	B	2300	NAI	O4B-C4B	2.44	1.50	1.45
2	A	1300	NAI	O4B-C4B	2.43	1.50	1.45
2	C	3300	NAI	C2D-C3D	-2.42	1.46	1.53
2	D	4300	NAI	O4B-C4B	2.40	1.50	1.45
2	B	2300	NAI	C2D-C3D	-2.40	1.46	1.53
2	E	5300	NAI	O4B-C4B	2.39	1.50	1.45
2	C	3300	NAI	O4B-C4B	2.39	1.50	1.45
2	A	1300	NAI	C2D-C3D	-2.38	1.46	1.53
2	C	3300	NAI	C2B-C3B	-2.36	1.46	1.53
2	D	4300	NAI	C2D-C3D	-2.36	1.46	1.53
2	A	1300	NAI	C2B-C3B	-2.35	1.46	1.53
2	B	2300	NAI	C2B-C3B	-2.33	1.47	1.53
2	D	4300	NAI	C2B-C3B	-2.31	1.47	1.53
2	E	5300	NAI	C2B-C3B	-2.30	1.47	1.53
2	D	4300	NAI	C5D-C4D	2.29	1.58	1.51
2	E	5300	NAI	PN-O1N	2.20	1.65	1.55
2	D	4300	NAI	C6A-N1A	2.13	1.36	1.32
2	C	3300	NAI	C6A-N1A	2.11	1.36	1.32
2	A	1300	NAI	C6A-N1A	2.09	1.36	1.32
2	B	2300	NAI	C6A-N1A	2.07	1.36	1.32
2	B	2300	NAI	O5D-C5D	2.04	1.52	1.44
2	A	1300	NAI	O5B-C5B	-2.02	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5300	NAI	C6A-N1A	2.01	1.36	1.32

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1300	NAI	C1B-N9A-C4A	20.66	162.94	126.64
2	E	5300	NAI	C1D-N1N-C6N	-19.23	79.40	120.83
2	E	5300	NAI	C1D-N1N-C2N	18.54	151.99	121.11
3	C	3301	GLU	CB-CG-CD	16.54	156.40	112.51
3	B	2301	GLU	CB-CG-CD	16.53	156.38	112.51
3	A	1301	GLU	CB-CG-CD	16.53	156.37	112.51
2	E	5300	NAI	O4D-C1D-N1N	15.13	137.63	108.06
2	A	1300	NAI	O4D-C1D-N1N	14.55	136.50	108.06
2	C	3300	NAI	O4B-C1B-C2B	-12.81	88.20	106.93
2	B	2300	NAI	O4B-C1B-C2B	-12.81	88.21	106.93
2	E	5300	NAI	O4B-C1B-C2B	-12.78	88.24	106.93
2	D	4300	NAI	O4B-C1B-C2B	-12.77	88.26	106.93
2	A	1300	NAI	O7N-C7N-N7N	-12.54	93.56	122.88
2	A	1300	NAI	C3N-C7N-N7N	11.70	138.46	117.67
2	B	2300	NAI	O4D-C1D-N1N	11.04	129.64	108.06
2	D	4300	NAI	O4D-C1D-N1N	11.03	129.63	108.06
2	C	3300	NAI	O4D-C1D-N1N	11.02	129.61	108.06
2	A	1300	NAI	O4B-C1B-C2B	-9.23	93.44	106.93
2	E	5300	NAI	PN-O3-PA	9.00	163.71	132.83
2	B	2300	NAI	PN-O3-PA	8.30	161.32	132.83
2	C	3300	NAI	PN-O3-PA	8.30	161.31	132.83
2	D	4300	NAI	PN-O3-PA	8.28	161.25	132.83
2	D	4300	NAI	O2A-PA-O5B	8.13	145.51	107.75
2	B	2300	NAI	O2A-PA-O5B	8.12	145.46	107.75
2	C	3300	NAI	O2A-PA-O5B	8.12	145.45	107.75
2	A	1300	NAI	O4B-C4B-C3B	-8.09	89.11	105.11
2	B	2300	NAI	O4B-C4B-C3B	-8.07	89.14	105.11
2	C	3300	NAI	O4B-C4B-C3B	-8.05	89.19	105.11
2	E	5300	NAI	O4B-C4B-C3B	-8.04	89.21	105.11
2	D	4300	NAI	O4B-C4B-C3B	-8.03	89.21	105.11
2	D	4300	NAI	O5B-C5B-C4B	7.78	135.77	108.99
2	B	2300	NAI	O5B-C5B-C4B	7.77	135.75	108.99
2	C	3300	NAI	O5B-C5B-C4B	7.77	135.73	108.99
2	A	1300	NAI	C4D-O4D-C1D	7.68	126.43	109.47
2	D	4300	NAI	C4D-O4D-C1D	7.67	126.39	109.47
2	B	2300	NAI	C4D-O4D-C1D	7.66	126.38	109.47
2	C	3300	NAI	C4D-O4D-C1D	7.64	126.34	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2300	NAI	C1B-N9A-C4A	-7.60	113.28	126.64
2	C	3300	NAI	C1B-N9A-C4A	-7.60	113.30	126.64
2	D	4300	NAI	C1B-N9A-C4A	-7.58	113.32	126.64
2	A	1300	NAI	O2A-PA-O5B	7.47	142.46	107.75
2	A	1300	NAI	C2D-C1D-N1N	7.12	131.15	113.30
2	E	5300	NAI	O5B-PA-O1A	6.69	135.21	109.07
2	D	4300	NAI	O4D-C1D-C2D	-6.58	92.31	106.64
2	A	1300	NAI	O4D-C1D-C2D	-6.57	92.32	106.64
2	B	2300	NAI	O4D-C1D-C2D	-6.57	92.32	106.64
2	C	3300	NAI	O4D-C1D-C2D	-6.57	92.32	106.64
2	C	3300	NAI	C5B-C4B-C3B	6.41	139.20	115.18
2	B	2300	NAI	C5B-C4B-C3B	6.41	139.18	115.18
2	D	4300	NAI	C5B-C4B-C3B	6.40	139.18	115.18
2	E	5300	NAI	C5D-C4D-C3D	6.30	138.80	115.18
2	E	5300	NAI	O4B-C4B-C5B	-6.27	88.75	109.37
2	E	5300	NAI	O1N-PN-O2N	-5.81	83.50	112.24
2	E	5300	NAI	PN-O5D-C5D	5.48	153.84	121.68
2	E	5300	NAI	O5B-C5B-C4B	5.39	127.53	108.99
2	E	5300	NAI	N1A-C2A-N3A	-5.15	121.06	127.65
2	E	5300	NAI	PA-O5B-C5B	-5.09	91.82	121.68
2	E	5300	NAI	C1B-N9A-C4A	5.08	135.56	126.64
2	D	4300	NAI	O5D-C5D-C4D	-5.06	91.57	108.99
2	C	3300	NAI	C5D-C4D-C3D	4.98	133.84	115.18
2	D	4300	NAI	C5D-C4D-C3D	4.92	133.60	115.18
2	C	3300	NAI	O2A-PA-O1A	-4.82	88.42	112.24
2	B	2300	NAI	O2A-PA-O1A	-4.82	88.42	112.24
2	D	4300	NAI	O2A-PA-O1A	-4.82	88.43	112.24
2	A	1300	NAI	O2A-PA-O1A	-4.82	88.43	112.24
2	A	1300	NAI	O5B-PA-O1A	-4.69	90.75	109.07
2	C	3300	NAI	O5D-C5D-C4D	-4.68	92.90	108.99
2	B	2300	NAI	C5D-C4D-C3D	4.62	132.49	115.18
3	D	4301	GLU	OXT-C-O	-4.53	113.81	124.09
2	D	4300	NAI	O5B-PA-O1A	-4.47	91.61	109.07
2	C	3300	NAI	O5B-PA-O1A	-4.46	91.63	109.07
2	B	2300	NAI	O5B-PA-O1A	-4.46	91.63	109.07
2	A	1300	NAI	O1N-PN-O2N	-4.41	90.44	112.24
2	E	5300	NAI	C5B-C4B-C3B	-4.40	98.70	115.18
2	A	1300	NAI	O4D-C4D-C5D	4.31	123.57	109.37
2	A	1300	NAI	C3B-C2B-C1B	4.26	107.39	100.98
2	B	2300	NAI	O4B-C4B-C5B	-4.20	95.55	109.37
2	D	4300	NAI	O4B-C4B-C5B	-4.20	95.57	109.37
2	C	3300	NAI	O4B-C4B-C5B	-4.19	95.58	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2300	NAI	O5D-C5D-C4D	-4.14	94.75	108.99
2	C	3300	NAI	O1N-PN-O5D	4.13	126.93	107.75
2	D	4300	NAI	O1N-PN-O5D	4.12	126.90	107.75
2	B	2300	NAI	O1N-PN-O5D	4.12	126.90	107.75
2	E	5300	NAI	O7N-C7N-N7N	-3.88	113.81	122.88
2	A	1300	NAI	C1D-N1N-C2N	-3.80	114.79	121.11
2	A	1300	NAI	PA-O5B-C5B	-3.66	100.20	121.68
2	B	2300	NAI	O1N-PN-O2N	-3.61	94.41	112.24
2	C	3300	NAI	O1N-PN-O2N	-3.61	94.41	112.24
2	D	4300	NAI	O1N-PN-O2N	-3.60	94.47	112.24
2	A	1300	NAI	O7N-C7N-C3N	3.54	127.57	120.90
3	E	5301	GLU	O-C-CA	-3.54	109.64	122.14
2	A	1300	NAI	O5B-C5B-C4B	3.48	120.96	108.99
2	E	5300	NAI	C6A-N1A-C2A	3.40	120.71	115.84
2	E	5300	NAI	O2A-PA-O5B	-3.36	92.14	107.75
2	A	1300	NAI	PN-O5D-C5D	3.32	141.13	121.68
2	E	5300	NAI	O4D-C4D-C3D	3.20	111.44	105.11
2	A	1300	NAI	C5D-C4D-C3D	3.19	127.14	115.18
3	E	5301	GLU	OXT-C-CA	3.02	123.67	113.38
3	B	2301	GLU	OXT-C-CA	3.02	123.66	113.38
3	D	4301	GLU	OXT-C-CA	3.01	123.64	113.38
3	C	3301	GLU	OXT-C-CA	3.00	123.60	113.38
2	A	1300	NAI	C5B-C4B-C3B	2.98	126.35	115.18
2	E	5300	NAI	O2A-PA-O1A	2.94	126.79	112.24
2	C	3300	NAI	C3N-C2N-N1N	-2.90	118.95	123.10
2	D	4300	NAI	C3N-C2N-N1N	-2.88	118.99	123.10
2	B	2300	NAI	C3N-C2N-N1N	-2.87	119.00	123.10
2	B	2300	NAI	O4D-C4D-C5D	2.85	118.77	109.37
2	E	5300	NAI	C3N-C2N-N1N	-2.85	119.03	123.10
2	C	3300	NAI	C1D-N1N-C6N	-2.83	114.74	120.83
2	B	2300	NAI	C1D-N1N-C6N	-2.82	114.75	120.83
2	D	4300	NAI	C1D-N1N-C6N	-2.80	114.80	120.83
2	A	1300	NAI	O1N-PN-O5D	-2.62	95.56	107.75
2	E	5300	NAI	C3D-C2D-C1D	2.55	106.28	101.43
2	E	5300	NAI	O7N-C7N-C3N	2.52	125.65	120.90
2	D	4300	NAI	O4D-C4D-C5D	2.49	117.58	109.37
2	E	5300	NAI	O3D-C3D-C4D	-2.48	103.87	111.05
2	E	5300	NAI	O5D-C5D-C4D	2.47	117.50	108.99
2	E	5300	NAI	O3D-C3D-C2D	2.45	119.73	111.82
2	C	3300	NAI	O4D-C4D-C5D	2.44	117.41	109.37
2	E	5300	NAI	O2D-C2D-C3D	-2.38	104.11	111.82
2	E	5300	NAI	O2D-C2D-C1D	2.38	117.97	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3300	NAI	C3B-C2B-C1B	2.32	104.47	100.98
2	E	5300	NAI	C3B-C2B-C1B	2.32	104.47	100.98
2	D	4300	NAI	C3B-C2B-C1B	2.31	104.45	100.98
2	B	2300	NAI	C3B-C2B-C1B	2.30	104.44	100.98
2	E	5300	NAI	C2D-C3D-C4D	2.04	106.60	102.64
2	A	1300	NAI	O4B-C4B-C5B	-2.01	102.76	109.37

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1300	NAI	C4D
2	A	1300	NAI	C1D
2	B	2300	NAI	C4D
2	C	3300	NAI	C4D
2	D	4300	NAI	C4D
2	E	5300	NAI	C4D
2	E	5300	NAI	C1B
2	E	5300	NAI	C1D

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1300	NAI	C5B-O5B-PA-O2A
2	A	1300	NAI	C5B-O5B-PA-O3
2	A	1300	NAI	O4B-C4B-C5B-O5B
2	A	1300	NAI	C3B-C4B-C5B-O5B
2	A	1300	NAI	C5D-O5D-PN-O3
2	A	1300	NAI	C5D-O5D-PN-O1N
2	A	1300	NAI	C4D-C5D-O5D-PN
2	A	1300	NAI	C3D-C4D-C5D-O5D
2	A	1300	NAI	C2D-C1D-N1N-C2N
2	B	2300	NAI	C5B-O5B-PA-O1A
2	B	2300	NAI	C5B-O5B-PA-O2A
2	B	2300	NAI	C4B-C5B-O5B-PA
2	B	2300	NAI	C5D-O5D-PN-O3
2	B	2300	NAI	C5D-O5D-PN-O1N
2	B	2300	NAI	C5D-O5D-PN-O2N
2	B	2300	NAI	C4D-C5D-O5D-PN
2	B	2300	NAI	C3D-C4D-C5D-O5D
2	C	3300	NAI	C5B-O5B-PA-O1A
2	C	3300	NAI	C5B-O5B-PA-O2A
2	C	3300	NAI	C4B-C5B-O5B-PA

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Mol	Chain	Res	Type	Atoms
2	C	3300	NAI	C5D-O5D-PN-O3
2	C	3300	NAI	C5D-O5D-PN-O1N
2	C	3300	NAI	C5D-O5D-PN-O2N
2	C	3300	NAI	C4D-C5D-O5D-PN
2	C	3300	NAI	C3D-C4D-C5D-O5D
2	D	4300	NAI	C5B-O5B-PA-O1A
2	D	4300	NAI	C5B-O5B-PA-O2A
2	D	4300	NAI	C4B-C5B-O5B-PA
2	D	4300	NAI	C5D-O5D-PN-O3
2	D	4300	NAI	C5D-O5D-PN-O1N
2	D	4300	NAI	C5D-O5D-PN-O2N
2	D	4300	NAI	C4D-C5D-O5D-PN
2	D	4300	NAI	C3D-C4D-C5D-O5D
2	E	5300	NAI	C4B-C5B-O5B-PA
3	A	1301	GLU	O-C-CA-N
3	A	1301	GLU	CA-CB-CG-CD
3	B	2301	GLU	O-C-CA-N
3	B	2301	GLU	CA-CB-CG-CD
3	C	3301	GLU	O-C-CA-N
3	C	3301	GLU	CA-CB-CG-CD
2	A	1300	NAI	O4D-C1D-N1N-C2N
2	B	2300	NAI	O4D-C1D-N1N-C2N
2	C	3300	NAI	O4D-C1D-N1N-C2N
2	D	4300	NAI	O4D-C1D-N1N-C2N
3	B	2301	GLU	OXT-C-CA-N
3	C	3301	GLU	OXT-C-CA-N
3	D	4301	GLU	OXT-C-CA-N
3	E	5301	GLU	OXT-C-CA-N
2	A	1300	NAI	C2D-C1D-N1N-C6N
2	E	5300	NAI	C2D-C1D-N1N-C6N
3	A	1301	GLU	OXT-C-CA-N
2	E	5300	NAI	O4B-C4B-C5B-O5B
2	E	5300	NAI	C3D-C4D-C5D-O5D
2	E	5300	NAI	C4D-C5D-O5D-PN
2	B	2300	NAI	O4B-C4B-C5B-O5B
2	C	3300	NAI	O4B-C4B-C5B-O5B
2	D	4300	NAI	O4B-C4B-C5B-O5B
2	E	5300	NAI	O4D-C4D-C5D-O5D
2	E	5300	NAI	O4D-C1D-N1N-C2N
2	A	1300	NAI	C4B-C5B-O5B-PA
2	B	2300	NAI	PN-O3-PA-O2A
2	C	3300	NAI	PN-O3-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	D	4300	NAI	PN-O3-PA-O2A
2	A	1300	NAI	C5B-O5B-PA-O1A
2	E	5300	NAI	C5B-O5B-PA-O1A
2	E	5300	NAI	PA-O3-PN-O1N
3	B	2301	GLU	OE2-CD-CG-CB
3	A	1301	GLU	OE2-CD-CG-CB
3	C	3301	GLU	OE2-CD-CG-CB
3	A	1301	GLU	OE1-CD-CG-CB
3	B	2301	GLU	OE1-CD-CG-CB
3	C	3301	GLU	OE1-CD-CG-CB
2	E	5300	NAI	C5B-O5B-PA-O3
2	E	5300	NAI	C3B-C4B-C5B-O5B
2	B	2300	NAI	PA-O3-PN-O1N
2	C	3300	NAI	PA-O3-PN-O1N
2	D	4300	NAI	PA-O3-PN-O1N
2	A	1300	NAI	C5D-O5D-PN-O2N

There are no ring outliers.

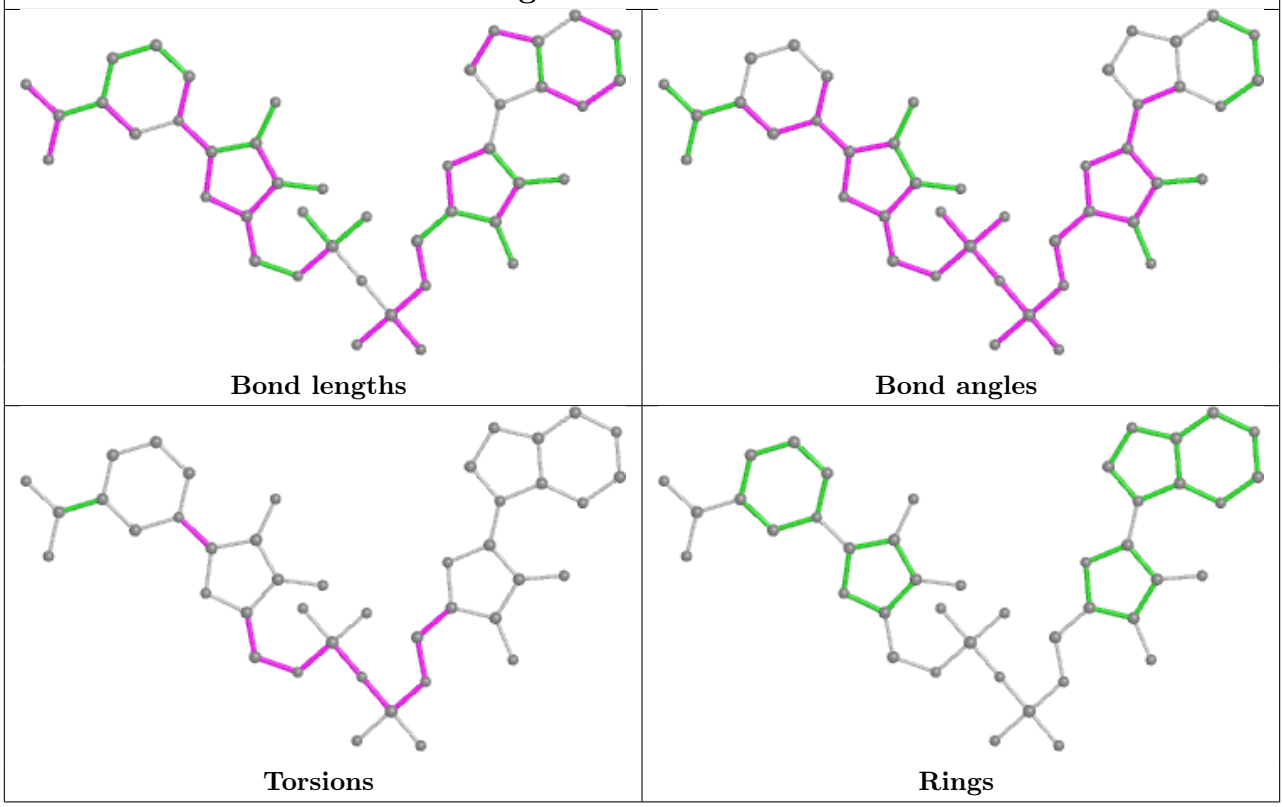
10 monomers are involved in 231 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2301	GLU	17	0
2	D	4300	NAI	40	0
2	E	5300	NAI	32	1
3	D	4301	GLU	21	0
3	A	1301	GLU	8	0
2	C	3300	NAI	39	4
3	C	3301	GLU	12	0
3	E	5301	GLU	11	0
2	A	1300	NAI	26	0
2	B	2300	NAI	67	5

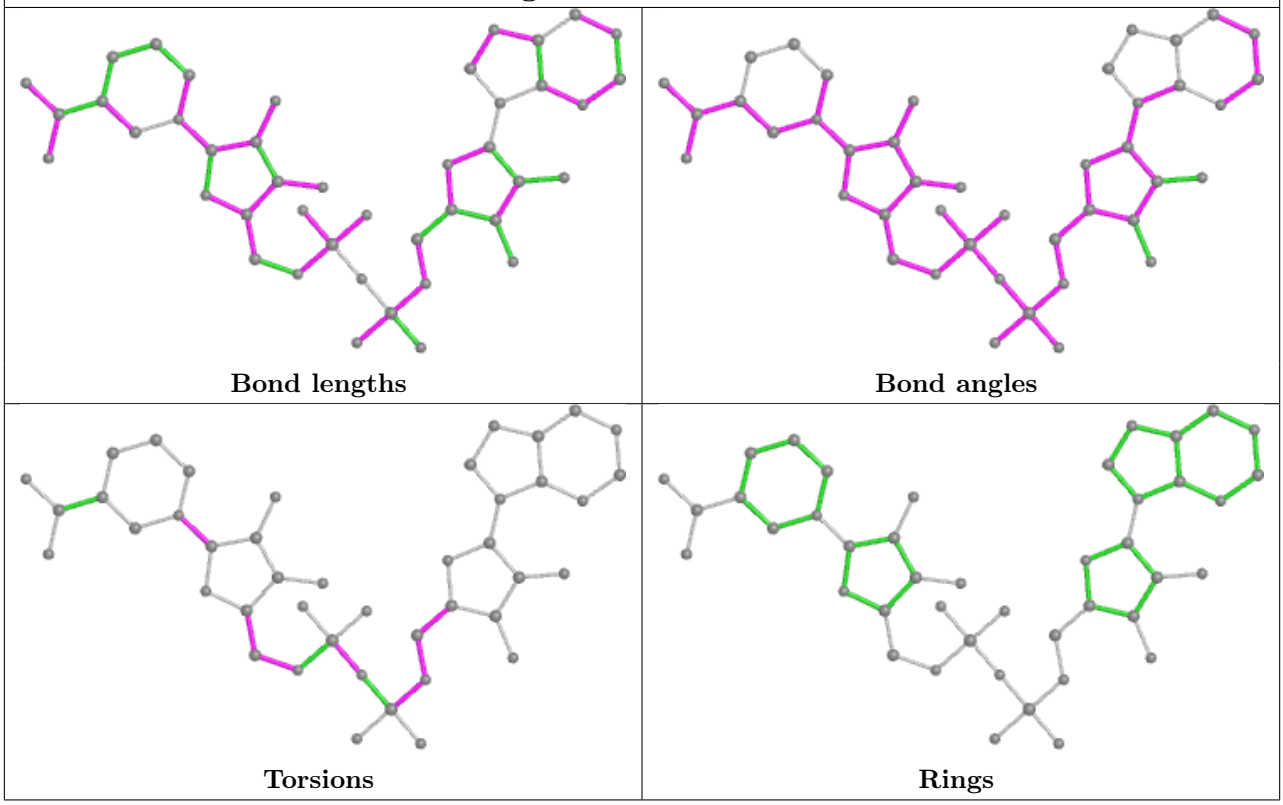
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

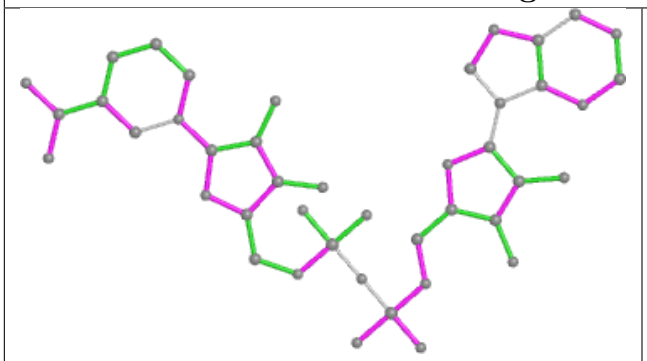
Ligand NAI D 4300



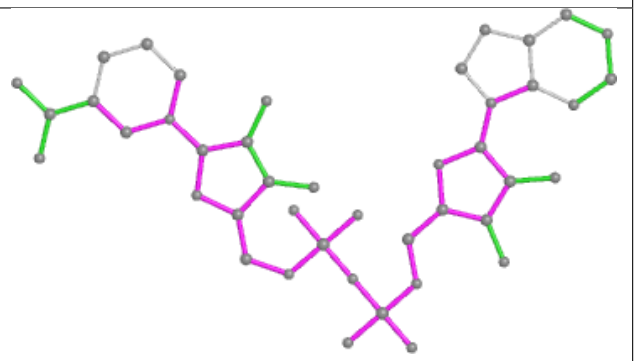
Ligand NAI E 5300



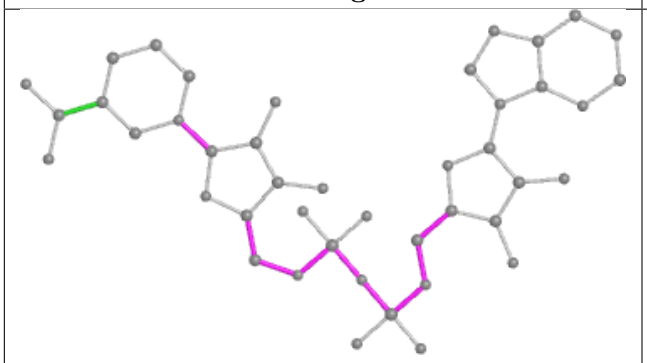
Ligand NAI C 3300



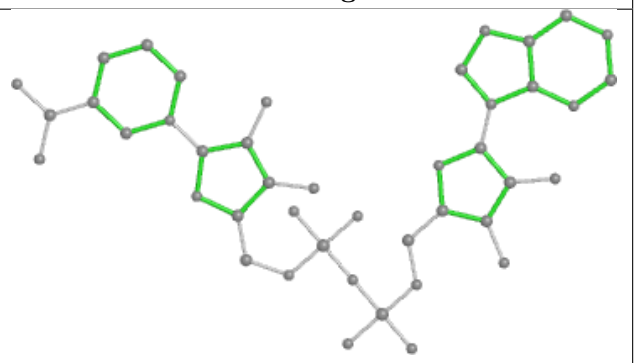
Bond lengths



Bond angles

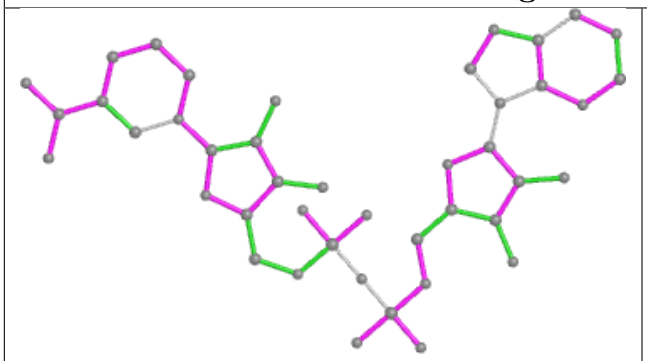


Torsions

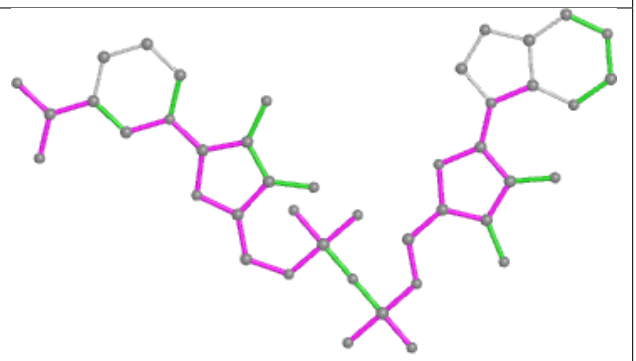


Rings

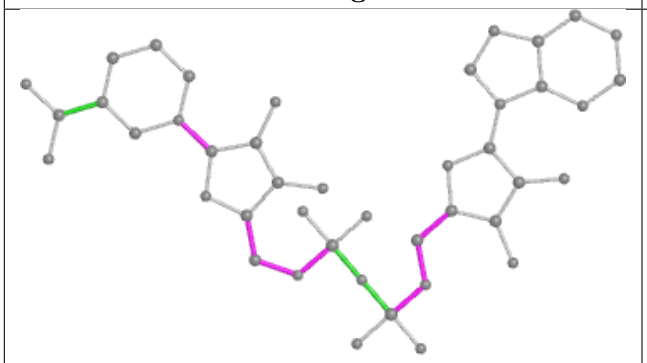
Ligand NAI A 1300



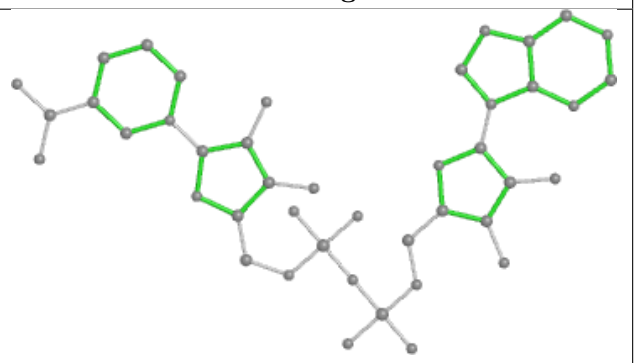
Bond lengths



Bond angles

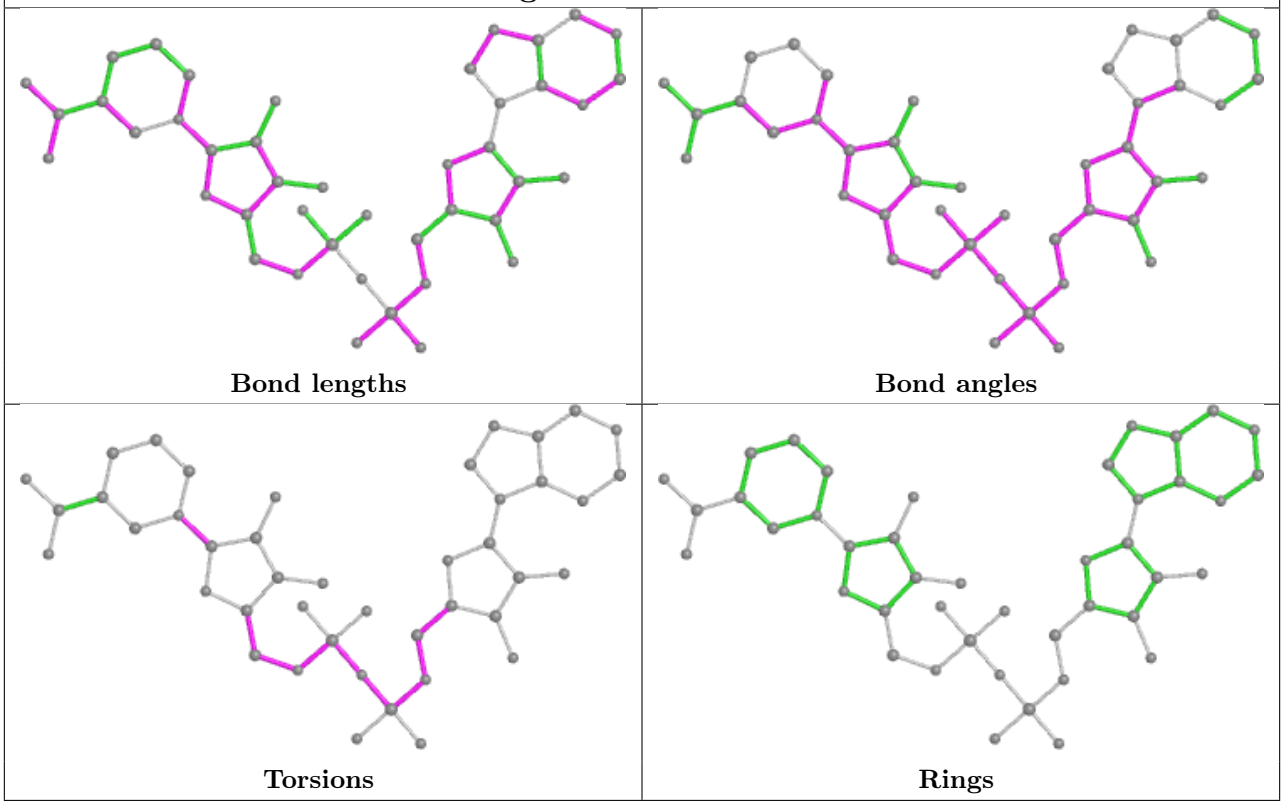


Torsions



Rings

Ligand NAI B 2300



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	277/277 (100%)	-0.36	1 (0%)	92	84	32, 82, 117, 153	0
1	B	276/277 (99%)	0.11	23 (8%)	11	4	39, 129, 183, 200	0
1	C	277/277 (100%)	0.12	20 (7%)	15	6	31, 125, 181, 195	0
1	D	277/277 (100%)	-0.43	2 (0%)	87	75	34, 76, 118, 191	0
1	E	277/277 (100%)	-0.40	5 (1%)	68	47	24, 80, 128, 142	0
All	All	1384/1385 (99%)	-0.19	51 (3%)	41	21	24, 87, 168, 200	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	275	GLU	4.8
1	C	95	CYS	4.7
1	C	36	ASP	4.7
1	C	32	ALA	4.6
1	C	274	GLN	3.7
1	B	52	LEU	3.6
1	C	275	GLU	3.6
1	B	93	VAL	3.6
1	B	38	ASP	3.5
1	B	24	VAL	3.5
1	C	94	SER	3.4
1	B	39	LEU	3.3
1	B	36	ASP	3.3
1	C	39	LEU	3.2
1	B	62	HIS	3.0
1	B	41	THR	3.0
1	C	93	VAL	2.8
1	E	39	LEU	2.7
1	C	96	ALA	2.7
1	C	64	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	66	LEU	2.6
1	C	54	PRO	2.6
1	C	146	GLY	2.6
1	B	136	ALA	2.5
1	B	47	LYS	2.5
1	E	272	ALA	2.5
1	B	67	PHE	2.4
1	C	25	LEU	2.4
1	B	35	PRO	2.4
1	B	34	SER	2.4
1	C	47	LYS	2.4
1	A	275	GLU	2.4
1	E	73	HIS	2.4
1	B	116	ARG	2.3
1	B	28	HIS	2.3
1	C	52	LEU	2.3
1	B	80	ASP	2.3
1	C	143	VAL	2.3
1	C	138	GLY	2.3
1	E	95	CYS	2.2
1	E	143	VAL	2.2
1	B	43	SER	2.2
1	B	55	HIS	2.1
1	B	122	THR	2.1
1	C	78	ILE	2.1
1	C	145	ASP	2.1
1	B	113	PRO	2.1
1	B	95	CYS	2.1
1	D	274	GLN	2.0
1	B	76	PRO	2.0
1	B	274	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

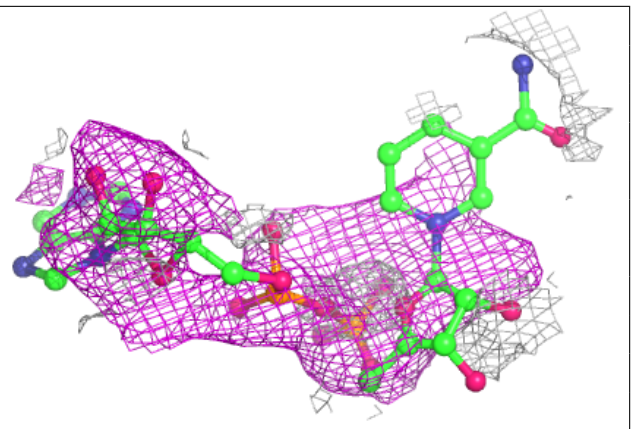
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

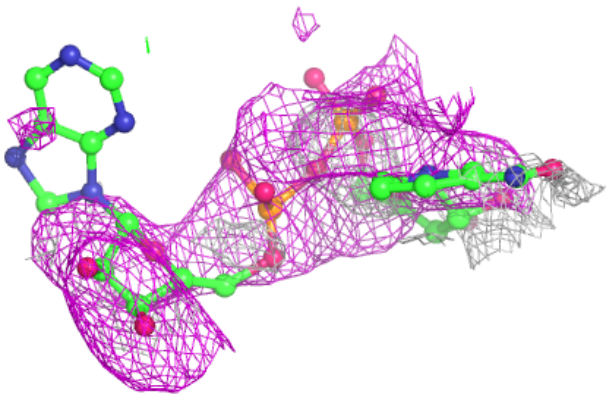
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLU	C	3301	10/10	0.09	1.45	200,200,200,200	0
3	GLU	B	2301	10/10	0.41	0.87	192,200,200,200	0
2	NAI	C	3300	43/44	0.54	0.97	189,195,195,195	0
3	GLU	D	4301	10/10	0.58	0.73	182,193,196,198	0
3	GLU	A	1301	10/10	0.64	0.61	120,131,140,140	0
2	NAI	B	2300	43/44	0.66	0.73	192,195,195,195	0
2	NAI	D	4300	43/44	0.74	0.65	81,91,95,95	0
2	NAI	A	1300	43/44	0.78	0.57	63,93,95,95	0
3	GLU	E	5301	10/10	0.78	0.56	195,200,200,200	0
2	NAI	E	5300	43/44	0.80	0.54	69,94,95,95	0

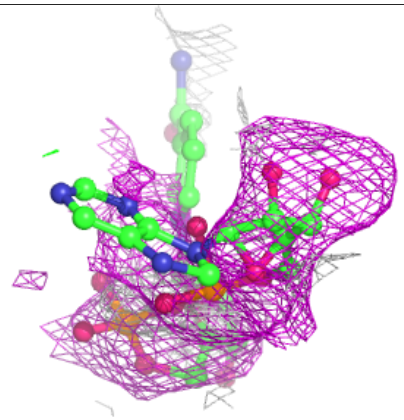
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI C 3300:

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

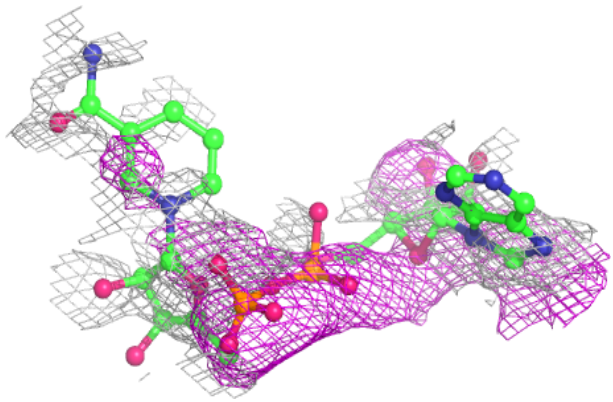


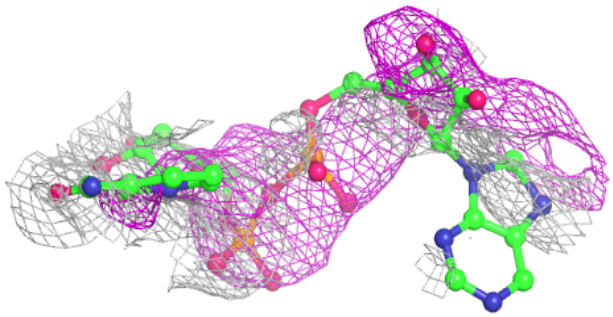


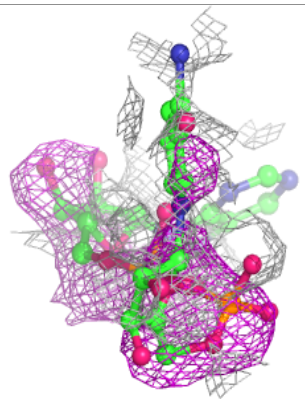


Electron density around NAI B 2300:

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

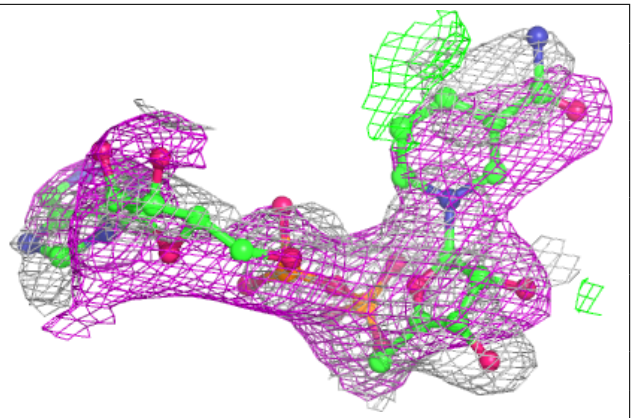


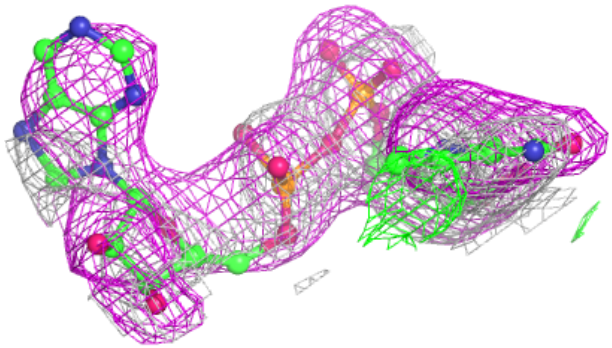


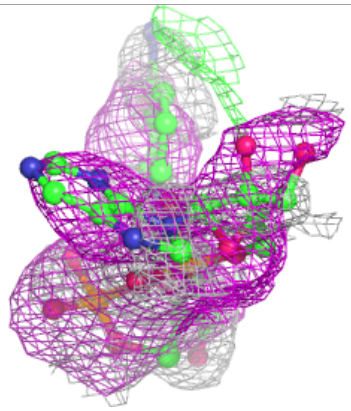


Electron density around NAI D 4300:

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

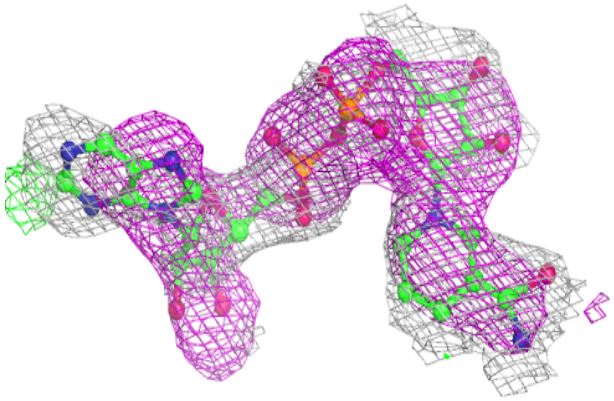


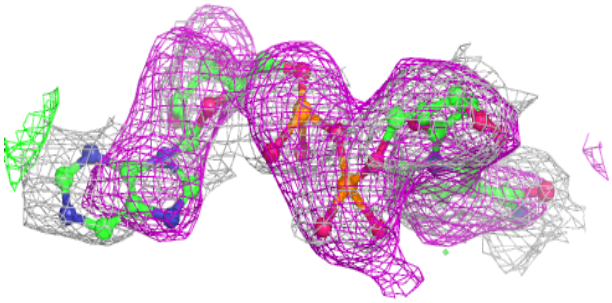


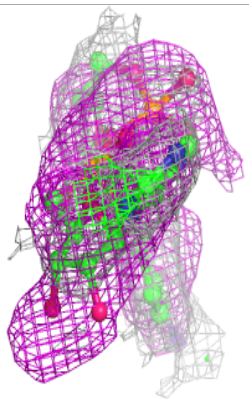


Electron density around NAI A 1300:

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

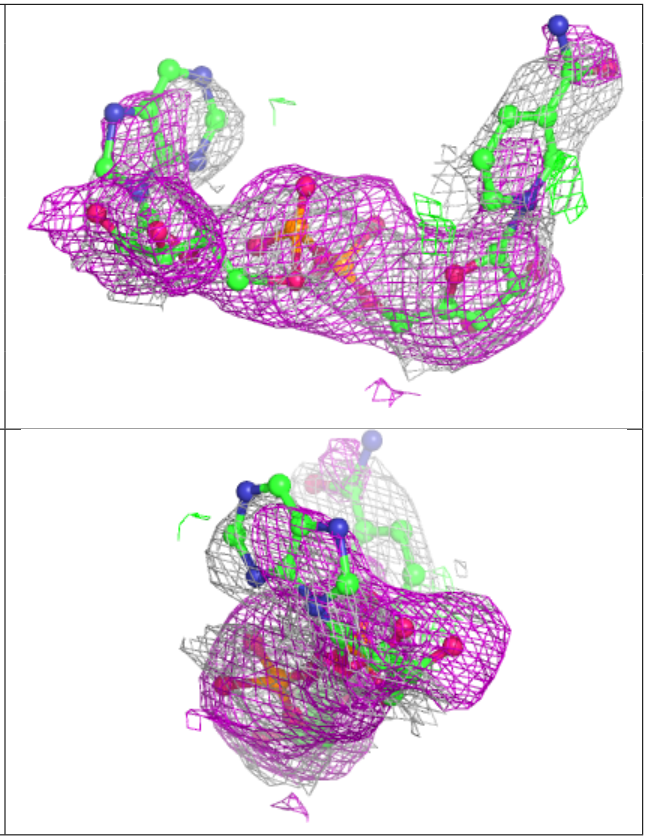






Electron density around NAI E 5300:

$2mF_o$-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 (i)

There are no such residues in this entry.