Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 05:48 PM EDT

PDB ID	:	3T35
Title	:	Arabidopsis thaliana dynamin-related protein 1A in postfission state
Authors	:	Yan, L.M.; Ma, Y.Y.; Sun, Y.N.; Lou, Z.Y.
Deposited on	:	2011-07-24
Resolution	:	3.59 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:

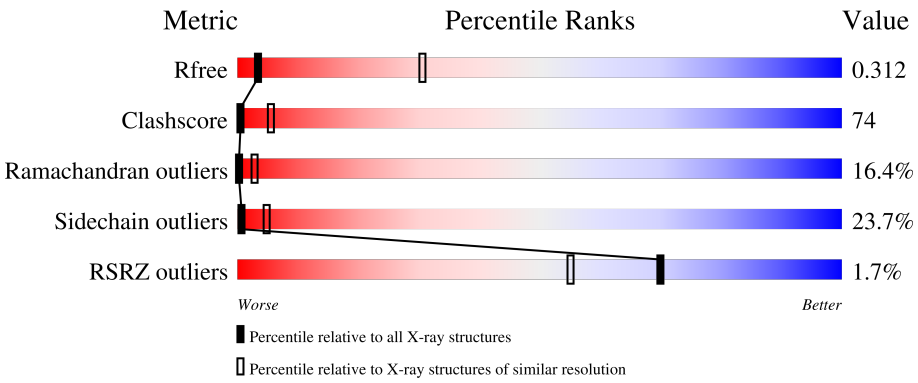
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.59 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	360	2%, 18%, 48%, 25%, •, 6%
1	B	360	2%, 19%, 49%, 23%, •, 6%
1	C	360	21%, 43%, 27%, •, 6%
1	D	360	2%, 18%, 51%, 22%, •, 6%

2 Entry composition (i)

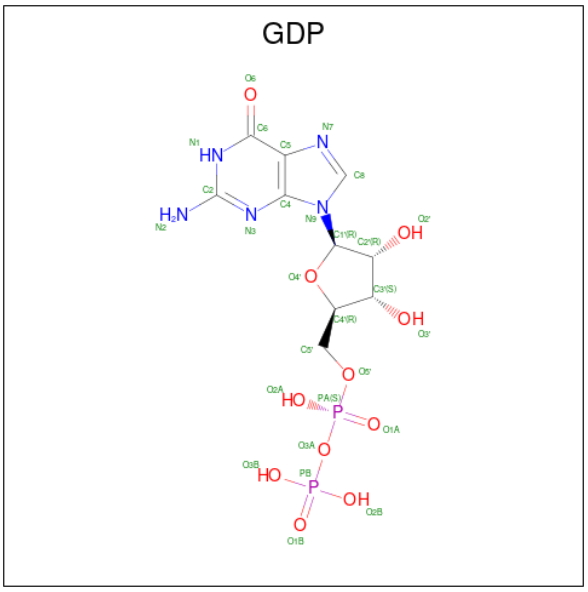
There are 3 unique types of molecules in this entry. The entry contains 11037 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dynamin-related protein 1A, LINKER, Dynamin-related protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	339	2636	1649	472	508	7	0	0	0
1	B	339	2636	1649	472	508	7	0	0	0
1	C	339	2636	1649	472	508	7	0	0	0
1	D	339	2636	1649	472	508	7	0	0	0

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	28	10	5	11	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
2	C	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
2	D	1	28	10	5	11	2	0	0

- Molecule 3 is water.

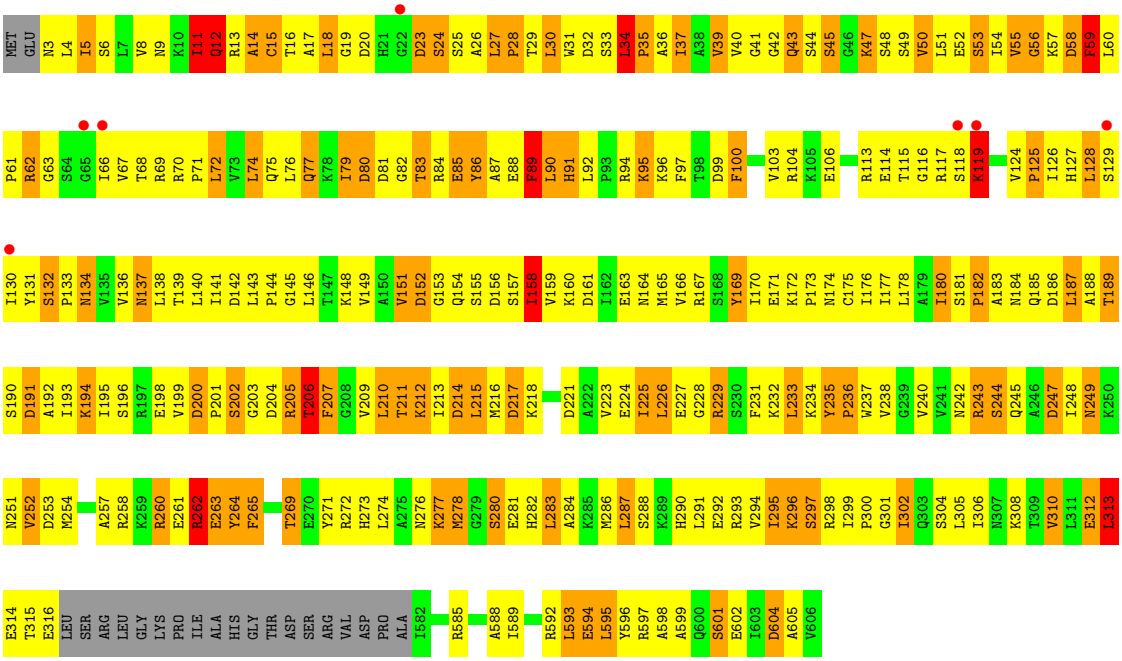
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	87	87	87	0	0
			Total	O		
3	B	121	121	121	0	0
			Total	O		
3	C	93	93	93	0	0
			Total	O		
3	D	80	80	80	0	0

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.

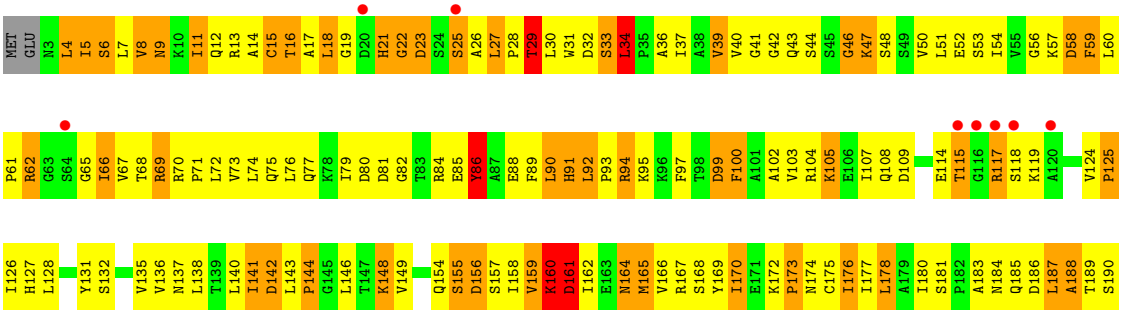
• Molecule 1: Dynamin-related protein 1A, LINKER, Dynamin-related protein 1A

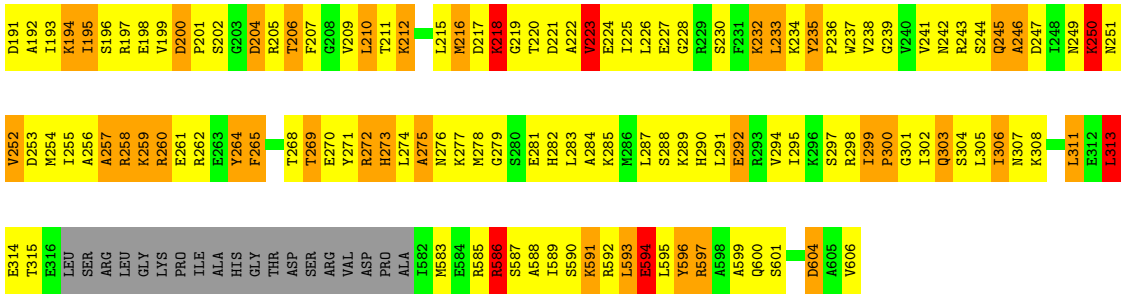
Chain A: 2% 18% 48% 25% 6%



• Molecule 1: Dynamin-related protein 1A, LINKER, Dynamin-related protein 1A

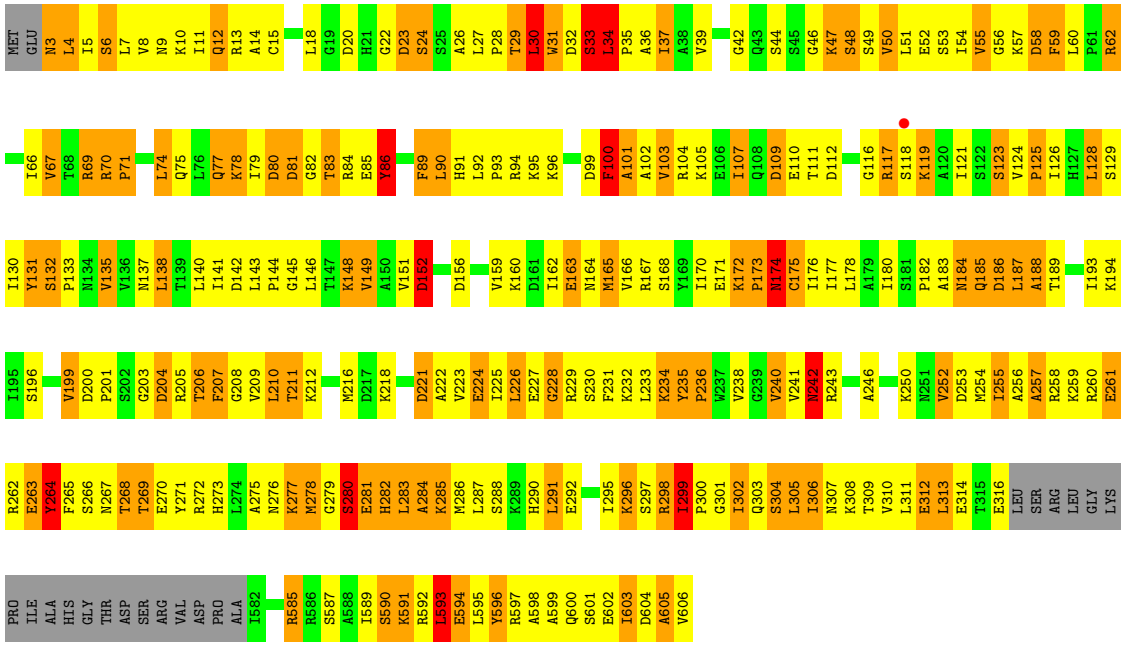
Chain B: 2% 19% 49% 23% 6%





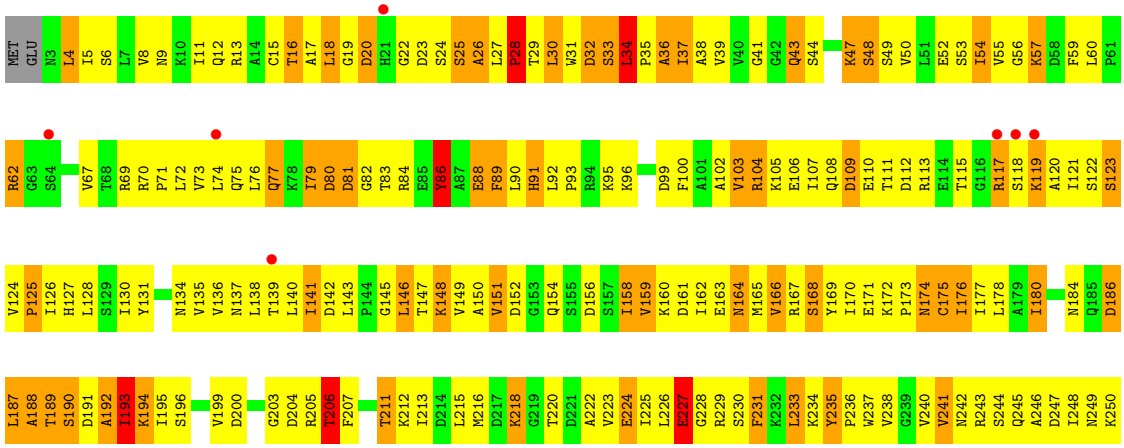
• Molecule 1: Dynamin-related protein 1A, LINKER, Dynamin-related protein 1A

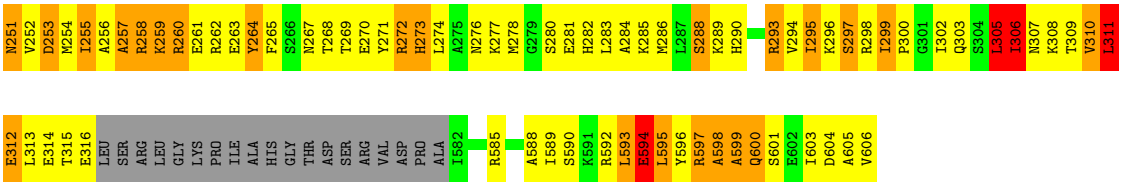
Chain C: 21% 43% 27% • 6%



• Molecule 1: Dynamin-related protein 1A, LINKER, Dynamin-related protein 1A

Chain D: 2% 18% 51% 22% • 6%




M251
V252
D253
M254
I255
A256
A257
R258
K259
R260
E261
R262
E263
Y264
F265
S266
N267
T268
T269
E270
Y271
R272
H273
L274
A275
N276
K277
M278
G279
S280
E281
H282
L283
A284
K285
M286
L287
S288
K289
H290
R293
V294
I295
K296
S297
R298
I299
P300
G301
I302
Q303
S304
L305
I306
N307
K308
T309
V310
L311
E312
L313
E314
T315
E316
LEU
SER
ARG
LEU
GLY
LYS
PRO
ILE
ALA
HIS
GLY
THR
ASP
SER
ARG
VAL
ASP
PRO
ALA
I582
R585
A588
I589
S590
K591
R592
L593
E594
L595
Y596
R597
A598
A599
Q600
S601
E602
I603
D604
A605
V606

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	146.16Å 146.16Å 204.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.32 – 3.59 49.82 – 3.59	Depositor EDS
% Data completeness (in resolution range)	87.2 (43.32-3.59) 98.6 (49.82-3.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.238 , 0.291 0.275 , 0.312	Depositor DCC
R_{free} test set	1449 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	50.3	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 58.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.066 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	11037	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.60% 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: GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.54	0/2671	0.80	3/3605 (0.1%)
1	B	0.60	0/2671	0.86	2/3605 (0.1%)
1	C	0.58	1/2671 (0.0%)	0.78	0/3605
1	D	0.50	0/2671	0.75	2/3605 (0.1%)
All	All	0.56	1/10684 (0.0%)	0.80	7/14420 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	235	TYR	CD1-CE1	-5.48	1.31	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	210	LEU	CA-CB-CG	7.92	133.53	115.30
1	B	311	LEU	CA-CB-CG	7.32	132.14	115.30
1	D	311	LEU	CA-CB-CG	6.19	129.53	115.30
1	B	313	LEU	CA-CB-CG	5.93	128.93	115.30
1	A	313	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	138	LEU	CA-CB-CG	5.34	127.58	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	36	ALA	N-CA-C	-5.34	96.58	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	34	LEU	Peptide
1	D	26	ALA	Peptide
1	D	28	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2636	0	2705	426	0
1	B	2636	0	2705	380	1
1	C	2636	0	2705	407	0
1	D	2636	0	2705	413	1
2	A	28	0	12	7	0
2	B	28	0	12	7	0
2	C	28	0	12	5	0
2	D	28	0	12	7	0
3	A	87	0	0	13	0
3	B	121	0	0	17	0
3	C	93	0	0	33	0
3	D	80	0	0	31	0
All	All	11037	0	10868	1591	1

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 74.

All (1591) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASN:OD1	1:A:277:LYS:HD3	1.27	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:SER:O	1:B:308:LYS:CE	1.86	1.23
1:D:32:ASP:O	1:D:35:PRO:HD3	1.44	1.15
1:B:29:THR:HA	1:B:32:ASP:HB2	1.26	1.15
1:A:276:ASN:OD1	1:A:277:LYS:CD	1.95	1.14
1:D:170:ILE:HG22	1:D:199:VAL:HG11	1.29	1.13
1:A:11:ILE:HG22	1:A:12:GLN:H	1.05	1.12
1:B:313:LEU:HD23	1:B:597:ARG:NH2	1.65	1.11
1:D:16:THR:HA	1:D:20:ASP:H	1.03	1.11
1:B:40:VAL:HG21	1:B:170:ILE:HD11	1.34	1.08
1:B:25:SER:O	1:B:308:LYS:HE3	1.53	1.07
1:D:140:LEU:HA	3:D:675:HOH:O	1.55	1.05
1:D:299:ILE:HG13	1:D:300:PRO:HD3	1.11	1.05
1:B:25:SER:O	1:B:308:LYS:NZ	1.90	1.02
1:B:60:LEU:HD23	1:B:61:PRO:HD2	1.42	1.01
1:C:27:LEU:HB3	1:C:31:TRP:HB2	1.37	1.01
1:D:16:THR:HA	1:D:20:ASP:N	1.76	1.01
1:C:83:THR:HG22	1:C:133:PRO:HG2	1.44	1.00
1:B:43:GLN:HE22	1:B:66:ILE:HB	1.26	1.00
1:A:11:ILE:HG22	1:A:12:GLN:N	1.75	1.00
1:A:92:LEU:HD13	1:A:95:LYS:HE3	1.41	0.99
1:A:23:ASP:HB2	1:A:26:ALA:HB3	1.45	0.99
1:B:92:LEU:HD11	1:B:95:LYS:HB3	1.43	0.99
1:C:66:ILE:HG22	1:C:119:LYS:HD2	1.45	0.99
1:B:313:LEU:HD23	1:B:597:ARG:HH22	1.21	0.99
1:C:42:GLY:HA2	1:C:146:LEU:HB2	1.39	0.98
1:A:183:ALA:HB2	1:A:210:LEU:HD22	1.42	0.98
1:C:189:THR:HA	1:D:148:LYS:HG2	1.45	0.98
1:A:293:ARG:HD3	1:C:306:ILE:HG21	1.46	0.97
1:D:299:ILE:CG1	1:D:300:PRO:HD3	1.94	0.97
1:C:298:ARG:HH11	1:C:298:ARG:HB2	1.26	0.97
1:D:299:ILE:HG13	1:D:300:PRO:CD	1.95	0.95
1:C:305:LEU:O	1:C:307:ASN:N	1.98	0.95
1:D:140:LEU:HD23	3:D:675:HOH:O	1.66	0.94
1:A:12:GLN:O	1:A:15:CYS:HB3	1.68	0.94
1:D:176:ILE:H	1:D:176:ILE:HD12	1.30	0.94
1:B:585:ARG:HE	1:B:589:ILE:HD11	1.31	0.94
1:B:308:LYS:HD3	1:B:311:LEU:HD23	1.47	0.93
1:A:301:GLY:O	1:A:305:LEU:HB2	1.66	0.93
1:D:79:ILE:HD13	1:D:84:ARG:HD2	1.48	0.93
1:D:23:ASP:HB3	1:D:592:ARG:HD3	1.50	0.92
1:A:172:LYS:HE3	1:A:175:CYS:HB3	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:VAL:HG12	1:B:125:PRO:HD2	1.52	0.92
1:B:215:LEU:HD11	2:B:9001:GDP:C2	2.05	0.92
1:D:19:GLY:HA2	1:D:22:GLY:HA2	1.52	0.92
1:D:82:GLY:O	1:D:84:ARG:HG3	1.72	0.90
1:D:39:VAL:HG22	1:D:141:ILE:O	1.72	0.89
1:C:74:LEU:O	1:C:75:GLN:HG3	1.72	0.89
1:D:35:PRO:HA	1:D:174:ASN:O	1.73	0.89
1:A:32:ASP:O	1:A:35:PRO:HD3	1.71	0.89
1:B:39:VAL:HG13	1:B:142:ASP:HA	1.53	0.89
1:C:28:PRO:O	1:C:32:ASP:HB3	1.73	0.89
1:C:255:ILE:O	1:C:259:LYS:HB2	1.73	0.89
1:D:258:ARG:HE	1:D:281:GLU:HG2	1.38	0.89
1:A:234:LYS:HE2	1:C:597:ARG:CZ	2.01	0.89
1:B:212:LYS:HB3	1:B:215:LEU:HD12	1.52	0.89
1:A:238:VAL:HG11	1:A:283:LEU:HD13	1.55	0.88
1:D:75:GLN:HA	3:D:667:HOH:O	1.71	0.88
1:D:77:GLN:HG3	1:D:131:TYR:CE1	2.08	0.88
1:C:74:LEU:HD23	1:C:75:GLN:H	1.37	0.88
1:A:224:GLU:N	1:A:224:GLU:OE1	2.07	0.88
1:B:252:VAL:HG11	1:B:260:ARG:NH2	1.89	0.87
1:A:224:GLU:HG3	1:A:229:ARG:NH1	1.90	0.86
1:B:583:MET:HA	1:B:586:ARG:CZ	2.06	0.86
1:C:596:TYR:O	1:C:599:ALA:HB3	1.76	0.85
1:D:17:ALA:O	1:D:18:LEU:HB2	1.76	0.85
1:A:37:ILE:HG13	1:A:140:LEU:HD23	1.56	0.84
1:D:11:ILE:HG22	3:D:625:HOH:O	1.76	0.84
1:D:193:ILE:HD12	1:D:193:ILE:H	1.40	0.84
1:D:193:ILE:HD12	1:D:193:ILE:N	1.93	0.84
1:D:256:ALA:HA	1:D:259:LYS:HB2	1.58	0.84
1:B:252:VAL:HG11	1:B:260:ARG:HH21	1.43	0.83
1:A:37:ILE:HG22	1:A:176:ILE:HB	1.60	0.83
1:B:174:ASN:HD22	1:B:298:ARG:CD	1.91	0.83
1:A:183:ALA:HB2	1:A:210:LEU:CD2	2.08	0.83
1:B:183:ALA:HB1	1:B:216:MET:HE3	1.59	0.82
1:B:23:ASP:OD2	1:B:26:ALA:HB3	1.80	0.82
1:C:290:HIS:HE1	3:C:673:HOH:O	1.62	0.82
1:B:29:THR:CA	1:B:32:ASP:HB2	2.08	0.82
1:A:302:ILE:C	1:A:304:SER:H	1.80	0.82
1:D:69:ARG:HB3	1:D:121:ILE:HG22	1.61	0.82
1:B:174:ASN:HD22	1:B:298:ARG:HD3	1.41	0.82
1:A:29:THR:C	1:A:31:TRP:H	1.81	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:VAL:HB	1:A:178:LEU:HD23	1.62	0.82
1:B:257:ALA:O	1:B:259:LYS:N	2.13	0.82
1:C:100:PHE:O	1:C:103:VAL:HG23	1.79	0.82
1:A:45:SER:O	1:A:182:PRO:HG3	1.77	0.81
1:A:42:GLY:HA2	1:A:146:LEU:H	1.43	0.81
1:B:5:ILE:HG23	1:B:6:SER:H	1.44	0.81
1:B:58:ASP:HB3	1:B:104:ARG:HH21	1.45	0.81
1:A:209:VAL:O	1:A:210:LEU:HB3	1.79	0.81
1:C:34:LEU:HD13	1:C:36:ALA:HB3	1.63	0.81
1:B:174:ASN:ND2	1:B:298:ARG:HE	1.77	0.81
1:C:276:ASN:OD1	1:C:277:LYS:HG3	1.81	0.81
1:D:224:GLU:OE2	1:D:229:ARG:HD3	1.80	0.80
1:C:234:LYS:O	1:C:235:TYR:CD2	2.34	0.80
1:C:238:VAL:HG11	1:C:283:LEU:HB2	1.63	0.80
1:A:24:SER:HB3	1:A:585:ARG:HH21	1.46	0.80
1:D:27:LEU:O	1:D:31:TRP:N	2.14	0.80
1:C:307:ASN:O	1:C:311:LEU:HG	1.80	0.80
1:A:152:ASP:CG	1:A:153:GLY:H	1.82	0.80
1:C:55:VAL:HG21	1:C:59:PHE:CE2	2.16	0.80
1:C:234:LYS:O	1:C:235:TYR:HD2	1.64	0.80
1:A:588:ALA:O	1:A:592:ARG:HG3	1.82	0.80
1:D:131:TYR:HB2	3:D:640:HOH:O	1.82	0.80
1:D:138:LEU:HD11	1:D:288:SER:OG	1.80	0.80
1:B:34:LEU:HD11	1:B:36:ALA:HB3	1.63	0.80
1:B:159:VAL:HG12	1:B:160:LYS:N	1.94	0.79
1:B:176:ILE:HG22	1:B:177:ILE:H	1.47	0.79
1:B:290:HIS:O	1:B:294:VAL:HG23	1.82	0.79
1:C:69:ARG:HH21	1:C:119:LYS:HD3	1.47	0.79
1:A:15:CYS:HA	1:A:595:LEU:HD21	1.64	0.79
1:B:37:ILE:HD11	1:B:291:LEU:HD22	1.63	0.79
1:B:583:MET:HA	1:B:586:ARG:NE	1.98	0.79
1:D:309:THR:HA	1:D:312:GLU:HB2	1.64	0.79
1:A:133:PRO:HG2	1:A:134:ASN:HD21	1.48	0.78
1:B:92:LEU:HD13	1:B:92:LEU:O	1.83	0.78
1:B:225:ILE:HG12	1:B:230:SER:OG	1.83	0.78
1:C:86:TYR:CE1	1:C:96:LYS:HD2	2.19	0.78
1:D:260:ARG:O	1:D:263:GLU:HB3	1.83	0.78
1:D:169:TYR:O	1:D:175:CYS:SG	2.41	0.78
1:C:183:ALA:HB1	1:C:216:MET:HE3	1.64	0.78
1:D:79:ILE:O	1:D:81:ASP:N	2.16	0.78
1:C:32:ASP:C	1:C:34:LEU:H	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:ILE:O	1:D:166:VAL:HG23	1.84	0.77
1:A:50:VAL:HG13	1:A:242:ASN:HD21	1.48	0.77
1:D:204:ASP:HA	1:D:234:LYS:CD	2.14	0.77
1:A:11:ILE:CG2	1:A:12:GLN:H	1.83	0.77
1:A:29:THR:O	1:A:31:TRP:N	2.18	0.77
1:C:291:LEU:O	1:C:291:LEU:HG	1.83	0.77
1:C:160:LYS:O	1:C:164:ASN:HB2	1.85	0.76
1:D:24:SER:HB2	1:D:592:ARG:NH1	1.99	0.76
1:C:74:LEU:HD23	1:C:75:GLN:N	2.00	0.76
1:C:240:VAL:HG12	1:C:261:GLU:OE2	1.84	0.76
1:C:600:GLN:O	1:C:600:GLN:HG2	1.85	0.76
1:C:302:ILE:HD11	1:C:603:ILE:HB	1.66	0.76
1:A:45:SER:HA	1:A:182:PRO:HG2	1.67	0.76
1:B:149:VAL:HA	3:B:682:HOH:O	1.86	0.75
1:C:66:ILE:CG2	1:C:119:LYS:HD2	2.16	0.75
1:D:282:HIS:O	1:D:282:HIS:ND1	2.19	0.75
1:B:15:CYS:O	1:B:17:ALA:N	2.13	0.75
1:B:606:VAL:HG13	3:B:676:HOH:O	1.85	0.75
1:A:82:GLY:O	1:A:84:ARG:N	2.16	0.75
1:A:276:ASN:HB3	3:A:624:HOH:O	1.86	0.74
1:C:260:ARG:O	1:C:263:GLU:HB2	1.86	0.74
1:B:29:THR:HA	1:B:32:ASP:CB	2.14	0.74
1:C:305:LEU:C	1:C:307:ASN:H	1.90	0.74
1:B:305:LEU:O	1:B:307:ASN:N	2.21	0.74
1:B:178:LEU:O	1:B:180:ILE:HD12	1.87	0.74
1:C:39:VAL:HG22	1:C:142:ASP:HA	1.69	0.74
1:A:29:THR:C	1:A:31:TRP:N	2.41	0.73
1:C:70:ARG:HH11	1:C:126:ILE:HD11	1.52	0.73
1:C:600:GLN:HA	1:C:603:ILE:HG13	1.69	0.73
1:C:137:ASN:O	1:C:138:LEU:HB3	1.88	0.73
1:D:193:ILE:H	1:D:193:ILE:CD1	2.00	0.73
1:C:27:LEU:O	1:C:31:TRP:N	2.21	0.73
1:C:69:ARG:NH2	1:C:119:LYS:HD3	2.03	0.73
1:C:598:ALA:O	1:C:602:GLU:HG3	1.89	0.73
1:D:86:TYR:CE1	1:D:96:LYS:HD3	2.24	0.73
1:B:212:LYS:CB	1:B:215:LEU:HD12	2.18	0.73
1:A:87:ALA:HB2	1:A:130:ILE:HG23	1.71	0.72
1:A:302:ILE:HA	1:A:305:LEU:HB3	1.72	0.72
1:C:27:LEU:HD22	1:C:31:TRP:CD1	2.23	0.72
1:C:39:VAL:CG2	1:C:142:ASP:HA	2.19	0.72
1:A:247:ASP:HB3	1:A:252:VAL:HG21	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:VAL:HG12	1:A:314:GLU:HB2	1.70	0.72
1:D:204:ASP:HA	1:D:234:LYS:HD2	1.71	0.72
1:A:13:ARG:O	1:A:15:CYS:N	2.23	0.72
1:D:307:ASN:HA	1:D:310:VAL:HG12	1.71	0.72
1:D:100:PHE:HA	1:D:103:VAL:HG23	1.71	0.72
1:A:119:LYS:HG3	1:A:154:GLN:HE21	1.53	0.72
1:D:24:SER:HB2	1:D:592:ARG:HH12	1.55	0.72
1:D:141:ILE:HD11	3:D:656:HOH:O	1.88	0.72
1:A:79:ILE:HD11	1:A:132:SER:HA	1.72	0.71
1:C:183:ALA:HB1	1:C:216:MET:CE	2.19	0.71
1:A:27:LEU:HD22	1:A:31:TRP:NE1	2.05	0.71
1:A:190:SER:HB2	1:A:193:ILE:HB	1.71	0.71
1:D:5:ILE:HD12	1:D:137:ASN:O	1.91	0.71
1:D:191:ASP:HB3	1:D:195:ILE:HD12	1.70	0.71
1:A:290:HIS:O	1:A:294:VAL:HG23	1.90	0.71
1:D:8:VAL:HG21	1:D:295:ILE:HD13	1.72	0.71
1:C:94:ARG:HD3	3:C:358:HOH:O	1.90	0.71
1:B:67:VAL:HG11	1:B:108:GLN:HE21	1.55	0.71
1:A:207:PHE:CZ	1:A:235:TYR:CE1	2.79	0.71
1:B:170:ILE:CG2	1:B:199:VAL:HG21	2.21	0.71
1:C:86:TYR:HE1	1:C:96:LYS:HD2	1.53	0.71
1:B:216:MET:HE1	1:B:222:ALA:HB2	1.73	0.71
1:C:22:GLY:HA2	1:C:26:ALA:HB3	1.72	0.71
1:A:70:ARG:NH2	1:A:124:VAL:O	2.23	0.71
1:A:282:HIS:O	1:A:283:LEU:C	2.28	0.71
1:B:294:VAL:O	1:B:298:ARG:HG3	1.90	0.70
1:D:31:TRP:HA	1:D:172:LYS:HE2	1.73	0.70
1:A:27:LEU:N	1:A:28:PRO:CD	2.55	0.70
1:D:80:ASP:O	1:D:82:GLY:N	2.25	0.70
1:D:187:LEU:HB2	1:D:231:PHE:CD2	2.25	0.70
1:A:300:PRO:C	1:A:302:ILE:H	1.95	0.70
1:B:590:SER:O	1:B:594:GLU:HG3	1.91	0.70
1:A:137:ASN:ND2	3:A:659:HOH:O	2.22	0.70
1:D:241:VAL:HG12	1:D:241:VAL:O	1.90	0.70
1:A:6:SER:HB2	3:A:659:HOH:O	1.91	0.70
1:B:6:SER:HB2	1:B:77:GLN:OE1	1.91	0.70
1:A:89:PHE:HE1	1:A:106:GLU:HG2	1.56	0.70
1:C:8:VAL:HG21	1:C:295:ILE:HD13	1.74	0.70
1:D:49:SER:HA	1:D:62:ARG:HH12	1.56	0.70
1:A:234:LYS:HE2	1:C:597:ARG:NE	2.06	0.69
1:B:59:PHE:HD1	1:B:59:PHE:O	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ASP:O	1:B:143:LEU:HD23	1.92	0.69
1:B:303:GLN:HA	1:B:306:ILE:HG22	1.72	0.69
1:A:36:ALA:HB1	1:A:139:THR:HG22	1.74	0.69
1:B:260:ARG:HG3	1:B:261:GLU:N	2.05	0.69
1:A:212:LYS:HG3	2:A:9001:GDP:C5	2.27	0.69
1:C:207:PHE:HD1	1:C:208:GLY:N	1.91	0.69
1:C:309:THR:N	3:C:675:HOH:O	2.24	0.69
1:C:11:ILE:O	1:C:12:GLN:C	2.31	0.69
1:D:192:ALA:HB3	1:D:193:ILE:HD12	1.74	0.69
1:A:182:PRO:HB3	1:A:212:LYS:HD3	1.74	0.69
1:B:67:VAL:HA	1:B:69:ARG:CZ	2.23	0.69
1:C:226:LEU:C	1:C:228:GLY:H	1.96	0.69
1:C:301:GLY:C	1:C:302:ILE:O	2.29	0.69
1:B:13:ARG:HB3	3:B:655:HOH:O	1.92	0.69
1:D:32:ASP:C	1:D:34:LEU:H	1.96	0.69
1:D:299:ILE:O	1:D:302:ILE:HG22	1.93	0.69
1:B:70:ARG:NH2	1:B:124:VAL:H	1.90	0.69
2:C:9001:GDP:PA	3:C:667:HOH:O	2.49	0.69
1:C:225:ILE:HG12	1:C:230:SER:CB	2.23	0.69
1:D:105:LYS:O	1:D:109:ASP:HB2	1.93	0.69
1:A:272:ARG:HG3	1:A:272:ARG:HH11	1.56	0.69
1:D:227:GLU:HG2	1:D:229:ARG:CZ	2.23	0.69
1:D:300:PRO:HB3	1:D:303:GLN:OE1	1.92	0.69
1:A:71:PRO:HB2	1:A:125:PRO:HA	1.76	0.68
1:A:77:GLN:NE2	1:A:137:ASN:HD21	1.91	0.68
1:A:148:LYS:HB2	1:B:194:LYS:HG3	1.74	0.68
1:C:34:LEU:HG	1:C:172:LYS:HE2	1.72	0.68
1:C:55:VAL:HG12	1:C:57:LYS:H	1.58	0.68
1:D:264:TYR:O	1:D:268:THR:HG23	1.93	0.68
1:B:31:TRP:CE3	1:B:172:LYS:HD3	2.28	0.68
1:C:200:ASP:OD2	1:C:206:THR:HB	1.92	0.68
1:A:226:LEU:HD22	1:A:278:MET:HE1	1.75	0.68
1:A:243:ARG:HG2	1:A:247:ASP:HB2	1.75	0.68
1:C:12:GLN:HB3	1:C:75:GLN:HE22	1.58	0.68
1:C:29:THR:O	1:C:33:SER:HB3	1.94	0.68
1:D:30:LEU:O	1:D:30:LEU:HD23	1.93	0.68
1:C:148:LYS:HG2	1:D:189:THR:HA	1.76	0.68
1:C:269:THR:HA	1:C:272:ARG:HB2	1.74	0.68
1:B:90:LEU:HB2	1:B:127:HIS:HB2	1.75	0.68
1:C:57:LYS:HG2	1:C:100:PHE:CE1	2.28	0.68
1:A:23:ASP:CB	1:A:26:ALA:HB3	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLY:HA2	1:A:146:LEU:HB2	1.74	0.68
1:A:63:GLY:HA3	1:A:67:VAL:HG22	1.76	0.68
1:B:56:GLY:O	1:B:57:LYS:HD3	1.92	0.68
1:C:173:PRO:O	1:C:175:CYS:N	2.25	0.68
1:B:34:LEU:CD1	1:B:36:ALA:HB3	2.22	0.68
1:B:253:ASP:HB3	3:B:632:HOH:O	1.91	0.68
1:B:295:ILE:O	1:B:299:ILE:HG22	1.93	0.68
1:C:27:LEU:HB3	1:C:31:TRP:CB	2.21	0.68
1:D:25:SER:O	1:D:28:PRO:HB2	1.93	0.68
1:D:36:ALA:C	3:D:656:HOH:O	2.33	0.68
1:B:143:LEU:HD11	1:B:169:TYR:HD2	1.59	0.68
1:A:126:ILE:HG22	1:A:126:ILE:O	1.94	0.67
1:B:37:ILE:HD12	1:B:37:ILE:H	1.58	0.67
1:C:90:LEU:HD23	1:C:90:LEU:O	1.92	0.67
1:D:103:VAL:O	1:D:104:ARG:C	2.33	0.67
1:B:26:ALA:HB1	1:B:596:TYR:CE2	2.30	0.67
1:B:257:ALA:O	1:B:260:ARG:HG2	1.93	0.67
1:C:32:ASP:O	1:C:35:PRO:HD3	1.93	0.67
1:B:29:THR:O	1:B:33:SER:HB3	1.94	0.67
1:C:34:LEU:O	1:C:36:ALA:N	2.27	0.67
1:A:293:ARG:HD3	1:C:306:ILE:CG2	2.21	0.67
1:B:114:GLU:O	1:B:115:THR:HG23	1.95	0.67
1:D:23:ASP:N	1:D:26:ALA:HB3	2.10	0.67
1:D:244:SER:HB3	1:D:247:ASP:OD2	1.95	0.67
1:C:207:PHE:HD1	1:C:208:GLY:H	1.43	0.67
1:A:296:LYS:HG2	1:A:297:SER:N	2.10	0.67
1:A:13:ARG:HG3	1:A:14:ALA:N	2.10	0.67
1:A:15:CYS:C	1:A:17:ALA:H	1.97	0.67
1:A:48:SER:HB2	2:A:9001:GDP:PA	2.34	0.67
1:C:44:SER:HA	2:C:9001:GDP:O3B	1.95	0.67
1:A:27:LEU:N	1:A:28:PRO:HD2	2.09	0.67
1:B:143:LEU:HD21	1:B:169:TYR:CE2	2.29	0.67
1:D:180:ILE:HD13	1:D:180:ILE:H	1.59	0.67
1:C:275:ALA:C	3:C:662:HOH:O	2.33	0.66
1:D:36:ALA:HB1	1:D:139:THR:HG22	1.77	0.66
1:A:5:ILE:HG22	1:A:137:ASN:HD22	1.61	0.66
1:C:183:ALA:HB2	1:C:210:LEU:CD2	2.26	0.66
1:C:241:VAL:HG12	1:C:241:VAL:O	1.93	0.66
2:C:9001:GDP:O1A	3:C:667:HOH:O	2.12	0.66
1:D:176:ILE:HD12	1:D:176:ILE:N	2.08	0.66
1:D:227:GLU:HG2	1:D:229:ARG:NH1	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ASN:HB3	3:D:662:HOH:O	1.96	0.66
1:C:30:LEU:HD23	1:C:34:LEU:HD23	1.76	0.66
1:C:55:VAL:HG11	1:C:59:PHE:CD2	2.30	0.66
1:A:210:LEU:HB2	1:A:237:TRP:CZ3	2.31	0.66
1:D:23:ASP:OD2	1:D:26:ALA:HB2	1.95	0.66
1:D:230:SER:OG	1:D:231:PHE:N	2.29	0.66
1:A:190:SER:CB	1:A:193:ILE:HB	2.25	0.66
1:B:257:ALA:HA	1:B:260:ARG:HD2	1.76	0.66
1:D:37:ILE:HG23	1:D:176:ILE:HB	1.78	0.66
1:D:167:ARG:C	1:D:169:TYR:H	1.99	0.66
1:B:243:ARG:HA	1:B:260:ARG:HH12	1.61	0.66
1:D:36:ALA:HB3	3:D:656:HOH:O	1.96	0.66
1:B:70:ARG:O	1:B:72:LEU:N	2.28	0.66
1:B:265:PHE:HB3	1:B:275:ALA:HB2	1.78	0.66
1:C:130:ILE:HG22	1:C:131:TYR:N	2.10	0.66
1:C:257:ALA:O	1:C:261:GLU:N	2.22	0.66
2:C:9001:GDP:H3'	3:C:667:HOH:O	1.96	0.66
1:A:29:THR:O	1:A:33:SER:HB3	1.96	0.65
1:A:235:TYR:HB3	1:A:236:PRO:CD	2.26	0.65
1:C:252:VAL:HG12	1:C:253:ASP:N	2.11	0.65
1:D:260:ARG:HA	1:D:263:GLU:HB2	1.77	0.65
1:A:227:GLU:HG2	1:A:229:ARG:HE	1.62	0.65
1:A:13:ARG:CG	1:A:14:ALA:H	2.09	0.65
1:B:244:SER:OG	1:B:246:ALA:HB3	1.96	0.65
1:C:30:LEU:CD2	1:C:34:LEU:HD23	2.26	0.65
1:D:151:VAL:N	1:D:154:GLN:OE1	2.29	0.65
1:B:25:SER:HB2	1:B:308:LYS:HZ2	1.60	0.65
1:B:174:ASN:ND2	1:B:298:ARG:NE	2.43	0.65
1:C:149:VAL:HG22	1:D:188:ALA:HA	1.79	0.65
1:D:88:GLU:OE1	1:D:96:LYS:HE2	1.96	0.65
1:A:133:PRO:HG2	1:A:134:ASN:ND2	2.10	0.65
1:C:3:ASN:O	1:C:6:SER:OG	2.13	0.65
1:A:119:LYS:HG3	1:A:154:GLN:NE2	2.10	0.65
1:B:21:HIS:CD2	1:B:592:ARG:HH22	2.15	0.65
1:D:170:ILE:HG23	1:D:177:ILE:CD1	2.26	0.65
1:B:594:GLU:O	1:B:595:LEU:HD23	1.97	0.65
1:C:183:ALA:HB2	1:C:210:LEU:HD21	1.77	0.65
1:A:143:LEU:HD21	1:A:169:TYR:HD2	1.61	0.65
1:B:59:PHE:O	1:B:59:PHE:CD1	2.50	0.65
1:B:80:ASP:O	1:B:82:GLY:N	2.30	0.65
1:B:303:GLN:N	1:B:303:GLN:HE21	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ARG:O	1:D:121:ILE:HG22	1.97	0.65
1:B:73:VAL:HG22	1:B:141:ILE:HG23	1.79	0.65
1:A:212:LYS:HB3	1:A:215:LEU:CD1	2.27	0.65
1:C:6:SER:HB2	1:C:77:GLN:NE2	2.11	0.65
1:A:13:ARG:HH12	1:A:129:SER:HB2	1.62	0.64
1:A:27:LEU:HD22	1:A:31:TRP:HE1	1.60	0.64
1:A:136:VAL:HG11	1:A:288:SER:HB3	1.80	0.64
1:B:174:ASN:HD22	1:B:298:ARG:NE	1.95	0.64
1:C:89:PHE:CD2	1:C:91:HIS:HB2	2.33	0.64
1:B:26:ALA:HB1	1:B:596:TYR:HE2	1.62	0.64
1:C:186:ASP:HB2	1:D:44:SER:HB2	1.79	0.64
1:A:174:ASN:HB3	1:A:298:ARG:HH22	1.62	0.64
1:A:201:PRO:HB3	3:A:674:HOH:O	1.97	0.64
1:B:305:LEU:C	1:B:307:ASN:N	2.50	0.64
1:C:30:LEU:O	1:C:32:ASP:N	2.27	0.64
1:D:154:GLN:HE21	1:D:158:ILE:HG12	1.62	0.64
1:D:186:ASP:HB2	1:D:189:THR:HG23	1.77	0.64
1:C:252:VAL:HG12	1:C:253:ASP:H	1.63	0.64
1:D:37:ILE:O	3:D:675:HOH:O	2.15	0.64
1:A:9:ASN:OD1	1:A:75:GLN:HG2	1.98	0.64
1:A:215:LEU:HD21	2:A:9001:GDP:N2	2.13	0.64
1:B:162:ILE:O	1:B:166:VAL:HG23	1.98	0.64
1:D:240:VAL:HG12	1:D:241:VAL:H	1.62	0.64
1:C:166:VAL:O	1:C:170:ILE:HG12	1.98	0.64
1:D:49:SER:HA	1:D:62:ARG:NH1	2.13	0.64
1:A:188:ALA:HB2	1:A:231:PHE:HZ	1.63	0.63
1:A:282:HIS:CE1	1:A:286:MET:HG3	2.33	0.63
1:B:70:ARG:NH1	3:B:679:HOH:O	2.31	0.63
1:C:33:SER:C	1:C:35:PRO:HD2	2.19	0.63
1:C:301:GLY:HA2	1:C:304:SER:OG	1.97	0.63
1:C:589:ILE:HG22	1:C:589:ILE:O	1.98	0.63
1:A:58:ASP:O	1:A:59:PHE:CD2	2.52	0.63
1:B:275:ALA:HA	1:B:278:MET:HB2	1.79	0.63
1:C:302:ILE:HD13	3:C:658:HOH:O	1.98	0.63
1:A:77:GLN:HG3	3:A:356:HOH:O	1.97	0.63
1:B:274:LEU:O	1:B:276:ASN:N	2.32	0.63
1:B:308:LYS:CD	1:B:311:LEU:HD23	2.27	0.63
1:C:302:ILE:O	1:C:304:SER:N	2.30	0.63
1:A:11:ILE:CG2	1:A:12:GLN:N	2.48	0.63
1:B:313:LEU:CD2	1:B:597:ARG:NH2	2.52	0.63
1:C:123:SER:HB3	1:C:165:MET:CE	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:THR:HA	1:D:148:LYS:CG	2.23	0.63
1:D:77:GLN:HG3	1:D:131:TYR:CD1	2.34	0.63
1:A:18:LEU:HD11	1:A:595:LEU:HG	1.79	0.63
1:A:57:LYS:O	1:A:58:ASP:O	2.17	0.63
1:A:195:ILE:HD13	1:A:198:GLU:HG3	1.81	0.63
1:B:265:PHE:HB3	1:B:275:ALA:CB	2.28	0.63
1:C:302:ILE:C	1:C:304:SER:H	2.00	0.63
1:A:45:SER:O	1:A:182:PRO:CG	2.47	0.63
1:B:12:GLN:NE2	1:B:73:VAL:HG11	2.14	0.63
1:C:7:LEU:O	1:C:10:LYS:N	2.32	0.63
1:C:101:ALA:O	1:C:104:ARG:HB3	1.99	0.63
1:B:589:ILE:O	1:B:592:ARG:HB2	1.99	0.62
1:D:191:ASP:HA	1:D:194:LYS:HB3	1.81	0.62
1:A:95:LYS:HG2	1:A:96:LYS:N	2.13	0.62
1:A:254:MET:O	1:A:257:ALA:HB3	1.99	0.62
1:D:190:SER:HB3	1:D:192:ALA:HB3	1.81	0.62
1:A:34:LEU:O	1:A:36:ALA:N	2.32	0.62
1:A:245:GLN:O	1:A:249:ASN:ND2	2.33	0.62
1:B:25:SER:O	1:B:308:LYS:CD	2.46	0.62
1:B:32:ASP:C	1:B:34:LEU:H	2.02	0.62
1:B:146:LEU:HD11	1:B:195:ILE:HG21	1.82	0.62
1:B:260:ARG:HG3	1:B:261:GLU:H	1.63	0.62
1:D:189:THR:O	1:D:189:THR:OG1	2.17	0.62
1:D:238:VAL:HG13	1:D:278:MET:HG2	1.80	0.62
1:A:283:LEU:O	1:A:284:ALA:C	2.38	0.62
1:D:16:THR:HG21	1:D:125:PRO:CG	2.30	0.62
1:D:27:LEU:O	1:D:29:THR:N	2.33	0.62
1:A:5:ILE:HG21	1:A:137:ASN:C	2.18	0.62
1:B:13:ARG:O	1:B:17:ALA:HB2	1.99	0.62
1:B:167:ARG:HH21	1:B:195:ILE:HD11	1.65	0.62
1:D:257:ALA:O	1:D:261:GLU:N	2.29	0.62
1:D:69:ARG:HB3	1:D:121:ILE:CG2	2.30	0.62
1:D:593:LEU:O	1:D:594:GLU:C	2.36	0.62
1:A:79:ILE:O	1:A:81:ASP:N	2.30	0.62
1:D:265:PHE:CE2	1:D:278:MET:HE1	2.34	0.62
1:A:45:SER:HA	1:A:182:PRO:CG	2.30	0.62
1:D:70:ARG:NH2	1:D:126:ILE:CD1	2.63	0.62
1:D:70:ARG:HG2	1:D:71:PRO:HD2	1.82	0.62
1:A:265:PHE:N	1:A:265:PHE:CD1	2.62	0.62
1:B:92:LEU:HD22	1:B:93:PRO:O	2.00	0.62
1:B:239:GLY:H	1:B:278:MET:HE1	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LEU:H	1:C:28:PRO:CD	2.11	0.62
1:D:16:THR:HG21	1:D:125:PRO:HG2	1.82	0.62
1:B:261:GLU:O	1:B:264:TYR:HB3	1.98	0.61
1:D:255:ILE:HD12	1:D:259:LYS:NZ	2.15	0.61
1:A:174:ASN:HA	1:A:298:ARG:HH12	1.65	0.61
1:B:257:ALA:HA	1:B:260:ARG:CD	2.30	0.61
1:C:32:ASP:C	1:C:34:LEU:N	2.53	0.61
1:C:290:HIS:C	1:C:292:GLU:H	2.04	0.61
1:D:213:ILE:HG13	3:D:654:HOH:O	2.01	0.61
1:A:16:THR:HA	1:A:20:ASP:HB2	1.81	0.61
1:A:55:VAL:HG11	1:A:59:PHE:CE2	2.35	0.61
1:A:185:GLN:NE2	1:B:185:GLN:NE2	2.49	0.61
1:A:200:ASP:C	1:A:202:SER:H	2.03	0.61
1:A:223:VAL:HA	1:A:226:LEU:HD12	1.82	0.61
1:C:33:SER:C	1:C:35:PRO:CD	2.68	0.61
1:D:13:ARG:HG3	1:D:75:GLN:OE1	2.00	0.61
1:D:76:LEU:HD23	1:D:130:ILE:HB	1.81	0.61
1:B:204:ASP:HB2	3:B:681:HOH:O	2.00	0.61
1:C:51:LEU:N	3:C:634:HOH:O	2.32	0.61
1:C:238:VAL:HG21	1:C:283:LEU:HD13	1.82	0.61
1:B:303:GLN:HE21	1:B:303:GLN:H	1.48	0.61
1:C:42:GLY:HA2	1:C:146:LEU:CB	2.25	0.61
1:C:148:LYS:HE2	1:D:148:LYS:HE2	1.82	0.61
1:D:88:GLU:CD	1:D:96:LYS:HE2	2.21	0.61
1:B:243:ARG:HA	1:B:260:ARG:NH1	2.14	0.61
1:B:260:ARG:CG	1:B:261:GLU:H	2.13	0.61
1:C:600:GLN:HA	1:C:603:ILE:CG1	2.30	0.61
1:D:37:ILE:HD12	1:D:176:ILE:HD13	1.83	0.61
1:B:79:ILE:HD11	1:B:132:SER:HA	1.83	0.61
1:D:161:ASP:HA	1:D:164:ASN:OD1	2.00	0.61
1:D:241:VAL:O	1:D:241:VAL:CG1	2.48	0.61
1:A:13:ARG:HB2	1:A:90:LEU:HD21	1.82	0.61
1:B:585:ARG:NE	1:B:589:ILE:HD11	2.11	0.61
1:C:37:ILE:HG22	1:C:37:ILE:O	2.01	0.61
1:C:278:MET:N	3:C:662:HOH:O	2.34	0.61
1:B:60:LEU:HD23	1:B:61:PRO:CD	2.25	0.61
1:C:66:ILE:HG23	1:C:69:ARG:HE	1.66	0.61
1:C:70:ARG:HG2	1:C:71:PRO:HD2	1.83	0.61
1:D:34:LEU:N	1:D:35:PRO:CD	2.64	0.60
1:A:23:ASP:HB3	1:A:592:ARG:HD3	1.81	0.60
1:C:27:LEU:N	1:C:28:PRO:CD	2.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:THR:CG2	1:A:30:LEU:HD13	2.31	0.60
1:A:79:ILE:HD11	1:A:132:SER:CA	2.31	0.60
1:C:266:SER:O	1:C:272:ARG:HG3	2.00	0.60
1:D:193:ILE:O	1:D:196:SER:N	2.31	0.60
1:A:13:ARG:CG	1:A:14:ALA:N	2.64	0.60
1:B:175:CYS:O	1:B:205:ARG:HD2	2.01	0.60
1:C:290:HIS:CE1	3:C:673:HOH:O	2.44	0.60
1:D:70:ARG:NH2	1:D:126:ILE:HD11	2.16	0.60
1:A:128:LEU:HD11	1:A:130:ILE:HG12	1.83	0.60
1:B:260:ARG:CG	1:B:261:GLU:N	2.63	0.60
1:A:13:ARG:HG3	1:A:14:ALA:H	1.66	0.60
1:D:186:ASP:HB2	3:D:659:HOH:O	2.01	0.60
1:D:187:LEU:O	1:D:189:THR:N	2.31	0.60
1:A:24:SER:CB	1:A:585:ARG:HH21	2.12	0.60
1:A:224:GLU:HG3	1:A:229:ARG:CZ	2.32	0.60
1:B:596:TYR:O	1:B:599:ALA:HB3	2.00	0.60
1:C:194:LYS:HA	1:D:149:VAL:CG1	2.32	0.60
1:D:15:CYS:O	1:D:17:ALA:N	2.35	0.60
1:D:276:ASN:OD1	1:D:277:LYS:HG3	2.01	0.60
1:D:294:VAL:O	1:D:297:SER:HB3	2.01	0.60
1:B:215:LEU:HD11	2:B:9001:GDP:N2	2.16	0.60
1:B:239:GLY:H	1:B:278:MET:CE	2.15	0.60
1:C:23:ASP:OD1	1:C:26:ALA:HB2	2.02	0.60
1:D:263:GLU:O	1:D:267:ASN:HB2	2.02	0.60
1:A:30:LEU:HG	1:A:34:LEU:HD22	1.84	0.60
1:A:53:SER:O	1:A:280:SER:HB3	2.00	0.60
1:D:29:THR:C	1:D:31:TRP:H	2.05	0.59
1:D:72:LEU:HD12	1:D:126:ILE:HB	1.84	0.59
1:A:16:THR:HG21	1:A:127:HIS:NE2	2.17	0.59
1:A:36:ALA:HB1	1:A:139:THR:CG2	2.32	0.59
1:A:207:PHE:N	1:A:207:PHE:CD2	2.70	0.59
1:B:285:LYS:O	1:B:289:LYS:HG2	2.03	0.59
1:C:186:ASP:O	1:C:188:ALA:N	2.34	0.59
1:B:92:LEU:HD21	1:B:95:LYS:HB2	1.83	0.59
1:B:207:PHE:CZ	1:B:235:TYR:CE1	2.90	0.59
1:C:302:ILE:HG13	1:C:603:ILE:HD12	1.83	0.59
1:D:234:LYS:HD3	1:D:235:TYR:CE2	2.37	0.59
1:B:235:TYR:N	1:B:235:TYR:CD2	2.69	0.59
1:D:15:CYS:HA	1:D:595:LEU:HD21	1.84	0.59
1:D:312:GLU:C	1:D:314:GLU:N	2.55	0.59
1:A:227:GLU:HG2	1:A:229:ARG:NE	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LYS:HB2	1:B:154:GLN:HE21	1.68	0.59
1:B:247:ASP:O	1:B:252:VAL:HG23	2.02	0.59
1:C:44:SER:HB2	1:D:186:ASP:OD2	2.02	0.59
1:C:128:LEU:HD12	1:C:128:LEU:C	2.22	0.59
1:D:27:LEU:C	1:D:29:THR:H	2.05	0.59
1:D:312:GLU:C	1:D:314:GLU:H	2.03	0.59
1:A:24:SER:HB3	1:A:585:ARG:NH2	2.16	0.59
1:C:593:LEU:HD23	1:C:593:LEU:H	1.68	0.59
1:B:46:GLY:O	1:B:47:LYS:C	2.40	0.59
1:C:7:LEU:CD2	1:C:11:ILE:HG12	2.33	0.59
1:C:80:ASP:O	1:C:82:GLY:N	2.36	0.59
1:C:225:ILE:HG12	1:C:230:SER:HB2	1.84	0.59
1:D:88:GLU:O	1:D:89:PHE:HB2	2.02	0.59
1:D:151:VAL:HG22	1:D:152:ASP:CG	2.23	0.59
1:A:42:GLY:HA2	1:A:146:LEU:N	2.16	0.58
1:A:204:ASP:OD1	1:A:234:LYS:NZ	2.36	0.58
1:D:189:THR:HG23	3:D:659:HOH:O	2.01	0.58
1:A:176:ILE:HD12	1:A:176:ILE:H	1.67	0.58
1:C:6:SER:CB	1:C:77:GLN:NE2	2.66	0.58
1:D:15:CYS:O	1:D:19:GLY:N	2.30	0.58
1:A:257:ALA:O	1:A:260:ARG:HB3	2.04	0.58
1:A:3:ASN:HA	1:A:137:ASN:ND2	2.19	0.58
1:A:59:PHE:HA	1:A:104:ARG:HB2	1.84	0.58
1:A:97:PHE:CD2	1:A:103:VAL:HG22	2.38	0.58
1:A:283:LEU:O	1:A:286:MET:N	2.36	0.58
1:B:92:LEU:HD22	1:B:92:LEU:C	2.24	0.58
1:B:183:ALA:HB1	1:B:216:MET:CE	2.32	0.58
1:B:591:LYS:O	1:B:595:LEU:HD12	2.04	0.58
1:C:7:LEU:HD23	1:C:11:ILE:HG12	1.86	0.58
1:D:259:LYS:HE3	3:D:643:HOH:O	2.02	0.58
1:A:31:TRP:HE3	1:A:172:LYS:HD3	1.68	0.58
1:A:34:LEU:HD23	1:A:172:LYS:HZ2	1.68	0.58
1:A:233:LEU:HD22	1:A:237:TRP:NE1	2.18	0.58
1:B:215:LEU:HD11	2:B:9001:GDP:N3	2.17	0.58
1:C:57:LYS:O	1:C:58:ASP:O	2.22	0.58
1:B:66:ILE:HG12	1:B:67:VAL:N	2.19	0.58
1:B:68:THR:O	1:B:68:THR:HG22	2.03	0.58
1:C:6:SER:HB3	1:C:137:ASN:ND2	2.19	0.58
1:D:187:LEU:C	1:D:189:THR:H	2.06	0.58
1:C:148:LYS:HB3	1:D:194:LYS:HD2	1.84	0.58
1:D:313:LEU:HG	1:D:593:LEU:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PHE:CE1	1:A:106:GLU:HG2	2.39	0.58
1:B:77:GLN:HB2	1:B:131:TYR:CD1	2.38	0.58
1:B:232:LYS:HD3	3:B:649:HOH:O	2.02	0.58
1:B:257:ALA:HA	1:B:260:ARG:NE	2.19	0.58
1:C:132:SER:HB3	1:C:135:VAL:HG13	1.85	0.58
1:D:26:ALA:N	1:D:28:PRO:HD2	2.17	0.58
1:D:52:GLU:O	1:D:254:MET:HE1	2.04	0.58
1:B:167:ARG:NH2	1:B:195:ILE:HD11	2.18	0.58
1:D:25:SER:HA	1:D:28:PRO:HG2	1.86	0.58
1:B:5:ILE:O	1:B:7:LEU:N	2.37	0.58
1:B:271:TYR:O	1:B:272:ARG:C	2.43	0.58
1:D:235:TYR:HE1	3:D:628:HOH:O	1.87	0.58
1:A:37:ILE:HG23	1:A:176:ILE:HD13	1.85	0.57
1:A:234:LYS:HE2	1:C:597:ARG:NH2	2.18	0.57
1:A:258:ARG:HH21	1:A:281:GLU:HG2	1.68	0.57
1:A:300:PRO:C	1:A:302:ILE:N	2.58	0.57
1:B:5:ILE:HG23	1:B:6:SER:N	2.17	0.57
1:B:40:VAL:HG21	1:B:170:ILE:CD1	2.24	0.57
1:B:306:ILE:HG13	1:B:306:ILE:O	2.04	0.57
1:A:166:VAL:O	1:A:170:ILE:HG12	2.04	0.57
1:B:249:ASN:C	1:B:251:ASN:H	2.07	0.57
1:D:205:ARG:O	1:D:206:THR:HG23	2.04	0.57
1:D:274:LEU:HD23	1:D:277:LYS:HZ3	1.69	0.57
1:A:89:PHE:CE2	1:A:128:LEU:HB2	2.39	0.57
1:A:276:ASN:OD1	1:A:277:LYS:CE	2.52	0.57
1:B:176:ILE:HG22	1:B:177:ILE:N	2.19	0.57
1:C:82:GLY:O	1:C:84:ARG:N	2.33	0.57
1:A:33:SER:O	1:A:35:PRO:HD2	2.04	0.57
1:A:235:TYR:HB3	1:A:236:PRO:HD3	1.87	0.57
1:B:593:LEU:O	1:B:597:ARG:N	2.37	0.57
1:D:204:ASP:HA	1:D:234:LYS:CE	2.33	0.57
1:B:195:ILE:HG23	1:B:195:ILE:O	2.04	0.57
1:C:590:SER:C	1:C:592:ARG:H	2.06	0.57
1:A:200:ASP:H	1:A:201:PRO:HD3	1.68	0.57
1:A:228:GLY:O	1:A:232:LYS:HG3	2.04	0.57
1:D:15:CYS:C	1:D:17:ALA:H	2.08	0.57
1:D:29:THR:O	1:D:31:TRP:N	2.38	0.57
1:A:86:TYR:CZ	1:A:131:TYR:CD2	2.93	0.57
1:C:27:LEU:CB	1:C:31:TRP:HB2	2.24	0.57
1:D:204:ASP:CA	1:D:234:LYS:HD2	2.33	0.57
1:A:37:ILE:CG1	1:A:140:LEU:HD23	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:PHE:CD2	1:B:103:VAL:HG23	2.40	0.57
1:C:89:PHE:O	1:C:90:LEU:HB2	2.03	0.57
1:C:100:PHE:O	1:C:103:VAL:N	2.38	0.57
1:D:49:SER:HB3	2:D:9001:GDP:O1A	2.05	0.57
1:A:296:LYS:C	1:A:298:ARG:H	2.06	0.56
1:B:305:LEU:O	1:B:308:LYS:N	2.38	0.56
1:D:47:LYS:NZ	1:D:145:GLY:N	2.53	0.56
1:D:236:PRO:HD2	3:D:670:HOH:O	2.05	0.56
1:D:597:ARG:NH1	1:D:597:ARG:HG3	2.19	0.56
1:C:162:ILE:O	1:C:166:VAL:HG23	2.05	0.56
1:A:261:GLU:HG3	1:A:262:ARG:N	2.20	0.56
1:B:92:LEU:HD21	1:B:95:LYS:CB	2.36	0.56
1:B:157:SER:O	1:B:161:ASP:HB2	2.04	0.56
1:C:29:THR:O	1:C:33:SER:CB	2.53	0.56
1:C:46:GLY:HA2	1:C:49:SER:OG	2.05	0.56
1:C:52:GLU:O	1:C:254:MET:HE2	2.04	0.56
1:D:256:ALA:CA	1:D:259:LYS:HB2	2.31	0.56
1:A:59:PHE:CD1	1:A:59:PHE:C	2.78	0.56
1:A:136:VAL:CG1	1:A:288:SER:HB3	2.35	0.56
1:C:593:LEU:HD23	1:C:593:LEU:N	2.20	0.56
1:D:29:THR:O	1:D:33:SER:N	2.38	0.56
1:A:85:GLU:O	1:A:86:TYR:CD2	2.58	0.56
1:A:172:LYS:O	1:A:172:LYS:HG2	2.05	0.56
1:C:162:ILE:HG22	1:C:163:GLU:N	2.20	0.56
1:D:302:ILE:CG1	1:D:600:GLN:HE21	2.18	0.56
1:A:293:ARG:NH1	1:C:604:ASP:OD2	2.39	0.56
1:D:215:LEU:HD11	2:D:9001:GDP:C2	2.40	0.56
1:A:8:VAL:HG21	1:A:295:ILE:HD13	1.88	0.56
1:A:24:SER:CB	1:A:585:ARG:NH2	2.68	0.56
1:B:223:VAL:O	1:B:227:GLU:HG3	2.06	0.56
1:C:121:ILE:HD12	1:C:121:ILE:O	2.05	0.56
1:C:253:ASP:CG	1:C:254:MET:H	2.08	0.56
1:C:307:ASN:OD1	1:C:311:LEU:HD11	2.05	0.56
1:C:590:SER:C	1:C:592:ARG:N	2.59	0.56
1:D:167:ARG:C	1:D:169:TYR:N	2.59	0.56
1:D:282:HIS:C	3:D:660:HOH:O	2.44	0.56
1:A:39:VAL:HG22	1:A:39:VAL:O	2.06	0.56
1:A:296:LYS:NZ	1:C:303:GLN:NE2	2.54	0.56
1:B:65:GLY:O	1:B:66:ILE:O	2.23	0.56
1:C:89:PHE:HD2	1:C:91:HIS:H	1.53	0.55
1:C:29:THR:O	1:C:33:SER:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:LYS:C	1:C:235:TYR:CD2	2.79	0.55
1:C:292:GLU:O	1:C:295:ILE:N	2.38	0.55
1:D:172:LYS:O	1:D:174:ASN:N	2.38	0.55
1:D:187:LEU:HD21	1:D:225:ILE:HD13	1.88	0.55
1:D:215:LEU:HD11	2:D:9001:GDP:N2	2.20	0.55
1:A:42:GLY:O	1:A:43:GLN:O	2.25	0.55
1:B:39:VAL:CG1	1:B:142:ASP:HA	2.32	0.55
1:C:30:LEU:C	1:C:32:ASP:H	2.09	0.55
1:C:49:SER:HB3	1:C:242:ASN:HD22	1.69	0.55
1:D:187:LEU:HD23	1:D:231:PHE:HD2	1.71	0.55
1:A:118:SER:C	1:A:119:LYS:HG2	2.26	0.55
1:B:11:ILE:HG22	1:B:12:GLN:N	2.21	0.55
1:D:69:ARG:HD3	1:D:120:ALA:H	1.71	0.55
1:D:300:PRO:C	1:D:302:ILE:H	2.09	0.55
1:B:592:ARG:O	1:B:596:TYR:HB2	2.06	0.55
1:D:122:SER:O	1:D:123:SER:HB3	2.06	0.55
1:D:178:LEU:HD12	1:D:207:PHE:O	2.07	0.55
1:B:59:PHE:CD1	1:B:59:PHE:C	2.80	0.55
1:C:235:TYR:O	1:C:236:PRO:C	2.43	0.55
1:C:295:ILE:O	1:C:297:SER:N	2.40	0.55
1:A:157:SER:O	1:A:161:ASP:N	2.39	0.55
1:A:306:ILE:HG22	1:A:306:ILE:O	2.07	0.55
1:B:14:ALA:O	1:B:15:CYS:O	2.25	0.55
1:B:253:ASP:O	1:B:256:ALA:HB3	2.07	0.55
1:C:27:LEU:H	1:C:28:PRO:HD2	1.71	0.55
1:C:137:ASN:O	1:C:138:LEU:CB	2.54	0.55
1:D:62:ARG:NH2	1:D:248:ILE:HD11	2.22	0.55
1:D:70:ARG:CZ	1:D:126:ILE:HD11	2.37	0.55
1:A:72:LEU:HG	1:A:74:LEU:HD13	1.88	0.55
1:B:59:PHE:HA	1:B:104:ARG:HB2	1.88	0.55
1:B:232:LYS:HD2	1:B:233:LEU:N	2.22	0.55
1:C:30:LEU:O	1:C:34:LEU:HB2	2.07	0.55
1:C:46:GLY:O	1:C:49:SER:HB2	2.07	0.55
1:D:289:LYS:N	3:D:636:HOH:O	2.17	0.55
1:D:604:ASP:O	1:D:606:VAL:HG12	2.06	0.55
1:A:51:LEU:HD22	1:A:140:LEU:HD13	1.89	0.55
1:A:92:LEU:HD13	1:A:95:LYS:CE	2.28	0.55
1:A:296:LYS:CG	1:A:297:SER:N	2.69	0.55
1:B:159:VAL:O	1:B:161:ASP:N	2.40	0.55
1:C:221:ASP:OD1	1:C:223:VAL:HB	2.06	0.55
1:D:142:ASP:O	1:D:143:LEU:HD23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:LYS:O	1:D:298:ARG:N	2.41	0.55
1:A:8:VAL:O	1:A:12:GLN:HB2	2.07	0.54
1:A:585:ARG:HA	1:A:588:ALA:HB3	1.87	0.54
1:B:70:ARG:HH21	1:B:124:VAL:H	1.55	0.54
1:D:308:LYS:O	1:D:312:GLU:HG2	2.07	0.54
1:A:18:LEU:HG	1:A:19:GLY:H	1.72	0.54
1:A:77:GLN:NE2	1:A:137:ASN:ND2	2.55	0.54
1:A:228:GLY:O	1:A:232:LYS:HE3	2.06	0.54
1:B:32:ASP:O	1:B:34:LEU:N	2.41	0.54
1:B:217:ASP:O	1:B:219:GLY:N	2.40	0.54
1:D:274:LEU:HD23	1:D:277:LYS:NZ	2.23	0.54
1:A:51:LEU:HA	1:A:54:ILE:HG22	1.88	0.54
1:B:593:LEU:C	1:B:595:LEU:H	2.10	0.54
1:C:226:LEU:C	1:C:228:GLY:N	2.60	0.54
1:C:279:GLY:O	1:C:281:GLU:N	2.41	0.54
1:D:90:LEU:HB3	1:D:127:HIS:HB2	1.89	0.54
1:D:170:ILE:CG2	1:D:199:VAL:HG11	2.21	0.54
1:D:223:VAL:O	1:D:227:GLU:HB2	2.07	0.54
1:A:596:TYR:O	1:A:599:ALA:HB3	2.08	0.54
1:B:88:GLU:HG3	1:B:95:LYS:O	2.07	0.54
1:C:592:ARG:O	1:C:593:LEU:C	2.46	0.54
1:D:47:LYS:HZ2	1:D:145:GLY:N	2.05	0.54
1:D:172:LYS:C	1:D:174:ASN:H	2.10	0.54
1:A:30:LEU:O	1:A:34:LEU:HD22	2.07	0.54
1:A:33:SER:C	1:A:35:PRO:CD	2.76	0.54
1:A:174:ASN:CB	1:A:298:ARG:HH22	2.19	0.54
1:A:223:VAL:O	1:A:225:ILE:N	2.39	0.54
1:B:268:THR:O	1:B:270:GLU:N	2.41	0.54
1:D:70:ARG:HH21	1:D:126:ILE:HD13	1.71	0.54
1:D:298:ARG:HG3	1:D:298:ARG:HH11	1.73	0.54
1:A:23:ASP:O	1:A:25:SER:N	2.41	0.54
1:A:25:SER:C	1:A:28:PRO:HD2	2.28	0.54
1:C:52:GLU:N	3:C:636:HOH:O	2.41	0.54
1:C:148:LYS:HB3	1:C:148:LYS:HZ2	1.73	0.54
1:D:227:GLU:HB3	1:D:229:ARG:HD2	1.90	0.54
1:D:283:LEU:C	3:D:660:HOH:O	2.46	0.54
1:B:124:VAL:HB	3:B:679:HOH:O	2.06	0.54
1:B:276:ASN:OD1	1:B:277:LYS:HG2	2.07	0.54
1:C:57:LYS:HG2	1:C:100:PHE:CD1	2.43	0.54
1:A:176:ILE:HG21	1:A:207:PHE:HE2	1.73	0.54
1:B:299:ILE:O	1:B:302:ILE:HB	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:LYS:HE2	1:D:148:LYS:CE	2.38	0.54
1:C:148:LYS:CG	1:D:189:THR:HA	2.38	0.54
1:D:39:VAL:CG2	1:D:142:ASP:HA	2.37	0.54
1:B:72:LEU:HD12	1:B:72:LEU:C	2.28	0.54
1:C:302:ILE:HA	1:C:600:GLN:HE21	1.73	0.54
1:A:34:LEU:HG	1:A:172:LYS:HZ1	1.73	0.54
1:A:206:THR:HG22	1:A:206:THR:O	2.06	0.54
1:B:43:GLN:O	1:B:44:SER:HB2	2.07	0.54
1:B:190:SER:HB3	1:B:193:ILE:HB	1.89	0.54
1:B:305:LEU:C	1:B:307:ASN:H	2.11	0.54
1:B:22:GLY:HA3	1:B:27:LEU:HD12	1.90	0.53
1:C:109:ASP:HA	1:C:112:ASP:HB2	1.90	0.53
1:C:148:LYS:HE2	1:D:148:LYS:NZ	2.24	0.53
1:A:27:LEU:H	1:A:28:PRO:CD	2.21	0.53
1:A:97:PHE:HD2	1:A:103:VAL:HG22	1.73	0.53
1:A:160:LYS:HA	1:A:163:GLU:HG2	1.89	0.53
1:B:99:ASP:O	1:B:102:ALA:HB3	2.08	0.53
1:C:6:SER:HB2	1:C:77:GLN:HE21	1.70	0.53
1:C:51:LEU:C	3:C:636:HOH:O	2.47	0.53
1:C:223:VAL:HG13	1:C:224:GLU:N	2.22	0.53
1:D:70:ARG:HH21	1:D:126:ILE:CD1	2.21	0.53
1:D:289:LYS:O	1:D:293:ARG:HB3	2.09	0.53
1:A:265:PHE:O	1:A:272:ARG:HA	2.08	0.53
1:C:89:PHE:CE2	1:C:91:HIS:HB2	2.44	0.53
1:C:224:GLU:HB3	1:C:229:ARG:NH1	2.23	0.53
1:D:59:PHE:HD1	1:D:107:ILE:CD1	2.22	0.53
1:A:205:ARG:O	1:A:206:THR:CB	2.56	0.53
1:C:264:TYR:CD1	1:C:264:TYR:C	2.82	0.53
1:D:36:ALA:CB	3:D:656:HOH:O	2.55	0.53
1:B:209:VAL:HA	1:B:238:VAL:O	2.08	0.53
1:D:6:SER:HA	1:D:9:ASN:HB2	1.90	0.53
1:D:43:GLN:HG3	1:D:147:THR:HG22	1.90	0.53
1:D:47:LYS:HB3	2:D:9001:GDP:O1B	2.08	0.53
1:A:30:LEU:HB3	3:A:664:HOH:O	2.08	0.53
1:A:91:HIS:CE1	1:A:106:GLU:OE2	2.61	0.53
1:B:5:ILE:HG21	1:B:137:ASN:HB2	1.89	0.53
1:B:294:VAL:O	1:B:297:SER:HB3	2.08	0.53
1:C:121:ILE:HD12	1:C:121:ILE:C	2.28	0.53
1:C:170:ILE:HG23	1:C:177:ILE:HD11	1.90	0.53
1:C:205:ARG:O	1:C:205:ARG:HG3	2.08	0.53
1:C:308:LYS:HE2	3:C:627:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:MET:C	1:D:167:ARG:H	2.11	0.53
1:D:593:LEU:O	1:D:596:TYR:N	2.42	0.53
1:A:89:PHE:CD2	1:A:128:LEU:HB2	2.44	0.53
1:B:9:ASN:HD22	1:B:77:GLN:NE2	2.07	0.53
1:B:172:LYS:HG2	1:B:175:CYS:HB2	1.90	0.53
1:C:193:ILE:HA	1:C:196:SER:HB3	1.91	0.53
1:D:39:VAL:HG12	1:D:178:LEU:HD23	1.89	0.53
1:D:246:ALA:O	1:D:249:ASN:HB2	2.09	0.53
1:D:600:GLN:O	1:D:600:GLN:HG2	2.08	0.53
1:A:185:GLN:HE21	1:B:185:GLN:NE2	2.07	0.53
1:A:193:ILE:HA	1:A:196:SER:HB2	1.91	0.53
1:A:247:ASP:HB3	1:A:252:VAL:CG2	2.39	0.53
1:B:47:LYS:HG3	2:B:9001:GDP:O2B	2.09	0.53
1:B:207:PHE:CE1	1:B:235:TYR:CD1	2.97	0.53
1:B:313:LEU:HB3	1:B:597:ARG:HH21	1.73	0.53
1:C:9:ASN:O	3:C:351:HOH:O	2.18	0.53
1:C:11:ILE:O	1:C:14:ALA:N	2.41	0.53
1:B:29:THR:HG21	1:B:596:TYR:CE1	2.44	0.53
1:B:583:MET:HA	1:B:586:ARG:CD	2.38	0.53
1:B:595:LEU:HD22	3:B:626:HOH:O	2.09	0.53
1:C:148:LYS:NZ	1:D:148:LYS:HZ1	2.07	0.53
1:C:253:ASP:OD2	1:C:255:ILE:HG12	2.09	0.53
1:C:295:ILE:C	1:C:297:SER:N	2.63	0.53
1:D:82:GLY:O	1:D:84:ARG:CG	2.52	0.53
1:D:166:VAL:HG12	1:D:166:VAL:O	2.08	0.53
1:D:34:LEU:O	1:D:36:ALA:N	2.42	0.52
1:A:312:GLU:N	1:A:315:THR:OG1	2.42	0.52
1:C:83:THR:CG2	1:C:133:PRO:HG2	2.29	0.52
1:D:204:ASP:N	1:D:234:LYS:HD2	2.23	0.52
1:A:58:ASP:O	1:A:59:PHE:CB	2.57	0.52
1:A:302:ILE:C	1:A:304:SER:N	2.53	0.52
1:B:586:ARG:O	1:B:588:ALA:N	2.42	0.52
1:B:590:SER:C	1:B:592:ARG:H	2.12	0.52
1:C:49:SER:CB	1:C:242:ASN:HD22	2.22	0.52
1:A:194:LYS:O	1:A:198:GLU:HG2	2.10	0.52
1:C:298:ARG:HB2	1:C:298:ARG:NH1	2.09	0.52
1:D:71:PRO:O	1:D:125:PRO:HA	2.08	0.52
1:D:172:LYS:C	1:D:174:ASN:N	2.63	0.52
1:D:271:TYR:O	1:D:273:HIS:N	2.42	0.52
1:A:42:GLY:O	1:A:43:GLN:C	2.48	0.52
1:A:226:LEU:HB2	1:A:274:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ARG:HG3	1:A:260:ARG:HH11	1.74	0.52
1:B:252:VAL:O	1:B:253:ASP:C	2.48	0.52
1:C:53:SER:HB3	1:C:280:SER:CB	2.40	0.52
1:C:599:ALA:O	1:C:603:ILE:HG12	2.09	0.52
1:D:34:LEU:O	1:D:35:PRO:C	2.42	0.52
1:A:3:ASN:HA	1:A:137:ASN:HD21	1.75	0.52
1:B:302:ILE:HG22	1:B:303:GLN:NE2	2.24	0.52
1:C:54:ILE:N	3:C:636:HOH:O	2.41	0.52
1:C:130:ILE:C	1:C:131:TYR:CD2	2.83	0.52
1:D:158:ILE:C	1:D:160:LYS:H	2.13	0.52
1:A:56:GLY:O	1:A:57:LYS:HD2	2.10	0.52
1:B:301:GLY:HA3	3:B:708:HOH:O	2.09	0.52
1:C:77:GLN:O	1:C:131:TYR:HA	2.10	0.52
1:C:301:GLY:HA3	3:C:635:HOH:O	2.10	0.52
1:D:255:ILE:HD12	1:D:259:LYS:HZ3	1.74	0.52
1:A:47:LYS:HA	1:A:180:ILE:CD1	2.40	0.52
1:A:50:VAL:O	1:A:54:ILE:HB	2.09	0.52
1:B:601:SER:HA	1:B:604:ASP:HB2	1.91	0.52
1:C:37:ILE:CG2	1:C:140:LEU:HG	2.39	0.52
1:C:111:THR:HG22	1:C:111:THR:O	2.10	0.52
1:D:29:THR:C	1:D:31:TRP:N	2.61	0.52
1:D:170:ILE:HD12	1:D:177:ILE:HG12	1.92	0.52
1:D:309:THR:CA	1:D:312:GLU:HB2	2.35	0.52
1:A:42:GLY:HA2	1:A:146:LEU:CB	2.38	0.52
1:B:233:LEU:HD23	1:B:237:TRP:NE1	2.24	0.52
1:D:31:TRP:HZ3	1:D:171:GLU:O	1.92	0.52
1:D:298:ARG:HG3	1:D:298:ARG:NH1	2.25	0.52
1:A:124:VAL:O	1:A:125:PRO:O	2.28	0.51
1:A:301:GLY:O	1:A:305:LEU:CB	2.49	0.51
1:A:313:LEU:HD13	1:A:314:GLU:HG3	1.92	0.51
1:B:40:VAL:HG12	1:B:40:VAL:O	2.09	0.51
1:B:272:ARG:HB3	3:B:688:HOH:O	2.09	0.51
1:C:52:GLU:OE2	1:C:60:LEU:HB2	2.11	0.51
1:D:31:TRP:CE3	1:D:172:LYS:HG2	2.45	0.51
1:D:76:LEU:CD2	1:D:130:ILE:HB	2.40	0.51
1:D:170:ILE:HG22	1:D:199:VAL:CG1	2.19	0.51
1:A:244:SER:HB3	1:A:247:ASP:OD2	2.11	0.51
1:A:296:LYS:O	1:A:298:ARG:N	2.43	0.51
1:C:50:VAL:HG11	1:C:240:VAL:HG21	1.93	0.51
1:D:25:SER:C	1:D:28:PRO:HD2	2.31	0.51
1:D:86:TYR:CD1	1:D:86:TYR:C	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:SER:N	3:D:636:HOH:O	2.43	0.51
1:D:307:ASN:HA	1:D:310:VAL:CG1	2.39	0.51
1:D:599:ALA:C	1:D:601:SER:H	2.12	0.51
1:D:37:ILE:CD1	1:D:176:ILE:HD13	2.40	0.51
1:D:187:LEU:HB2	1:D:231:PHE:CE2	2.45	0.51
1:D:192:ALA:CB	1:D:193:ILE:HD12	2.40	0.51
1:D:309:THR:HA	1:D:312:GLU:HG2	1.92	0.51
1:A:58:ASP:O	1:A:59:PHE:HB3	2.10	0.51
1:C:37:ILE:HG21	1:C:140:LEU:HG	1.92	0.51
1:C:200:ASP:N	1:C:201:PRO:HD3	2.24	0.51
1:C:308:LYS:CE	3:C:627:HOH:O	2.58	0.51
1:D:23:ASP:CG	1:D:26:ALA:CB	2.79	0.51
1:D:27:LEU:C	1:D:29:THR:N	2.64	0.51
1:D:231:PHE:O	1:D:237:TRP:NE1	2.43	0.51
1:D:305:LEU:O	1:D:306:ILE:C	2.48	0.51
1:A:15:CYS:C	1:A:17:ALA:N	2.63	0.51
1:B:85:GLU:O	1:B:86:TYR:O	2.28	0.51
1:B:254:MET:O	1:B:257:ALA:N	2.25	0.51
1:C:51:LEU:HG	3:C:634:HOH:O	2.10	0.51
1:C:309:THR:O	1:C:313:LEU:HG	2.10	0.51
1:D:37:ILE:CG2	1:D:176:ILE:HB	2.40	0.51
1:D:163:GLU:O	1:D:167:ARG:HG3	2.10	0.51
2:D:9001:GDP:O2B	3:D:668:HOH:O	2.19	0.51
1:A:54:ILE:HG23	1:A:54:ILE:O	2.08	0.51
1:A:143:LEU:HD13	1:A:166:VAL:HA	1.92	0.51
1:A:293:ARG:HH22	1:C:604:ASP:CG	2.14	0.51
1:C:165:MET:HG2	1:C:166:VAL:N	2.26	0.51
1:C:183:ALA:O	1:C:216:MET:HG2	2.10	0.51
1:A:182:PRO:HA	1:A:211:THR:O	2.09	0.51
1:C:309:THR:HB	1:C:313:LEU:HD23	1.92	0.51
1:D:32:ASP:C	1:D:34:LEU:N	2.64	0.51
1:D:213:ILE:O	1:D:216:MET:HB3	2.11	0.51
1:A:27:LEU:H	1:A:28:PRO:HD2	1.75	0.51
1:B:277:LYS:O	1:B:282:HIS:CE1	2.64	0.51
1:D:90:LEU:O	1:D:93:PRO:HD3	2.10	0.51
1:D:256:ALA:HA	1:D:259:LYS:CB	2.34	0.51
1:D:302:ILE:HG13	1:D:600:GLN:HE21	1.75	0.51
1:A:238:VAL:CG1	1:A:283:LEU:HD13	2.35	0.51
1:A:310:VAL:C	1:A:312:GLU:H	2.13	0.51
1:C:54:ILE:HB	3:C:636:HOH:O	2.10	0.51
1:D:203:GLY:C	1:D:234:LYS:HD2	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ILE:HD12	1:A:300:PRO:HD3	1.92	0.51
1:A:589:ILE:HA	1:A:592:ARG:HB2	1.93	0.51
1:B:215:LEU:CD1	2:B:9001:GDP:C2	2.87	0.51
1:C:235:TYR:O	1:C:236:PRO:O	2.29	0.51
1:D:23:ASP:H	1:D:26:ALA:HB3	1.75	0.51
1:A:134:ASN:ND2	1:A:134:ASN:N	2.59	0.50
1:A:189:THR:HA	1:B:148:LYS:CG	2.42	0.50
1:B:21:HIS:CD2	1:B:592:ARG:NH2	2.79	0.50
1:B:313:LEU:CD2	1:B:597:ARG:HH22	2.08	0.50
1:B:593:LEU:N	1:B:593:LEU:HD23	2.26	0.50
1:C:3:ASN:HA	1:C:6:SER:HB3	1.93	0.50
1:C:12:GLN:HB3	1:C:75:GLN:NE2	2.26	0.50
1:C:184:ASN:OD1	1:C:184:ASN:N	2.44	0.50
1:D:76:LEU:HB2	1:D:138:LEU:O	2.11	0.50
1:D:258:ARG:O	1:D:260:ARG:N	2.44	0.50
1:D:302:ILE:HD11	1:D:600:GLN:HE21	1.76	0.50
1:B:92:LEU:CD1	1:B:95:LYS:HB3	2.28	0.50
1:C:600:GLN:HA	1:C:603:ILE:CD1	2.42	0.50
1:D:253:ASP:OD2	1:D:255:ILE:HG13	2.10	0.50
1:D:264:TYR:C	1:D:264:TYR:HD1	2.15	0.50
1:A:170:ILE:HG23	1:A:177:ILE:HD11	1.92	0.50
1:A:207:PHE:N	1:A:207:PHE:HD2	2.09	0.50
1:A:221:ASP:OD1	1:A:221:ASP:C	2.50	0.50
1:C:77:GLN:HE22	1:C:137:ASN:HD21	1.57	0.50
1:C:162:ILE:C	1:C:164:ASN:H	2.13	0.50
1:C:226:LEU:CD2	1:C:278:MET:SD	2.99	0.50
1:A:180:ILE:HA	1:A:209:VAL:HB	1.92	0.50
1:B:34:LEU:HD12	1:B:172:LYS:HE3	1.93	0.50
1:B:108:GLN:O	1:B:108:GLN:HG2	2.11	0.50
1:B:593:LEU:O	1:B:595:LEU:N	2.44	0.50
1:D:34:LEU:HG	1:D:172:LYS:NZ	2.26	0.50
1:D:195:ILE:HG22	1:D:195:ILE:O	2.11	0.50
1:A:47:LYS:HB3	1:A:180:ILE:HD12	1.93	0.50
1:B:15:CYS:C	1:B:17:ALA:H	2.09	0.50
1:B:77:GLN:HG3	1:B:131:TYR:CE1	2.46	0.50
1:B:257:ALA:O	1:B:258:ARG:C	2.50	0.50
1:C:86:TYR:HD1	1:C:96:LYS:HB3	1.75	0.50
1:A:23:ASP:HB2	1:A:26:ALA:CB	2.29	0.50
1:A:299:ILE:C	1:A:301:GLY:H	2.14	0.50
1:B:66:ILE:CG1	1:B:67:VAL:N	2.75	0.50
1:C:585:ARG:C	1:C:587:SER:N	2.63	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ARG:CB	1:D:121:ILE:HG22	2.39	0.50
1:D:204:ASP:HA	1:D:234:LYS:HE2	1.92	0.50
1:A:30:LEU:O	1:A:34:LEU:CD2	2.59	0.50
1:A:214:ASP:OD2	1:A:214:ASP:N	2.41	0.50
1:B:243:ARG:HG2	1:B:260:ARG:NH1	2.26	0.50
1:C:257:ALA:O	1:C:260:ARG:N	2.44	0.50
1:D:306:ILE:O	1:D:307:ASN:C	2.49	0.50
1:A:226:LEU:CD2	1:A:278:MET:HE1	2.42	0.50
1:A:245:GLN:OE1	1:A:248:ILE:HD11	2.11	0.50
1:A:286:MET:O	1:A:287:LEU:C	2.49	0.50
1:B:211:THR:O	1:B:212:LYS:O	2.29	0.50
1:C:100:PHE:HA	1:C:103:VAL:HG23	1.94	0.50
1:C:276:ASN:N	3:C:662:HOH:O	2.43	0.50
1:A:49:SER:O	1:A:52:GLU:N	2.44	0.50
1:A:158:ILE:HG22	1:A:159:VAL:N	2.27	0.50
1:A:186:ASP:OD1	1:A:187:LEU:N	2.45	0.50
1:B:75:GLN:NE2	3:B:655:HOH:O	2.32	0.50
1:B:86:TYR:HA	1:B:97:PHE:O	2.12	0.50
1:B:190:SER:OG	1:B:192:ALA:HB3	2.12	0.50
1:B:299:ILE:C	1:B:301:GLY:H	2.15	0.50
1:C:132:SER:CB	1:C:135:VAL:HG13	2.41	0.50
1:D:9:ASN:OD1	1:D:75:GLN:HG2	2.11	0.50
1:A:69:ARG:HD3	1:A:119:LYS:HB3	1.92	0.49
1:B:196:SER:O	1:B:198:GLU:N	2.45	0.49
1:B:238:VAL:HG11	1:B:283:LEU:HD13	1.94	0.49
1:C:46:GLY:HA3	1:C:211:THR:HG21	1.94	0.49
1:C:142:ASP:OD2	1:C:143:LEU:N	2.45	0.49
1:D:37:ILE:N	1:D:37:ILE:HD13	2.26	0.49
1:D:170:ILE:CG2	1:D:177:ILE:CD1	2.89	0.49
1:D:236:PRO:HG2	1:D:238:VAL:CG2	2.42	0.49
1:D:286:MET:O	1:D:290:HIS:HD2	1.94	0.49
1:B:11:ILE:O	1:B:14:ALA:N	2.42	0.49
1:C:124:VAL:O	1:C:125:PRO:O	2.30	0.49
1:D:23:ASP:OD2	1:D:592:ARG:HB3	2.12	0.49
1:A:152:ASP:CG	1:A:153:GLY:N	2.56	0.49
1:A:308:LYS:HG3	3:A:650:HOH:O	2.12	0.49
1:C:48:SER:HB3	1:C:60:LEU:HD13	1.93	0.49
1:C:66:ILE:HG23	1:C:66:ILE:O	2.12	0.49
1:C:290:HIS:C	1:C:292:GLU:N	2.65	0.49
1:C:309:THR:OG1	3:C:675:HOH:O	2.18	0.49
1:D:309:THR:HA	1:D:312:GLU:CB	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:603:ILE:O	1:D:606:VAL:HB	2.12	0.49
1:A:157:SER:O	1:A:158:ILE:C	2.51	0.49
1:C:27:LEU:N	1:C:28:PRO:HD2	2.26	0.49
1:C:273:HIS:ND1	3:C:668:HOH:O	2.35	0.49
1:C:316:GLU:HA	3:C:684:HOH:O	2.13	0.49
1:D:311:LEU:O	1:D:315:THR:HG23	2.12	0.49
1:A:5:ILE:HD13	1:A:137:ASN:O	2.12	0.49
1:A:187:LEU:HB2	1:A:231:PHE:CD2	2.47	0.49
1:A:207:PHE:CE1	1:A:235:TYR:CD1	3.00	0.49
1:A:299:ILE:C	1:A:301:GLY:N	2.66	0.49
1:C:260:ARG:HD2	1:C:260:ARG:C	2.32	0.49
1:D:277:LYS:O	1:D:282:HIS:CE1	2.66	0.49
1:A:28:PRO:HB3	1:A:308:LYS:NZ	2.27	0.49
1:B:118:SER:O	1:B:119:LYS:HG2	2.13	0.49
1:B:143:LEU:HD21	1:B:169:TYR:HE2	1.75	0.49
1:B:282:HIS:CG	1:B:282:HIS:O	2.66	0.49
1:C:128:LEU:HD12	1:C:128:LEU:O	2.12	0.49
1:D:56:GLY:O	1:D:57:LYS:HB2	2.12	0.49
1:A:224:GLU:CG	1:A:229:ARG:NH1	2.71	0.49
1:A:235:TYR:CB	1:A:236:PRO:CD	2.91	0.49
1:B:12:GLN:HA	1:B:15:CYS:SG	2.53	0.49
1:B:261:GLU:O	1:B:262:ARG:C	2.51	0.49
1:C:79:ILE:O	1:C:79:ILE:HD12	2.12	0.49
1:C:82:GLY:O	1:C:84:ARG:HG3	2.12	0.49
1:C:148:LYS:NZ	1:D:148:LYS:NZ	2.60	0.49
1:C:312:GLU:O	1:C:314:GLU:N	2.46	0.49
1:D:28:PRO:HA	1:D:31:TRP:HB2	1.95	0.49
1:D:70:ARG:NH2	1:D:126:ILE:HD13	2.28	0.49
1:D:250:LYS:O	1:D:252:VAL:N	2.46	0.49
1:D:305:LEU:O	1:D:307:ASN:N	2.45	0.49
1:D:589:ILE:HA	1:D:592:ARG:HG3	1.93	0.49
1:B:124:VAL:CG1	1:B:125:PRO:HD2	2.34	0.49
1:C:302:ILE:HG12	1:C:600:GLN:HG3	1.95	0.49
1:D:27:LEU:N	1:D:28:PRO:CD	2.75	0.49
1:D:41:GLY:HA3	1:D:180:ILE:HG12	1.94	0.49
1:A:23:ASP:HB3	1:A:592:ARG:CD	2.43	0.49
1:A:167:ARG:O	1:A:171:GLU:HG3	2.13	0.49
1:A:272:ARG:HG3	1:A:272:ARG:NH1	2.27	0.49
1:B:158:ILE:HG23	1:B:159:VAL:H	1.78	0.49
1:D:136:VAL:HB	1:D:138:LEU:CD1	2.43	0.49
1:A:55:VAL:HG11	1:A:59:PHE:HE2	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:LYS:HA	1:C:299:ILE:HD13	1.95	0.49
1:A:31:TRP:CE3	1:A:172:LYS:HD3	2.46	0.48
1:A:51:LEU:HA	1:A:54:ILE:CG2	2.43	0.48
1:C:256:ALA:O	1:C:257:ALA:C	2.52	0.48
1:D:193:ILE:O	1:D:194:LYS:C	2.51	0.48
1:D:255:ILE:O	1:D:259:LYS:HB2	2.12	0.48
1:D:264:TYR:C	1:D:264:TYR:CD1	2.86	0.48
1:A:189:THR:HA	1:B:148:LYS:HG3	1.96	0.48
1:B:62:ARG:HD2	1:B:62:ARG:HA	1.47	0.48
1:B:217:ASP:O	1:B:218:LYS:C	2.52	0.48
1:B:222:ALA:O	1:B:223:VAL:C	2.51	0.48
1:C:39:VAL:HG12	1:C:178:LEU:HD23	1.95	0.48
1:C:228:GLY:O	1:C:232:LYS:HE2	2.13	0.48
1:C:305:LEU:C	1:C:307:ASN:N	2.56	0.48
1:D:35:PRO:HG3	1:D:174:ASN:HB3	1.95	0.48
1:A:296:LYS:HZ1	1:C:303:GLN:NE2	2.11	0.48
1:B:27:LEU:N	1:B:28:PRO:CD	2.77	0.48
1:B:89:PHE:HB3	1:B:91:HIS:HB3	1.95	0.48
1:B:233:LEU:HB3	1:B:234:LYS:H	1.44	0.48
1:B:257:ALA:CA	1:B:260:ARG:HD2	2.42	0.48
1:C:309:THR:O	1:C:313:LEU:N	2.46	0.48
1:D:597:ARG:O	1:D:598:ALA:O	2.31	0.48
1:B:42:GLY:HA2	1:B:146:LEU:HB2	1.94	0.48
1:C:301:GLY:O	1:C:305:LEU:HD12	2.13	0.48
1:D:15:CYS:SG	3:D:625:HOH:O	2.60	0.48
1:A:149:VAL:HB	1:B:188:ALA:HA	1.96	0.48
1:A:278:MET:HE3	1:A:278:MET:HB3	1.59	0.48
1:B:187:LEU:C	1:B:189:THR:H	2.16	0.48
1:B:586:ARG:N	1:B:586:ARG:HD2	2.29	0.48
1:C:263:GLU:O	1:C:265:PHE:N	2.47	0.48
1:C:310:VAL:HA	1:C:313:LEU:HG	1.96	0.48
1:A:34:LEU:HG	1:A:172:LYS:NZ	2.28	0.48
1:A:75:GLN:C	1:A:76:LEU:HD23	2.34	0.48
1:A:224:GLU:HG3	1:A:229:ARG:HH12	1.72	0.48
1:C:5:ILE:HG21	1:C:138:LEU:HA	1.95	0.48
1:D:191:ASP:O	1:D:192:ALA:C	2.50	0.48
1:A:100:PHE:HZ	1:A:130:ILE:HG21	1.77	0.48
1:A:151:VAL:O	1:A:152:ASP:HB3	2.14	0.48
1:B:119:LYS:CB	1:B:154:GLN:HE21	2.27	0.48
1:B:138:LEU:HD21	1:B:288:SER:HB2	1.95	0.48
1:B:299:ILE:C	1:B:301:GLY:N	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ASN:OD1	1:C:277:LYS:N	2.47	0.48
1:A:83:THR:HA	1:A:133:PRO:HG3	1.95	0.48
1:A:238:VAL:HG12	1:A:238:VAL:O	2.13	0.48
1:B:90:LEU:O	1:B:92:LEU:N	2.47	0.48
1:B:105:LYS:HG3	1:B:109:ASP:OD2	2.13	0.48
1:B:291:LEU:O	1:B:292:GLU:C	2.52	0.48
1:B:606:VAL:HA	3:B:676:HOH:O	2.13	0.48
1:A:89:PHE:HB3	1:A:91:HIS:HB3	1.95	0.48
1:A:187:LEU:C	1:A:189:THR:H	2.17	0.48
1:A:252:VAL:HG12	1:A:253:ASP:O	2.14	0.48
1:B:199:VAL:HG23	1:B:200:ASP:N	2.28	0.48
1:C:118:SER:C	1:C:119:LYS:HG2	2.33	0.48
1:C:130:ILE:HG22	1:C:131:TYR:H	1.77	0.48
1:C:593:LEU:O	1:C:595:LEU:N	2.47	0.48
1:D:296:LYS:O	1:D:297:SER:C	2.53	0.48
1:A:302:ILE:HA	1:A:305:LEU:CB	2.40	0.48
1:D:605:ALA:O	1:D:606:VAL:C	2.51	0.48
1:A:59:PHE:C	1:A:104:ARG:HG3	2.34	0.47
1:A:18:LEU:CD1	1:A:595:LEU:HG	2.44	0.47
1:A:66:ILE:HG23	1:A:119:LYS:HD2	1.95	0.47
1:A:82:GLY:O	1:A:84:ARG:HG3	2.14	0.47
1:A:172:LYS:CE	1:A:175:CYS:HB3	2.35	0.47
1:B:118:SER:C	1:B:119:LYS:HG2	2.34	0.47
1:D:8:VAL:O	1:D:11:ILE:HB	2.13	0.47
1:D:57:LYS:HE2	1:D:100:PHE:CD1	2.49	0.47
1:D:170:ILE:HG23	1:D:177:ILE:HD11	1.95	0.47
1:A:128:LEU:CD1	1:A:130:ILE:HG12	2.45	0.47
1:B:54:ILE:HG22	1:B:54:ILE:O	2.14	0.47
1:B:180:ILE:HD12	1:B:180:ILE:H	1.79	0.47
1:C:56:GLY:O	1:C:254:MET:HG3	2.14	0.47
1:C:591:LYS:O	1:C:595:LEU:HD12	2.14	0.47
1:D:23:ASP:CG	1:D:592:ARG:HB3	2.35	0.47
1:D:124:VAL:O	1:D:125:PRO:O	2.32	0.47
1:A:176:ILE:HG21	1:A:207:PHE:CE2	2.49	0.47
1:A:200:ASP:OD2	1:A:205:ARG:O	2.32	0.47
1:B:8:VAL:O	1:B:9:ASN:C	2.53	0.47
1:B:244:SER:HB3	2:B:9001:GDP:HN22	1.78	0.47
1:B:313:LEU:HD23	1:B:597:ARG:HH21	1.65	0.47
1:D:137:ASN:HA	3:D:655:HOH:O	2.15	0.47
1:D:302:ILE:CD1	1:D:600:GLN:HE21	2.27	0.47
1:D:597:ARG:HG3	1:D:597:ARG:HH11	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:HB3	1:A:142:ASP:HB3	1.95	0.47
1:A:143:LEU:CD2	1:A:169:TYR:HD2	2.24	0.47
1:B:243:ARG:HB3	1:B:247:ASP:HB2	1.96	0.47
1:B:256:ALA:O	1:B:257:ALA:O	2.33	0.47
1:C:279:GLY:C	1:C:281:GLU:N	2.68	0.47
1:D:99:ASP:OD2	1:D:102:ALA:HB2	2.14	0.47
1:D:265:PHE:CE2	1:D:278:MET:CE	2.97	0.47
1:D:299:ILE:CB	1:D:300:PRO:HD3	2.44	0.47
1:A:8:VAL:O	1:A:11:ILE:HB	2.15	0.47
1:A:47:LYS:O	1:A:48:SER:C	2.53	0.47
1:A:92:LEU:CD1	1:A:95:LYS:HE3	2.30	0.47
1:B:200:ASP:OD2	1:B:205:ARG:HG2	2.14	0.47
1:B:315:THR:HG21	1:B:589:ILE:HD13	1.96	0.47
1:C:246:ALA:O	1:C:250:LYS:HG3	2.15	0.47
1:A:43:GLN:H	1:A:146:LEU:N	2.12	0.47
1:A:217:ASP:CG	1:A:218:LYS:H	2.17	0.47
1:A:233:LEU:HD12	1:A:233:LEU:HA	1.69	0.47
1:B:37:ILE:O	1:B:140:LEU:HA	2.15	0.47
1:B:52:GLU:HG3	1:B:60:LEU:HD12	1.96	0.47
1:B:59:PHE:CE1	1:B:60:LEU:HG	2.49	0.47
1:C:11:ILE:O	1:C:13:ARG:N	2.48	0.47
1:C:13:ARG:NE	3:C:351:HOH:O	2.47	0.47
1:D:8:VAL:CG2	1:D:295:ILE:HG21	2.45	0.47
1:D:57:LYS:O	1:D:59:PHE:HD2	1.97	0.47
1:D:143:LEU:HD23	1:D:143:LEU:HA	1.46	0.47
1:D:205:ARG:O	1:D:205:ARG:HG3	2.15	0.47
1:D:211:THR:O	1:D:212:LYS:HB2	2.15	0.47
1:A:39:VAL:HG23	1:A:180:ILE:HD11	1.96	0.47
1:C:6:SER:HB3	1:C:137:ASN:HD21	1.79	0.47
1:C:182:PRO:HB2	1:C:212:LYS:HD2	1.97	0.47
1:A:215:LEU:HD21	2:A:9001:GDP:C2	2.49	0.47
1:A:601:SER:HA	1:A:604:ASP:HB2	1.97	0.47
1:B:172:LYS:CG	1:B:175:CYS:HB2	2.44	0.47
1:B:196:SER:C	1:B:198:GLU:N	2.67	0.47
1:C:263:GLU:O	1:C:264:TYR:C	2.53	0.47
1:D:146:LEU:HD12	1:D:191:ASP:HB3	1.96	0.47
1:A:44:SER:OG	1:B:186:ASP:HB2	2.14	0.47
1:A:47:LYS:HE3	1:A:143:LEU:O	2.14	0.47
1:A:90:LEU:HB3	3:A:646:HOH:O	2.14	0.47
1:C:140:LEU:HD23	1:C:141:ILE:N	2.30	0.47
1:D:285:LYS:N	3:D:660:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ASN:O	1:D:311:LEU:HD23	2.15	0.47
1:B:79:ILE:HG12	1:B:132:SER:C	2.35	0.46
1:C:189:THR:C	1:D:148:LYS:HD3	2.35	0.46
1:C:203:GLY:O	1:C:204:ASP:C	2.53	0.46
1:C:302:ILE:CG1	1:C:603:ILE:HD12	2.46	0.46
1:D:167:ARG:O	1:D:169:TYR:N	2.48	0.46
1:B:30:LEU:O	1:B:34:LEU:HB2	2.15	0.46
1:B:226:LEU:C	1:B:228:GLY:H	2.19	0.46
1:C:264:TYR:O	1:C:267:ASN:N	2.45	0.46
1:C:277:LYS:O	1:C:278:MET:HG2	2.15	0.46
1:D:15:CYS:C	1:D:17:ALA:N	2.68	0.46
1:D:141:ILE:CD1	3:D:656:HOH:O	2.57	0.46
1:D:244:SER:C	1:D:246:ALA:H	2.18	0.46
1:A:34:LEU:HD23	1:A:172:LYS:NZ	2.30	0.46
1:A:59:PHE:HD1	1:A:59:PHE:O	1.98	0.46
1:A:301:GLY:O	1:A:305:LEU:N	2.48	0.46
1:B:13:ARG:CB	3:B:655:HOH:O	2.57	0.46
1:C:95:LYS:HG3	1:C:96:LYS:N	2.31	0.46
1:C:199:VAL:O	1:C:200:ASP:HB3	2.15	0.46
1:C:241:VAL:HG21	1:C:264:TYR:CE2	2.50	0.46
1:C:279:GLY:C	1:C:281:GLU:H	2.19	0.46
1:D:165:MET:O	1:D:167:ARG:N	2.48	0.46
1:A:6:SER:HB2	1:A:77:GLN:HE21	1.80	0.46
1:C:57:LYS:HG2	1:C:100:PHE:HE1	1.79	0.46
1:C:100:PHE:C	1:C:102:ALA:N	2.69	0.46
1:C:103:VAL:O	1:C:107:ILE:HG12	2.15	0.46
1:C:130:ILE:CG2	1:C:131:TYR:N	2.77	0.46
1:D:12:GLN:O	1:D:13:ARG:C	2.54	0.46
1:A:69:ARG:HD3	1:A:119:LYS:HA	1.97	0.46
1:B:154:GLN:HB3	1:B:158:ILE:HG21	1.96	0.46
1:C:28:PRO:O	1:C:32:ASP:CB	2.53	0.46
1:C:148:LYS:HZ1	1:D:148:LYS:NZ	2.13	0.46
1:A:59:PHE:CZ	1:A:74:LEU:HD21	2.51	0.46
1:A:69:ARG:CD	1:A:119:LYS:HA	2.46	0.46
1:A:213:ILE:O	1:A:216:MET:HB3	2.15	0.46
1:B:155:SER:OG	1:B:156:ASP:N	2.47	0.46
1:B:606:VAL:CG1	3:B:676:HOH:O	2.54	0.46
1:C:34:LEU:O	1:C:35:PRO:C	2.50	0.46
1:C:132:SER:HB3	1:C:135:VAL:CG1	2.44	0.46
1:C:178:LEU:HD12	1:C:178:LEU:HA	1.80	0.46
1:D:222:ALA:C	1:D:224:GLU:N	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:HG11	1:A:59:PHE:CD2	2.51	0.46
1:A:62:ARG:HB2	1:A:62:ARG:HH11	1.80	0.46
1:A:191:ASP:HB2	3:A:649:HOH:O	2.15	0.46
1:B:103:VAL:O	1:B:107:ILE:HG13	2.15	0.46
1:B:159:VAL:HG12	1:B:160:LYS:HG3	1.97	0.46
1:B:261:GLU:O	1:B:265:PHE:N	2.48	0.46
1:C:233:LEU:HG	1:C:234:LYS:H	1.80	0.46
1:D:50:VAL:O	1:D:50:VAL:HG12	2.16	0.46
1:D:54:ILE:HG22	1:D:55:VAL:N	2.29	0.46
1:B:18:LEU:HD12	1:B:18:LEU:O	2.14	0.46
1:B:69:ARG:HD2	1:B:69:ARG:N	2.31	0.46
1:B:585:ARG:O	1:B:588:ALA:N	2.43	0.46
1:C:47:LYS:C	1:C:49:SER:N	2.69	0.46
1:A:183:ALA:HB1	1:A:216:MET:CE	2.45	0.46
1:B:52:GLU:CG	1:B:60:LEU:HD12	2.45	0.46
1:C:162:ILE:C	1:C:164:ASN:N	2.69	0.46
1:D:38:ALA:HA	1:D:141:ILE:HG13	1.98	0.46
1:D:151:VAL:HG22	1:D:152:ASP:OD2	2.16	0.46
1:A:286:MET:HE2	1:A:286:MET:HB3	1.77	0.46
1:B:5:ILE:CG2	1:B:6:SER:H	2.22	0.46
1:B:94:ARG:NH1	1:B:94:ARG:HB2	2.30	0.46
1:B:124:VAL:HG12	1:B:125:PRO:CD	2.33	0.46
1:D:34:LEU:N	1:D:35:PRO:HD3	2.30	0.46
1:D:136:VAL:HG23	1:D:284:ALA:HB1	1.96	0.46
1:A:79:ILE:HD11	1:A:132:SER:N	2.31	0.45
1:B:37:ILE:HD12	1:B:37:ILE:N	2.27	0.45
1:B:40:VAL:HG13	1:B:166:VAL:CG1	2.46	0.45
1:C:34:LEU:N	1:C:35:PRO:CD	2.79	0.45
1:C:295:ILE:C	1:C:297:SER:H	2.20	0.45
1:D:597:ARG:HH11	1:D:597:ARG:CG	2.29	0.45
1:A:234:LYS:CE	1:C:597:ARG:NH2	2.80	0.45
1:A:251:ASN:O	1:A:252:VAL:C	2.55	0.45
1:C:606:VAL:HG12	1:C:606:VAL:O	2.16	0.45
1:D:43:GLN:HE21	1:D:43:GLN:HB3	1.49	0.45
1:D:89:PHE:HE2	1:D:128:LEU:HB2	1.79	0.45
1:D:594:GLU:O	1:D:595:LEU:C	2.55	0.45
1:A:76:LEU:HD23	1:A:76:LEU:N	2.31	0.45
1:A:195:ILE:HA	1:A:198:GLU:HG2	1.97	0.45
1:B:252:VAL:CG1	1:B:260:ARG:HH21	2.23	0.45
1:D:585:ARG:O	1:D:588:ALA:N	2.50	0.45
1:A:39:VAL:HA	1:A:178:LEU:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:HG13	1:A:133:PRO:N	2.32	0.45
1:A:589:ILE:HG22	1:A:589:ILE:O	2.15	0.45
1:B:32:ASP:C	1:B:34:LEU:N	2.67	0.45
1:B:143:LEU:HD21	1:B:169:TYR:CD2	2.51	0.45
1:B:170:ILE:HG22	1:B:199:VAL:HG21	1.99	0.45
1:B:586:ARG:C	1:B:588:ALA:N	2.70	0.45
1:C:186:ASP:O	1:C:189:THR:N	2.47	0.45
1:C:216:MET:SD	1:C:222:ALA:HB2	2.55	0.45
1:D:99:ASP:O	1:D:102:ALA:HB3	2.16	0.45
1:B:39:VAL:HG23	1:B:180:ILE:HD11	1.98	0.45
1:B:67:VAL:O	1:B:69:ARG:HD2	2.15	0.45
1:B:93:PRO:O	1:B:94:ARG:C	2.55	0.45
1:D:199:VAL:HG12	1:D:200:ASP:N	2.30	0.45
1:A:8:VAL:CG1	1:A:33:SER:O	2.64	0.45
1:B:34:LEU:HA	1:B:34:LEU:HD22	1.44	0.45
1:C:78:LYS:HB2	1:C:135:VAL:O	2.16	0.45
1:D:47:LYS:NZ	1:D:145:GLY:H	2.15	0.45
1:D:598:ALA:O	1:D:601:SER:N	2.49	0.45
1:A:47:LYS:CA	1:A:180:ILE:HD12	2.47	0.45
1:A:68:THR:O	1:A:144:PRO:HB3	2.17	0.45
1:A:86:TYR:CZ	1:A:131:TYR:HD2	2.35	0.45
1:A:213:ILE:HG23	1:A:216:MET:CE	2.46	0.45
1:B:15:CYS:HB2	1:B:16:THR:H	1.46	0.45
1:B:90:LEU:C	1:B:92:LEU:N	2.69	0.45
1:B:170:ILE:HG21	1:B:199:VAL:HG21	1.96	0.45
1:B:283:LEU:HD12	1:B:283:LEU:HA	1.85	0.45
1:C:77:GLN:NE2	1:C:137:ASN:HD21	2.15	0.45
1:C:148:LYS:CE	1:D:148:LYS:NZ	2.80	0.45
1:C:283:LEU:HG	1:C:284:ALA:N	2.31	0.45
1:D:313:LEU:HD21	1:D:597:ARG:HH21	1.81	0.45
1:A:166:VAL:HG12	1:A:167:ARG:N	2.31	0.45
1:A:204:ASP:HA	1:A:234:LYS:NZ	2.32	0.45
1:B:16:THR:HG21	1:B:30:LEU:HD13	1.98	0.45
1:B:241:VAL:HG12	1:B:241:VAL:O	2.17	0.45
1:C:3:ASN:C	1:C:6:SER:OG	2.55	0.45
1:C:187:LEU:HA	1:C:187:LEU:HD12	1.71	0.45
1:C:225:ILE:HG22	1:C:225:ILE:O	2.17	0.45
1:D:74:LEU:N	1:D:140:LEU:O	2.47	0.45
1:D:250:LYS:O	1:D:251:ASN:C	2.55	0.45
1:D:300:PRO:C	1:D:302:ILE:N	2.70	0.45
1:A:95:LYS:HG2	1:A:96:LYS:H	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLU:C	1:A:225:ILE:HG12	2.34	0.45
1:B:25:SER:O	1:B:308:LYS:HD2	2.17	0.45
1:B:76:LEU:HD13	1:B:135:VAL:HB	1.98	0.45
1:B:593:LEU:O	1:B:596:TYR:N	2.41	0.45
1:C:86:TYR:HE1	1:C:96:LYS:CD	2.25	0.45
1:C:176:ILE:HD11	1:C:290:HIS:CE1	2.52	0.45
1:D:8:VAL:HG21	1:D:295:ILE:HG21	1.99	0.45
1:D:23:ASP:OD2	1:D:26:ALA:CB	2.63	0.45
1:D:73:VAL:HG12	3:D:653:HOH:O	2.17	0.45
1:D:226:LEU:C	1:D:228:GLY:N	2.70	0.45
1:B:7:LEU:O	1:B:11:ILE:N	2.48	0.45
1:B:257:ALA:C	1:B:260:ARG:HG2	2.38	0.45
1:B:291:LEU:HD12	1:B:291:LEU:HA	1.52	0.45
1:C:89:PHE:CD2	1:C:91:HIS:CB	3.00	0.45
1:C:183:ALA:HB1	1:C:216:MET:HE2	1.99	0.45
1:D:112:ASP:HA	1:D:115:THR:OG1	2.17	0.45
1:D:290:HIS:O	1:D:294:VAL:HB	2.17	0.45
1:A:43:GLN:H	1:A:146:LEU:H	1.65	0.44
1:A:273:HIS:CD2	1:A:274:LEU:HD23	2.52	0.44
1:B:27:LEU:H	1:B:28:PRO:CD	2.30	0.44
1:C:258:ARG:O	1:C:259:LYS:C	2.55	0.44
1:D:186:ASP:O	1:D:187:LEU:HD13	2.17	0.44
1:A:195:ILE:HA	1:A:198:GLU:CG	2.47	0.44
1:A:261:GLU:O	1:A:265:PHE:CE1	2.71	0.44
1:A:299:ILE:HD12	1:A:299:ILE:C	2.37	0.44
1:A:593:LEU:O	1:A:594:GLU:C	2.56	0.44
1:B:154:GLN:O	1:B:155:SER:C	2.56	0.44
1:D:170:ILE:CG2	1:D:177:ILE:HD11	2.47	0.44
1:D:604:ASP:O	1:D:605:ALA:C	2.55	0.44
1:A:291:LEU:O	1:A:295:ILE:HG13	2.17	0.44
1:C:23:ASP:HB2	1:C:24:SER:H	1.66	0.44
1:C:173:PRO:HB2	1:C:174:ASN:H	1.47	0.44
1:C:310:VAL:HG23	3:C:675:HOH:O	2.17	0.44
1:D:256:ALA:O	1:D:257:ALA:C	2.54	0.44
1:B:305:LEU:O	1:B:306:ILE:C	2.56	0.44
1:C:23:ASP:H	1:C:26:ALA:HB2	1.83	0.44
1:C:187:LEU:HB2	3:C:666:HOH:O	2.17	0.44
1:C:264:TYR:HE1	1:C:268:THR:HG1	1.62	0.44
1:D:16:THR:CG2	1:D:125:PRO:HG2	2.47	0.44
1:D:247:ASP:O	1:D:248:ILE:C	2.56	0.44
1:D:274:LEU:CD2	1:D:277:LYS:NZ	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:C	1:B:92:LEU:H	2.20	0.44
1:C:79:ILE:O	1:C:81:ASP:N	2.51	0.44
1:C:283:LEU:HD11	1:C:287:LEU:HD11	2.00	0.44
1:C:302:ILE:CD1	3:C:658:HOH:O	2.60	0.44
1:A:224:GLU:CG	1:A:229:ARG:HH12	2.31	0.44
1:B:172:LYS:O	1:B:174:ASN:N	2.50	0.44
1:B:212:LYS:HB3	1:B:215:LEU:CD1	2.37	0.44
1:B:300:PRO:C	1:B:302:ILE:H	2.21	0.44
1:B:315:THR:HG21	1:B:589:ILE:CD1	2.48	0.44
1:C:188:ALA:HA	1:D:149:VAL:HG23	1.98	0.44
1:D:59:PHE:O	1:D:104:ARG:HA	2.16	0.44
1:D:158:ILE:HD11	1:D:162:ILE:HD11	1.99	0.44
1:A:245:GLN:HA	1:A:248:ILE:HG12	1.98	0.44
1:B:41:GLY:O	1:B:47:LYS:HD3	2.18	0.44
1:D:168:SER:O	1:D:172:LYS:HE3	2.18	0.44
1:D:193:ILE:O	1:D:195:ILE:N	2.50	0.44
1:D:305:LEU:O	1:D:308:LYS:N	2.39	0.44
1:A:37:ILE:CD1	1:A:140:LEU:HD23	2.48	0.44
1:B:100:PHE:O	1:B:103:VAL:N	2.46	0.44
1:C:47:LYS:O	1:C:49:SER:N	2.51	0.44
1:C:171:GLU:HA	1:C:199:VAL:HG11	2.00	0.44
1:C:252:VAL:CG1	1:C:253:ASP:N	2.80	0.44
1:D:4:LEU:HD13	1:D:295:ILE:HB	1.99	0.44
1:D:23:ASP:CG	1:D:26:ALA:HB2	2.38	0.44
1:D:86:TYR:HE1	1:D:96:LYS:HD3	1.78	0.44
1:D:245:GLN:HG3	1:D:245:GLN:O	2.18	0.44
1:A:62:ARG:HA	1:A:62:ARG:HD3	1.71	0.44
1:A:169:TYR:HD1	1:A:169:TYR:HA	1.75	0.44
1:B:33:SER:O	1:B:33:SER:OG	2.31	0.44
1:B:42:GLY:O	1:B:43:GLN:C	2.54	0.44
1:B:250:LYS:H	1:B:250:LYS:HG2	1.45	0.44
1:C:167:ARG:O	1:C:170:ILE:N	2.43	0.44
1:C:186:ASP:O	1:C:187:LEU:C	2.55	0.44
1:D:80:ASP:C	1:D:82:GLY:N	2.72	0.44
1:A:47:LYS:CB	1:A:180:ILE:HD12	2.48	0.43
1:A:200:ASP:N	1:A:201:PRO:HD3	2.29	0.43
1:C:99:ASP:O	1:C:101:ALA:N	2.51	0.43
1:C:222:ALA:N	1:C:271:TYR:OH	2.48	0.43
1:D:227:GLU:OE2	1:D:274:LEU:HD11	2.18	0.43
1:D:310:VAL:O	1:D:310:VAL:HG13	2.18	0.43
1:A:212:LYS:CG	2:A:9001:GDP:C5	3.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:PRO:HB2	1:B:67:VAL:HB	2.00	0.43
1:B:222:ALA:O	1:B:224:GLU:N	2.51	0.43
1:C:51:LEU:HD23	1:C:51:LEU:HA	1.79	0.43
1:C:62:ARG:NE	3:C:667:HOH:O	2.50	0.43
1:C:313:LEU:HD12	1:C:314:GLU:HG3	2.00	0.43
1:C:600:GLN:HA	1:C:603:ILE:HD11	2.00	0.43
1:D:77:GLN:O	1:D:131:TYR:HA	2.18	0.43
1:D:245:GLN:O	1:D:249:ASN:OD1	2.36	0.43
1:A:71:PRO:O	1:A:72:LEU:HB2	2.16	0.43
1:A:203:GLY:O	1:A:234:LYS:HD3	2.18	0.43
1:C:235:TYR:HA	1:C:236:PRO:HD2	1.69	0.43
1:D:262:ARG:O	1:D:263:GLU:C	2.56	0.43
1:A:181:SER:O	1:A:210:LEU:HA	2.18	0.43
1:B:50:VAL:O	1:B:53:SER:HB2	2.19	0.43
1:C:151:VAL:O	1:C:152:ASP:HB2	2.17	0.43
1:D:62:ARG:HH21	1:D:248:ILE:HD11	1.82	0.43
1:D:91:HIS:HE2	1:D:110:GLU:CD	2.21	0.43
1:D:309:THR:HA	1:D:312:GLU:CG	2.48	0.43
1:A:4:LEU:HB2	3:A:609:HOH:O	2.18	0.43
1:A:41:GLY:O	1:A:145:GLY:HA2	2.18	0.43
1:A:258:ARG:HE	1:A:281:GLU:HG3	1.84	0.43
1:B:199:VAL:O	1:B:201:PRO:HD3	2.19	0.43
1:D:92:LEU:CD1	1:D:106:GLU:OE2	2.67	0.43
1:D:227:GLU:OE2	1:D:274:LEU:HD21	2.18	0.43
1:D:302:ILE:C	1:D:305:LEU:H	2.22	0.43
1:A:291:LEU:O	1:A:294:VAL:HB	2.19	0.43
1:A:296:LYS:C	1:A:298:ARG:N	2.70	0.43
1:B:168:SER:O	1:B:169:TYR:C	2.54	0.43
1:B:177:ILE:HB	1:B:206:THR:HG23	2.00	0.43
1:C:91:HIS:NE2	1:C:110:GLU:CD	2.72	0.43
1:C:160:LYS:O	1:C:164:ASN:CB	2.62	0.43
1:C:203:GLY:O	1:C:206:THR:N	2.52	0.43
1:D:235:TYR:N	1:D:235:TYR:CD2	2.86	0.43
1:A:48:SER:O	1:A:60:LEU:HD13	2.18	0.43
1:A:149:VAL:O	1:A:151:VAL:HG12	2.18	0.43
1:A:598:ALA:O	1:A:602:GLU:HB2	2.18	0.43
1:B:5:ILE:O	1:B:8:VAL:N	2.51	0.43
1:B:298:ARG:O	1:B:301:GLY:N	2.48	0.43
1:B:311:LEU:C	3:B:656:HOH:O	2.56	0.43
1:C:149:VAL:HG11	1:D:193:ILE:HB	1.99	0.43
1:C:187:LEU:C	1:C:189:THR:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:LYS:C	1:C:282:HIS:CE1	2.92	0.43
1:D:15:CYS:SG	1:D:595:LEU:HD11	2.58	0.43
1:D:117:ARG:HG3	1:D:117:ARG:HH11	1.82	0.43
1:A:99:ASP:O	1:A:99:ASP:OD2	2.36	0.43
1:A:143:LEU:HD12	1:A:166:VAL:HG22	2.00	0.43
1:A:588:ALA:HB1	1:A:592:ARG:HE	1.84	0.43
1:C:89:PHE:HB3	1:C:90:LEU:H	1.55	0.43
1:C:278:MET:HB2	3:C:662:HOH:O	2.18	0.43
1:D:131:TYR:CB	3:D:640:HOH:O	2.56	0.43
1:A:4:LEU:N	3:A:609:HOH:O	2.39	0.43
1:B:287:LEU:O	1:B:290:HIS:N	2.50	0.43
1:C:66:ILE:O	1:C:69:ARG:NE	2.51	0.43
1:C:260:ARG:O	1:C:263:GLU:N	2.52	0.43
1:D:113:ARG:HG2	1:D:113:ARG:HH11	1.83	0.43
1:D:222:ALA:C	1:D:224:GLU:H	2.21	0.43
1:A:74:LEU:HA	1:A:74:LEU:HD12	1.77	0.43
1:A:74:LEU:HD11	1:A:128:LEU:CD2	2.49	0.43
1:B:15:CYS:C	1:B:17:ALA:N	2.71	0.43
1:B:39:VAL:HG23	1:B:180:ILE:CD1	2.49	0.43
1:B:103:VAL:HG12	1:B:104:ARG:N	2.34	0.43
1:B:222:ALA:C	1:B:224:GLU:N	2.71	0.43
1:B:244:SER:HB3	2:B:9001:GDP:N2	2.33	0.43
1:B:264:TYR:O	1:B:268:THR:OG1	2.36	0.43
1:C:105:LYS:O	1:C:109:ASP:HB2	2.19	0.43
1:C:597:ARG:O	1:C:600:GLN:N	2.52	0.43
1:D:235:TYR:HB3	1:D:236:PRO:CD	2.48	0.43
1:D:593:LEU:HD23	1:D:593:LEU:HA	1.67	0.43
1:B:25:SER:HB2	1:B:308:LYS:NZ	2.31	0.42
1:C:205:ARG:O	1:C:205:ARG:CG	2.66	0.42
1:C:263:GLU:O	1:C:266:SER:N	2.39	0.42
1:D:59:PHE:CE1	1:D:60:LEU:HG	2.54	0.42
1:A:90:LEU:HB2	1:A:127:HIS:HB2	2.00	0.42
1:B:59:PHE:C	1:B:104:ARG:HB2	2.39	0.42
1:B:119:LYS:HD3	1:B:119:LYS:N	2.35	0.42
1:B:586:ARG:CD	1:B:586:ARG:H	2.29	0.42
1:C:86:TYR:CD2	1:C:86:TYR:O	2.73	0.42
1:C:283:LEU:O	1:C:285:LYS:N	2.51	0.42
1:D:50:VAL:HG22	1:D:242:ASN:HD21	1.83	0.42
1:D:106:GLU:HA	1:D:109:ASP:HB3	2.01	0.42
1:D:286:MET:N	3:D:660:HOH:O	2.17	0.42
1:A:113:ARG:C	1:A:114:GLU:HG3	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:O	1:A:286:MET:HB2	2.19	0.42
1:A:302:ILE:O	1:A:304:SER:N	2.52	0.42
1:B:72:LEU:HA	1:B:126:ILE:HB	2.01	0.42
1:B:295:ILE:C	1:B:297:SER:N	2.72	0.42
1:C:47:LYS:C	1:C:49:SER:H	2.22	0.42
1:C:116:GLY:O	1:C:117:ARG:HB2	2.18	0.42
1:C:143:LEU:HA	1:C:144:PRO:HD3	1.89	0.42
1:C:177:ILE:HB	1:C:206:THR:OG1	2.19	0.42
1:C:265:PHE:O	1:C:272:ARG:HA	2.19	0.42
1:A:293:ARG:HH21	1:C:600:GLN:HG2	1.85	0.42
1:C:58:ASP:HB3	1:C:59:PHE:H	1.57	0.42
1:D:4:LEU:HD23	1:D:4:LEU:HA	1.78	0.42
1:A:207:PHE:CZ	1:A:235:TYR:HE1	2.35	0.42
1:A:299:ILE:HD12	1:A:300:PRO:CD	2.50	0.42
1:B:216:MET:HE2	1:B:221:ASP:O	2.19	0.42
1:B:305:LEU:HB2	1:B:600:GLN:OE1	2.19	0.42
1:C:100:PHE:O	1:C:101:ALA:C	2.58	0.42
1:C:187:LEU:C	1:C:189:THR:N	2.73	0.42
1:C:262:ARG:O	1:C:263:GLU:O	2.37	0.42
1:C:295:ILE:O	1:C:298:ARG:N	2.52	0.42
1:D:56:GLY:HA2	1:D:254:MET:HE2	2.00	0.42
1:D:303:GLN:HA	1:D:306:ILE:HD11	2.01	0.42
1:A:593:LEU:HA	1:A:593:LEU:HD23	1.79	0.42
1:B:79:ILE:CD1	1:B:132:SER:HA	2.49	0.42
1:B:143:LEU:HD23	1:B:143:LEU:HA	1.70	0.42
1:B:283:LEU:O	1:B:284:ALA:C	2.56	0.42
1:D:5:ILE:HD12	1:D:137:ASN:C	2.40	0.42
1:D:71:PRO:HA	1:D:142:ASP:O	2.19	0.42
1:D:236:PRO:O	1:D:238:VAL:HG23	2.20	0.42
1:D:271:TYR:O	1:D:272:ARG:C	2.57	0.42
1:D:597:ARG:NH1	1:D:597:ARG:CG	2.82	0.42
1:A:23:ASP:O	1:A:24:SER:OG	2.30	0.42
1:A:56:GLY:HA2	1:A:254:MET:HE2	2.01	0.42
1:A:183:ALA:HB3	1:A:212:LYS:O	2.20	0.42
1:C:230:SER:OG	1:C:231:PHE:HD2	2.02	0.42
1:C:283:LEU:O	1:C:286:MET:N	2.52	0.42
1:D:57:LYS:N	1:D:254:MET:HG3	2.34	0.42
1:D:75:GLN:HG3	3:D:653:HOH:O	2.20	0.42
1:A:27:LEU:HD22	1:A:31:TRP:CD1	2.55	0.42
1:A:155:SER:HB2	3:A:638:HOH:O	2.20	0.42
1:B:4:LEU:O	1:B:4:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:SER:O	1:B:245:GLN:C	2.58	0.42
1:C:241:VAL:HG21	1:C:264:TYR:CD2	2.55	0.42
1:C:302:ILE:N	1:C:305:LEU:HD12	2.35	0.42
1:D:16:THR:HG21	1:D:125:PRO:HG3	2.02	0.42
1:D:233:LEU:HD13	1:D:233:LEU:HA	1.73	0.42
1:A:60:LEU:HA	1:A:61:PRO:HD3	1.93	0.42
1:A:216:MET:HG2	1:A:217:ASP:N	2.34	0.42
1:C:185:GLN:HB2	3:C:623:HOH:O	2.18	0.42
1:C:253:ASP:CG	1:C:254:MET:N	2.73	0.42
1:C:286:MET:O	1:C:290:HIS:HB2	2.20	0.42
1:C:296:LYS:HD2	1:C:296:LYS:O	2.20	0.42
1:D:218:LYS:NZ	1:D:218:LYS:HB3	2.35	0.42
1:D:299:ILE:N	1:D:300:PRO:CD	2.83	0.42
1:A:3:ASN:O	1:A:6:SER:HB3	2.20	0.42
1:A:263:GLU:O	1:A:264:TYR:O	2.38	0.42
1:B:50:VAL:HG12	1:B:51:LEU:N	2.34	0.42
1:B:67:VAL:C	1:B:69:ARG:HD2	2.40	0.42
1:C:92:LEU:HA	1:C:93:PRO:HD2	1.88	0.42
1:C:110:GLU:OE2	1:C:110:GLU:HA	2.20	0.42
1:C:187:LEU:HD11	1:C:193:ILE:HD11	2.01	0.42
1:D:118:SER:C	1:D:119:LYS:HG2	2.41	0.42
1:D:176:ILE:H	1:D:176:ILE:CD1	2.08	0.42
1:D:274:LEU:CD2	1:D:277:LYS:HZ1	2.32	0.42
2:D:9001:GDP:PB	3:D:631:HOH:O	2.77	0.42
1:A:300:PRO:O	1:A:302:ILE:O	2.38	0.41
1:B:249:ASN:C	1:B:251:ASN:N	2.74	0.41
1:D:80:ASP:O	1:D:81:ASP:C	2.57	0.41
1:D:147:THR:O	1:D:159:VAL:HG12	2.20	0.41
1:D:156:ASP:C	1:D:158:ILE:H	2.23	0.41
1:D:258:ARG:O	1:D:259:LYS:C	2.58	0.41
1:A:157:SER:C	1:A:159:VAL:N	2.70	0.41
1:A:244:SER:HB2	2:A:9001:GDP:N2	2.35	0.41
1:B:47:LYS:HB2	1:B:48:SER:H	1.75	0.41
1:B:235:TYR:N	1:B:235:TYR:HD2	2.16	0.41
1:C:4:LEU:O	1:C:4:LEU:HD22	2.20	0.41
1:C:207:PHE:CD1	1:C:208:GLY:N	2.81	0.41
1:C:225:ILE:HG12	1:C:230:SER:HB3	1.98	0.41
1:C:273:HIS:N	3:C:668:HOH:O	2.53	0.41
1:C:290:HIS:C	1:C:290:HIS:ND1	2.73	0.41
1:C:302:ILE:CA	1:C:305:LEU:HD12	2.50	0.41
1:C:593:LEU:C	1:C:595:LEU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:SER:N	2:D:9001:GDP:O1B	2.47	0.41
1:A:33:SER:C	1:A:35:PRO:HD2	2.41	0.41
1:A:34:LEU:HD12	1:A:36:ALA:HB3	2.01	0.41
1:A:70:ARG:HH22	1:A:124:VAL:HG23	1.84	0.41
1:C:223:VAL:CG1	1:C:224:GLU:N	2.83	0.41
1:C:598:ALA:O	1:C:602:GLU:CG	2.63	0.41
1:C:600:GLN:O	1:C:600:GLN:CG	2.60	0.41
1:A:16:THR:OG1	1:A:127:HIS:NE2	2.53	0.41
1:A:69:ARG:NH1	1:A:116:GLY:O	2.52	0.41
1:A:80:ASP:C	1:A:82:GLY:H	2.24	0.41
1:A:104:ARG:HG2	1:A:104:ARG:O	2.20	0.41
1:A:200:ASP:C	1:A:202:SER:N	2.70	0.41
1:A:299:ILE:O	1:A:302:ILE:HB	2.20	0.41
1:C:7:LEU:O	1:C:8:VAL:C	2.58	0.41
1:C:128:LEU:C	1:C:128:LEU:CD1	2.89	0.41
1:C:305:LEU:HB2	1:C:600:GLN:NE2	2.35	0.41
1:D:165:MET:C	1:D:167:ARG:N	2.74	0.41
1:A:56:GLY:O	1:A:254:MET:HB3	2.20	0.41
1:A:209:VAL:O	1:A:238:VAL:O	2.39	0.41
1:A:213:ILE:C	1:A:215:LEU:N	2.74	0.41
1:B:4:LEU:O	1:B:4:LEU:CD2	2.69	0.41
1:B:70:ARG:NH2	1:B:124:VAL:N	2.63	0.41
1:B:180:ILE:HA	1:B:209:VAL:HB	2.02	0.41
1:C:256:ALA:O	1:C:257:ALA:O	2.38	0.41
1:C:290:HIS:O	1:C:292:GLU:N	2.53	0.41
1:C:299:ILE:N	1:C:300:PRO:CD	2.84	0.41
1:C:605:ALA:O	1:C:606:VAL:C	2.58	0.41
1:D:310:VAL:O	1:D:314:GLU:OE1	2.38	0.41
1:A:53:SER:HA	1:A:254:MET:HE1	2.02	0.41
1:A:148:LYS:HE3	1:B:191:ASP:N	2.35	0.41
1:A:160:LYS:NZ	3:A:360:HOH:O	2.53	0.41
1:A:174:ASN:CG	1:A:298:ARG:HH22	2.24	0.41
1:A:593:LEU:O	1:A:595:LEU:N	2.53	0.41
1:C:185:GLN:HG3	3:C:623:HOH:O	2.21	0.41
1:C:599:ALA:O	1:C:603:ILE:CG1	2.68	0.41
1:D:103:VAL:O	1:D:106:GLU:N	2.35	0.41
1:D:108:GLN:O	1:D:110:GLU:N	2.53	0.41
1:D:187:LEU:C	1:D:189:THR:N	2.73	0.41
1:A:27:LEU:O	1:A:29:THR:N	2.47	0.41
1:A:57:LYS:CA	1:A:254:MET:HG3	2.51	0.41
1:A:233:LEU:HD22	1:A:237:TRP:HE1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:TYR:HE1	1:B:268:THR:HG21	1.85	0.41
1:C:12:GLN:O	1:C:15:CYS:HB2	2.21	0.41
1:C:32:ASP:O	1:C:34:LEU:N	2.54	0.41
1:C:69:ARG:HH21	1:C:119:LYS:CD	2.27	0.41
1:C:75:GLN:O	1:C:130:ILE:N	2.53	0.41
1:D:599:ALA:C	1:D:601:SER:N	2.73	0.41
1:A:272:ARG:NH1	1:A:272:ARG:CG	2.83	0.41
1:B:16:THR:HA	1:B:19:GLY:H	1.85	0.41
1:C:91:HIS:CE1	1:C:110:GLU:OE2	2.74	0.41
1:C:301:GLY:C	1:C:305:LEU:HD12	2.40	0.41
1:B:69:ARG:HH21	1:B:119:LYS:HD2	1.86	0.41
1:B:268:THR:O	1:B:268:THR:HG22	2.21	0.41
1:C:79:ILE:O	1:C:80:ASP:C	2.59	0.41
1:C:142:ASP:C	1:C:143:LEU:HG	2.42	0.41
1:C:312:GLU:O	1:C:313:LEU:C	2.59	0.41
1:A:45:SER:HA	1:A:182:PRO:CD	2.51	0.41
1:A:204:ASP:HA	1:A:234:LYS:HZ3	1.84	0.41
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.83	0.41
1:B:8:VAL:HG12	1:B:9:ASN:N	2.35	0.41
1:B:43:GLN:NE2	1:B:66:ILE:HB	2.11	0.41
1:B:58:ASP:CB	1:B:104:ARG:HH21	2.22	0.41
1:D:23:ASP:HB3	1:D:592:ARG:CD	2.36	0.41
1:D:264:TYR:HH	1:D:271:TYR:HE1	1.64	0.41
1:A:55:VAL:O	1:A:55:VAL:CG1	2.69	0.40
1:A:57:LYS:HG2	1:A:100:PHE:HD1	1.85	0.40
1:A:164:ASN:O	1:A:165:MET:C	2.60	0.40
1:A:225:ILE:HG22	1:A:237:TRP:CD1	2.56	0.40
1:A:293:ARG:HH21	1:C:600:GLN:CG	2.34	0.40
1:B:57:LYS:HD3	1:B:57:LYS:HA	1.93	0.40
1:B:128:LEU:O	1:B:128:LEU:HG	2.20	0.40
1:B:254:MET:O	1:B:254:MET:HE3	2.21	0.40
1:B:254:MET:O	1:B:257:ALA:CB	2.69	0.40
1:D:27:LEU:O	1:D:30:LEU:N	2.54	0.40
1:D:57:LYS:HG2	1:D:100:PHE:CE1	2.56	0.40
1:D:227:GLU:CG	1:D:229:ARG:NH1	2.83	0.40
1:A:30:LEU:HG	1:A:30:LEU:O	2.22	0.40
1:A:49:SER:O	1:A:52:GLU:HB2	2.21	0.40
1:A:245:GLN:HB2	2:A:9001:GDP:O3'	2.22	0.40
1:B:57:LYS:C	1:B:254:MET:HG3	2.41	0.40
1:C:124:VAL:HA	1:C:125:PRO:HD3	1.88	0.40
1:A:26:ALA:N	1:A:28:PRO:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:GLU:O	1:A:89:PHE:CG	2.74	0.40
1:A:167:ARG:NH2	1:A:195:ILE:CD1	2.84	0.40
1:B:161:ASP:HA	1:B:164:ASN:HD21	1.86	0.40
1:B:245:GLN:O	1:B:246:ALA:C	2.59	0.40
1:B:273:HIS:CG	3:B:688:HOH:O	2.74	0.40
1:B:284:ALA:O	1:B:285:LYS:C	2.60	0.40
1:B:586:ARG:C	1:B:588:ALA:H	2.25	0.40
1:C:49:SER:OG	2:C:9001:GDP:PA	2.80	0.40
1:C:299:ILE:HG12	1:C:300:PRO:HD3	2.02	0.40
1:D:9:ASN:HA	1:D:75:GLN:HE21	1.86	0.40
1:A:34:LEU:CG	1:A:172:LYS:NZ	2.85	0.40
1:A:59:PHE:CD1	1:A:59:PHE:O	2.74	0.40
1:B:79:ILE:HG12	1:B:132:SER:CA	2.51	0.40
1:B:94:ARG:HB2	1:B:94:ARG:HH11	1.86	0.40
1:B:143:LEU:HA	1:B:144:PRO:HD2	1.65	0.40
1:B:144:PRO:HG2	1:B:165:MET:SD	2.61	0.40
1:B:154:GLN:O	1:B:155:SER:O	2.39	0.40
1:B:252:VAL:CG1	1:B:260:ARG:NH2	2.72	0.40
1:A:23:ASP:OD2	1:A:26:ALA:HB3	2.22	0.40
1:A:90:LEU:HA	1:A:90:LEU:HD12	1.67	0.40
1:A:244:SER:N	1:A:247:ASP:OD2	2.55	0.40
1:A:249:ASN:C	1:A:251:ASN:H	2.25	0.40
1:B:146:LEU:CD1	1:B:195:ILE:HG21	2.50	0.40
1:B:172:LYS:HA	1:B:173:PRO:HD2	1.84	0.40
1:B:183:ALA:HB2	1:B:210:LEU:HD13	2.02	0.40
1:C:12:GLN:CB	1:C:75:GLN:NE2	2.84	0.40
1:C:22:GLY:HA2	1:C:26:ALA:CB	2.46	0.40
1:C:74:LEU:O	1:C:75:GLN:CG	2.57	0.40
1:C:149:VAL:HG12	1:D:194:LYS:HB2	2.03	0.40
1:C:302:ILE:C	1:C:304:SER:N	2.68	0.40
1:D:47:LYS:O	1:D:49:SER:N	2.55	0.40
1:D:84:ARG:O	1:D:86:TYR:HB3	2.22	0.40

All (1) 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:234:LYS:NZ	1:D:313:LEU:CD1[1_655]	1.86	0.34

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	335/360 (93%)	201 (60%)	80 (24%)	54 (16%)	0 3
1	B	335/360 (93%)	194 (58%)	81 (24%)	60 (18%)	0 2
1	C	335/360 (93%)	205 (61%)	73 (22%)	57 (17%)	0 2
1	D	335/360 (93%)	192 (57%)	94 (28%)	49 (15%)	0 3
All	All	1340/1440 (93%)	792 (59%)	328 (24%)	220 (16%)	0 3

All (220) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	14	ALA
1	A	43	GLN
1	A	58	ASP
1	A	72	LEU
1	A	80	ASP
1	A	83	THR
1	A	91	HIS
1	A	125	PRO
1	A	200	ASP
1	A	206	THR
1	A	235	TYR
1	A	236	PRO
1	A	264	TYR
1	A	605	ALA
1	B	6	SER
1	B	15	CYS
1	B	16	THR
1	B	25	SER
1	B	47	LYS
1	B	66	ILE
1	B	81	ASP

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Mol	Chain	Res	Type
1	B	86	TYR
1	B	91	HIS
1	B	155	SER
1	B	159	VAL
1	B	246	ALA
1	B	257	ALA
1	B	258	ARG
1	B	260	ARG
1	B	272	ARG
1	B	275	ALA
1	B	306	ILE
1	C	12	GLN
1	C	31	TRP
1	C	58	ASP
1	C	62	ARG
1	C	80	ASP
1	C	81	ASP
1	C	83	THR
1	C	85	GLU
1	C	90	LEU
1	C	100	PHE
1	C	117	ARG
1	C	125	PRO
1	C	173	PRO
1	C	174	ASN
1	C	187	LEU
1	C	204	ASP
1	C	236	PRO
1	C	263	GLU
1	C	264	TYR
1	C	284	ALA
1	C	296	LYS
1	C	306	ILE
1	C	605	ALA
1	D	16	THR
1	D	18	LEU
1	D	20	ASP
1	D	25	SER
1	D	80	ASP
1	D	81	ASP
1	D	91	HIS
1	D	123	SER

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Mol	Chain	Res	Type
1	D	125	PRO
1	D	194	LYS
1	D	235	TYR
1	D	251	ASN
1	D	257	ALA
1	D	272	ARG
1	D	306	ILE
1	D	598	ALA
1	D	599	ALA
1	A	12	GLN
1	A	15	CYS
1	A	30	LEU
1	A	34	LEU
1	A	59	PHE
1	A	85	GLU
1	A	152	ASP
1	A	158	ILE
1	A	192	ALA
1	A	252	VAL
1	A	283	LEU
1	A	296	LYS
1	B	18	LEU
1	B	22	GLY
1	B	33	SER
1	B	58	ASP
1	B	94	ARG
1	B	144	PRO
1	B	156	ASP
1	B	197	ARG
1	B	212	LYS
1	B	259	LYS
1	B	264	TYR
1	B	279	GLY
1	B	587	SER
1	B	594	GLU
1	B	597	ARG
1	C	6	SER
1	C	34	LEU
1	C	119	LYS
1	C	228	GLY
1	C	242	ASN
1	C	257	ALA

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Mol	Chain	Res	Type
1	C	280	SER
1	C	291	LEU
1	C	302	ILE
1	C	313	LEU
1	C	590	SER
1	C	591	LYS
1	C	593	LEU
1	C	594	GLU
1	D	30	LEU
1	D	47	LYS
1	D	48	SER
1	D	89	PHE
1	D	103	VAL
1	D	104	ARG
1	D	159	VAL
1	D	168	SER
1	D	188	ALA
1	D	206	THR
1	D	259	LYS
1	D	297	SER
1	A	23	ASP
1	A	24	SER
1	A	77	GLN
1	A	119	LYS
1	A	217	ASP
1	A	287	LEU
1	A	297	SER
1	A	313	LEU
1	A	604	ASP
1	B	29	THR
1	B	117	ARG
1	B	160	LYS
1	B	173	PRO
1	B	187	LEU
1	B	218	LYS
1	B	223	VAL
1	B	269	THR
1	B	586	ARG
1	C	33	SER
1	C	47	LYS
1	C	145	GLY
1	C	152	ASP

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Mol	Chain	Res	Type
1	C	188	ALA
1	C	252	VAL
1	D	119	LYS
1	D	173	PRO
1	D	186	ASP
1	D	594	GLU
1	A	28	PRO
1	A	56	GLY
1	A	89	PHE
1	A	94	ARG
1	A	115	THR
1	A	212	LYS
1	A	244	SER
1	A	262	ARG
1	A	269	THR
1	A	312	GLU
1	A	594	GLU
1	B	71	PRO
1	B	115	THR
1	B	125	PRO
1	B	188	ALA
1	B	252	VAL
1	B	265	PHE
1	B	300	PRO
1	B	591	LYS
1	C	30	LEU
1	C	48	SER
1	C	86	TYR
1	C	138	LEU
1	C	186	ASP
1	C	283	LEU
1	D	28	PRO
1	D	33	SER
1	D	57	LYS
1	D	86	TYR
1	D	109	ASP
1	D	150	ALA
1	D	166	VAL
1	D	192	ALA
1	D	258	ARG
1	D	305	LEU
1	D	600	GLN

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Mol	Chain	Res	Type
1	A	45	SER
1	A	55	VAL
1	A	263	GLU
1	B	99	ASP
1	B	161	ASP
1	B	250	LYS
1	B	593	LEU
1	C	269	THR
1	C	299	ILE
1	C	585	ARG
1	D	117	ARG
1	B	9	ASN
1	B	292	GLU
1	C	23	ASP
1	C	101	ALA
1	D	193	ILE
1	D	227	GLU
1	A	35	PRO
1	A	182	PRO
1	C	67	VAL
1	D	241	VAL
1	A	295	ILE
1	B	34	LEU
1	D	34	LEU
1	B	236	PRO
1	C	55	VAL
1	B	5	ILE
1	B	46	GLY
1	C	71	PRO
1	A	173	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	294/313 (94%)	224 (76%)	70 (24%)	0 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	294/313 (94%)	231 (79%)	63 (21%)	1 7
1	C	294/313 (94%)	213 (72%)	81 (28%)	0 3
1	D	294/313 (94%)	229 (78%)	65 (22%)	1 6
All	All	1176/1252 (94%)	897 (76%)	279 (24%)	1 5

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	11	ILE
1	A	12	GLN
1	A	18	LEU
1	A	27	LEU
1	A	34	LEU
1	A	37	ILE
1	A	39	VAL
1	A	40	VAL
1	A	47	LYS
1	A	50	VAL
1	A	53	SER
1	A	59	PHE
1	A	62	ARG
1	A	74	LEU
1	A	79	ILE
1	A	86	TYR
1	A	89	PHE
1	A	90	LEU
1	A	95	LYS
1	A	100	PHE
1	A	117	ARG
1	A	119	LYS
1	A	128	LEU
1	A	132	SER
1	A	134	ASN
1	A	137	ASN
1	A	141	ILE
1	A	151	VAL
1	A	156	ASP
1	A	158	ILE
1	A	169	TYR
1	A	180	ILE

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Mol	Chain	Res	Type
1	A	184	ASN
1	A	187	LEU
1	A	189	THR
1	A	191	ASP
1	A	194	LYS
1	A	199	VAL
1	A	202	SER
1	A	205	ARG
1	A	206	THR
1	A	207	PHE
1	A	211	THR
1	A	214	ASP
1	A	215	LEU
1	A	225	ILE
1	A	226	LEU
1	A	229	ARG
1	A	233	LEU
1	A	240	VAL
1	A	243	ARG
1	A	247	ASP
1	A	249	ASN
1	A	260	ARG
1	A	262	ARG
1	A	265	PHE
1	A	269	THR
1	A	271	TYR
1	A	277	LYS
1	A	278	MET
1	A	280	SER
1	A	292	GLU
1	A	302	ILE
1	A	310	VAL
1	A	316	GLU
1	A	593	LEU
1	A	595	LEU
1	A	597	ARG
1	A	601	SER
1	B	4	LEU
1	B	8	VAL
1	B	11	ILE
1	B	21	HIS
1	B	23	ASP

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Mol	Chain	Res	Type
1	B	27	LEU
1	B	29	THR
1	B	34	LEU
1	B	39	VAL
1	B	59	PHE
1	B	62	ARG
1	B	69	ARG
1	B	74	LEU
1	B	84	ARG
1	B	86	TYR
1	B	90	LEU
1	B	92	LEU
1	B	100	PHE
1	B	105	LYS
1	B	117	ARG
1	B	136	VAL
1	B	141	ILE
1	B	142	ASP
1	B	148	LYS
1	B	160	LYS
1	B	161	ASP
1	B	164	ASN
1	B	165	MET
1	B	170	ILE
1	B	176	ILE
1	B	178	LEU
1	B	181	SER
1	B	184	ASN
1	B	194	LYS
1	B	195	ILE
1	B	200	ASP
1	B	202	SER
1	B	204	ASP
1	B	206	THR
1	B	210	LEU
1	B	216	MET
1	B	218	LYS
1	B	220	THR
1	B	223	VAL
1	B	232	LYS
1	B	233	LEU
1	B	235	TYR

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Mol	Chain	Res	Type
1	B	242	ASN
1	B	245	GLN
1	B	250	LYS
1	B	255	ILE
1	B	269	THR
1	B	273	HIS
1	B	281	GLU
1	B	299	ILE
1	B	303	GLN
1	B	304	SER
1	B	313	LEU
1	B	314	GLU
1	B	586	ARG
1	B	594	GLU
1	B	596	TYR
1	B	604	ASP
1	C	3	ASN
1	C	4	LEU
1	C	18	LEU
1	C	20	ASP
1	C	24	SER
1	C	29	THR
1	C	30	LEU
1	C	33	SER
1	C	34	LEU
1	C	37	ILE
1	C	50	VAL
1	C	59	PHE
1	C	67	VAL
1	C	69	ARG
1	C	70	ARG
1	C	74	LEU
1	C	77	GLN
1	C	78	LYS
1	C	86	TYR
1	C	89	PHE
1	C	100	PHE
1	C	103	VAL
1	C	107	ILE
1	C	109	ASP
1	C	123	SER
1	C	128	LEU

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Mol	Chain	Res	Type
1	C	129	SER
1	C	131	TYR
1	C	132	SER
1	C	135	VAL
1	C	148	LYS
1	C	149	VAL
1	C	152	ASP
1	C	156	ASP
1	C	159	VAL
1	C	163	GLU
1	C	165	MET
1	C	168	SER
1	C	172	LYS
1	C	174	ASN
1	C	175	CYS
1	C	180	ILE
1	C	184	ASN
1	C	185	GLN
1	C	199	VAL
1	C	206	THR
1	C	207	PHE
1	C	209	VAL
1	C	210	LEU
1	C	211	THR
1	C	218	LYS
1	C	221	ASP
1	C	224	GLU
1	C	226	LEU
1	C	227	GLU
1	C	234	LYS
1	C	240	VAL
1	C	242	ASN
1	C	243	ARG
1	C	255	ILE
1	C	261	GLU
1	C	264	TYR
1	C	268	THR
1	C	270	GLU
1	C	277	LYS
1	C	278	MET
1	C	280	SER
1	C	281	GLU

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Mol	Chain	Res	Type
1	C	282	HIS
1	C	285	LYS
1	C	288	SER
1	C	298	ARG
1	C	299	ILE
1	C	304	SER
1	C	305	LEU
1	C	312	GLU
1	C	593	LEU
1	C	594	GLU
1	C	596	TYR
1	C	601	SER
1	C	603	ILE
1	D	4	LEU
1	D	32	ASP
1	D	34	LEU
1	D	37	ILE
1	D	43	GLN
1	D	53	SER
1	D	54	ILE
1	D	62	ARG
1	D	67	VAL
1	D	77	GLN
1	D	79	ILE
1	D	83	THR
1	D	86	TYR
1	D	88	GLU
1	D	95	LYS
1	D	111	THR
1	D	134	ASN
1	D	135	VAL
1	D	141	ILE
1	D	146	LEU
1	D	148	LYS
1	D	151	VAL
1	D	158	ILE
1	D	164	ASN
1	D	174	ASN
1	D	175	CYS
1	D	176	ILE
1	D	180	ILE
1	D	184	ASN

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Mol	Chain	Res	Type
1	D	187	LEU
1	D	189	THR
1	D	190	SER
1	D	193	ILE
1	D	206	THR
1	D	211	THR
1	D	218	LYS
1	D	220	THR
1	D	224	GLU
1	D	227	GLU
1	D	231	PHE
1	D	233	LEU
1	D	243	ARG
1	D	253	ASP
1	D	255	ILE
1	D	260	ARG
1	D	264	TYR
1	D	269	THR
1	D	270	GLU
1	D	273	HIS
1	D	280	SER
1	D	288	SER
1	D	293	ARG
1	D	295	ILE
1	D	299	ILE
1	D	305	LEU
1	D	306	ILE
1	D	310	VAL
1	D	311	LEU
1	D	312	GLU
1	D	316	GLU
1	D	590	SER
1	D	593	LEU
1	D	594	GLU
1	D	595	LEU
1	D	597	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	91	HIS

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Mol	Chain	Res	Type
1	A	134	ASN
1	A	154	GLN
1	A	174	ASN
1	A	185	GLN
1	A	242	ASN
1	A	273	HIS
1	A	282	HIS
1	B	12	GLN
1	B	21	HIS
1	B	43	GLN
1	B	77	GLN
1	B	108	GLN
1	B	154	GLN
1	B	164	ASN
1	B	174	ASN
1	B	185	GLN
1	B	245	GLN
1	B	249	ASN
1	B	303	GLN
1	C	12	GLN
1	C	75	GLN
1	C	137	ASN
1	C	242	ASN
1	C	245	GLN
1	C	290	HIS
1	C	303	GLN
1	D	43	GLN
1	D	290	HIS
1	D	600	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)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GDP	D	9001	-	24,30,30	0.90	1 (4%)	30,47,47	1.54	7 (23%)
2	GDP	A	9001	-	24,30,30	0.98	1 (4%)	30,47,47	1.59	8 (26%)
2	GDP	B	9001	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
2	GDP	C	9001	-	24,30,30	1.06	1 (4%)	30,47,47	1.46	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	D	9001	-	-	5/12/32/32	0/3/3/3
2	GDP	A	9001	-	-	6/12/32/32	0/3/3/3
2	GDP	B	9001	-	-	2/12/32/32	0/3/3/3
2	GDP	C	9001	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	9001	GDP	C6-N1	-2.90	1.33	1.37
2	A	9001	GDP	C6-N1	-2.82	1.33	1.37
2	D	9001	GDP	C6-N1	-2.31	1.34	1.37
2	B	9001	GDP	C6-N1	-2.29	1.34	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	9001	GDP	PA-O3A-PB	-4.62	116.97	132.83
2	B	9001	GDP	PA-O3A-PB	-4.08	118.81	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	9001	GDP	O4'-C1'-C2'	-3.86	101.29	106.93
2	D	9001	GDP	PA-O3A-PB	-3.57	120.57	132.83
2	A	9001	GDP	PA-O3A-PB	-3.50	120.80	132.83
2	D	9001	GDP	O6-C6-C5	-3.00	118.52	124.37
2	B	9001	GDP	O3B-PB-O3A	2.66	113.56	104.64
2	D	9001	GDP	C8-N7-C5	2.66	108.06	102.99
2	A	9001	GDP	C8-N7-C5	2.64	108.02	102.99
2	B	9001	GDP	C8-N7-C5	2.64	108.01	102.99
2	D	9001	GDP	O6-C6-N1	2.55	123.66	120.65
2	B	9001	GDP	C5-C6-N1	2.44	118.27	113.95
2	D	9001	GDP	O3B-PB-O3A	2.28	112.29	104.64
2	A	9001	GDP	O2B-PB-O3A	2.28	112.27	104.64
2	A	9001	GDP	C5-C6-N1	2.24	117.92	113.95
2	A	9001	GDP	C5'-C4'-C3'	-2.22	106.87	115.18
2	D	9001	GDP	C3'-C2'-C1'	-2.20	97.67	100.98
2	D	9001	GDP	C5-C6-N1	2.19	117.82	113.95
2	A	9001	GDP	O6-C6-C5	-2.16	120.16	124.37
2	C	9001	GDP	O6-C6-C5	-2.14	120.19	124.37
2	A	9001	GDP	C3'-C2'-C1'	-2.10	97.81	100.98
2	C	9001	GDP	C5-C6-N1	2.09	117.64	113.95
2	C	9001	GDP	C8-N7-C5	2.07	106.93	102.99

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	9001	GDP	C5'-O5'-PA-O3A
2	A	9001	GDP	O4'-C4'-C5'-O5'
2	A	9001	GDP	C3'-C4'-C5'-O5'
2	D	9001	GDP	C5'-O5'-PA-O3A
2	D	9001	GDP	C5'-O5'-PA-O2A
2	D	9001	GDP	C3'-C4'-C5'-O5'
2	D	9001	GDP	O4'-C4'-C5'-O5'
2	A	9001	GDP	C5'-O5'-PA-O1A
2	D	9001	GDP	C5'-O5'-PA-O1A
2	A	9001	GDP	PB-O3A-PA-O1A
2	A	9001	GDP	PB-O3A-PA-O2A
2	B	9001	GDP	PA-O3A-PB-O1B
2	B	9001	GDP	PA-O3A-PB-O3B

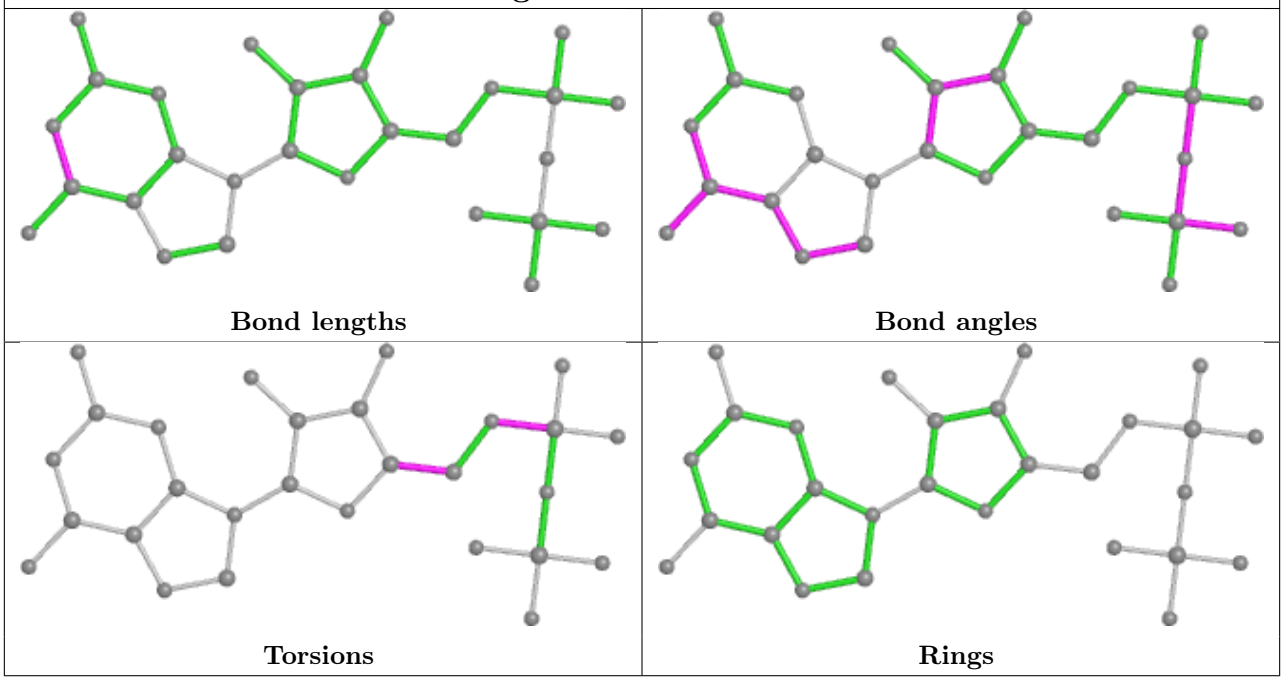
There are no ring outliers.

4 monomers are involved in 26 short contacts:

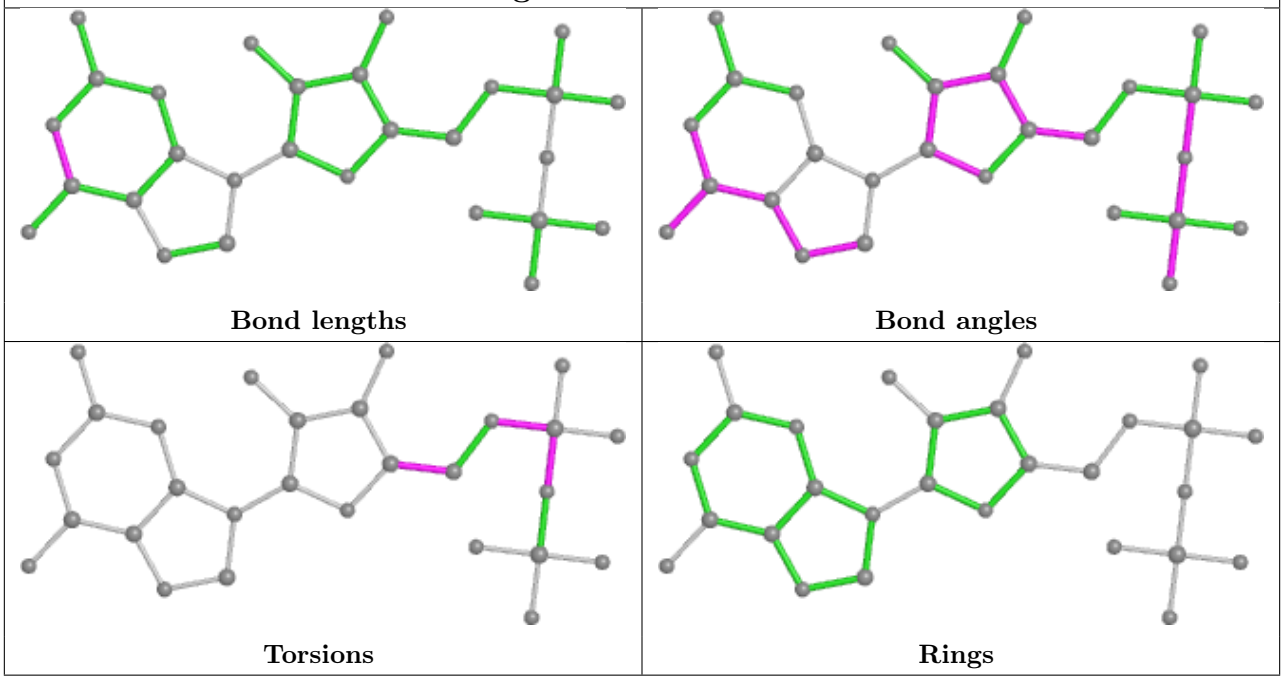
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	9001	GDP	7	0
2	A	9001	GDP	7	0
2	B	9001	GDP	7	0
2	C	9001	GDP	5	0

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

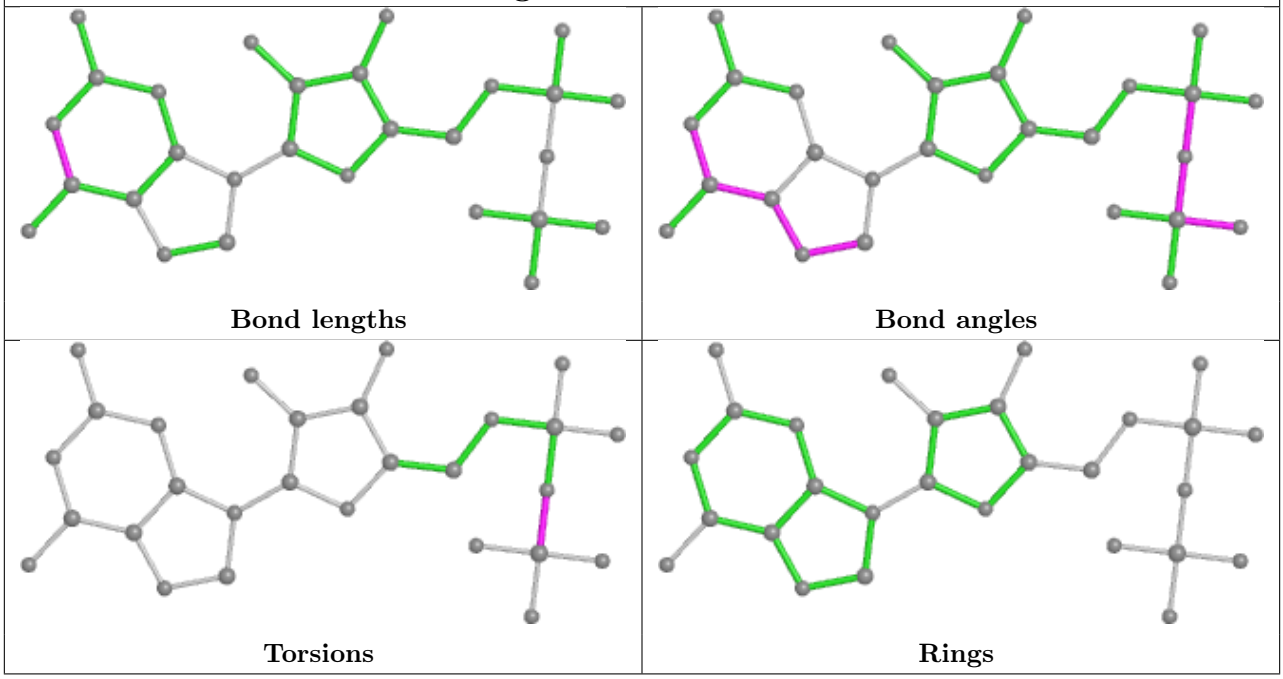
Ligand GDP D 9001



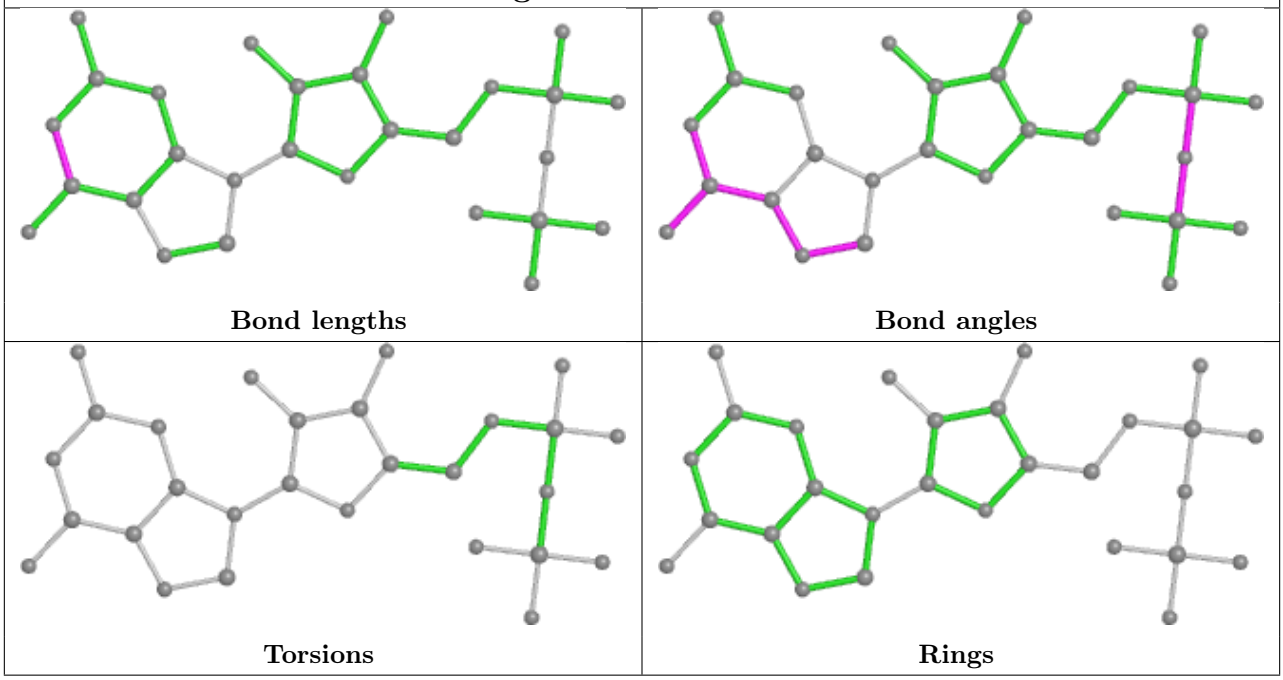
Ligand GDP A 9001



Ligand GDP B 9001



Ligand GDP C 9001



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	339/360 (94%)	-0.34	7 (2%)	63	48	20, 44, 118, 146	0
1	B	339/360 (94%)	-0.43	8 (2%)	59	42	18, 38, 104, 162	0
1	C	339/360 (94%)	-0.42	1 (0%)	94	88	22, 51, 130, 174	0
1	D	339/360 (94%)	-0.26	7 (2%)	63	48	31, 62, 118, 173	0
All	All	1356/1440 (94%)	-0.36	23 (1%)	70	55	18, 48, 118, 174	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	118	SER	5.3
1	A	118	SER	4.8
1	D	64	SER	3.6
1	A	22	GLY	3.6
1	B	118	SER	3.4
1	B	116	GLY	2.8
1	A	129	SER	2.6
1	B	20	ASP	2.6
1	A	65	GLY	2.5
1	D	117	ARG	2.5
1	D	21	HIS	2.5
1	A	66	ILE	2.4
1	C	118	SER	2.4
1	A	119	LYS	2.3
1	B	120	ALA	2.3
1	A	130	ILE	2.2
1	B	117	ARG	2.2
1	B	115	THR	2.2
1	D	74	LEU	2.2
1	D	139	THR	2.1
1	B	25	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	64	SER	2.0
1	D	119	LYS	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)

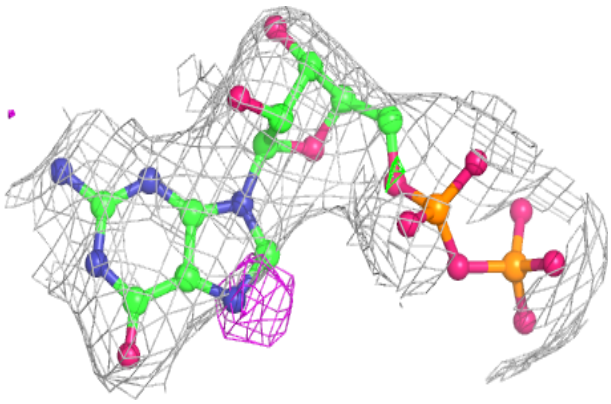
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

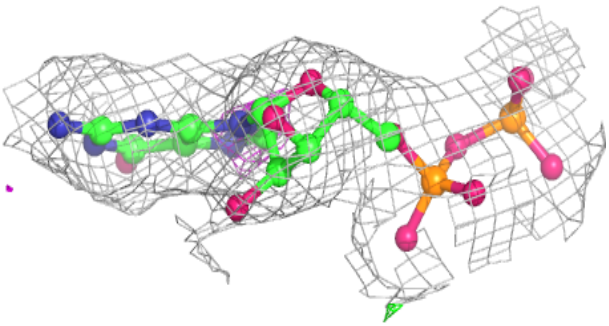
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GDP	A	9001	28/28	0.95	0.19	24,41,56,61	0
2	GDP	C	9001	28/28	0.95	0.16	33,47,52,54	0
2	GDP	D	9001	28/28	0.96	0.15	34,42,47,48	0
2	GDP	B	9001	28/28	0.97	0.14	22,27,33,37	0

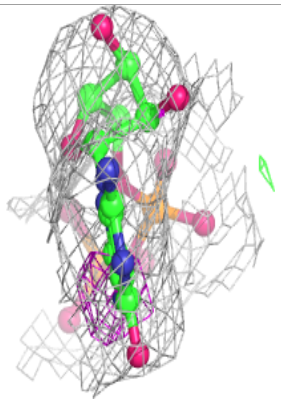
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP A 9001:

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

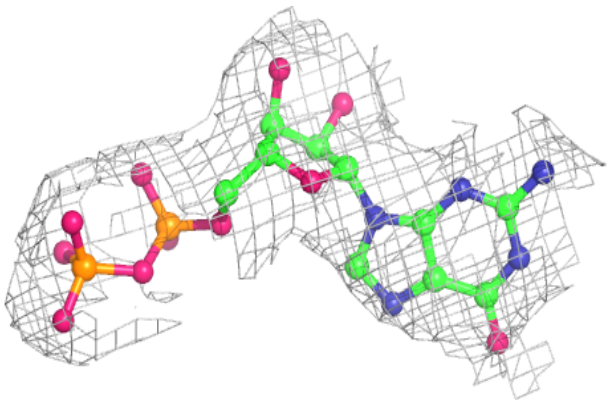


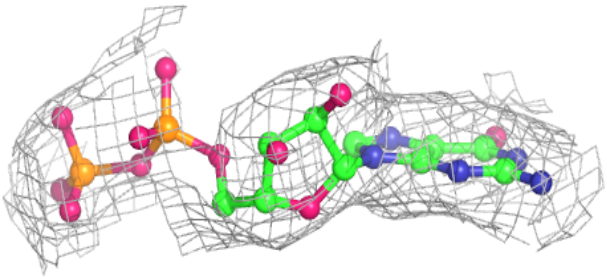


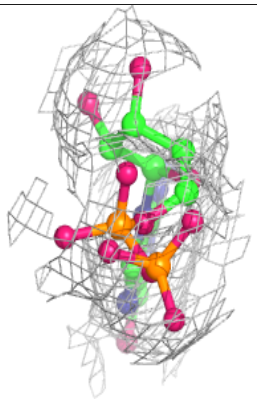


Electron density around GDP C 9001:

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

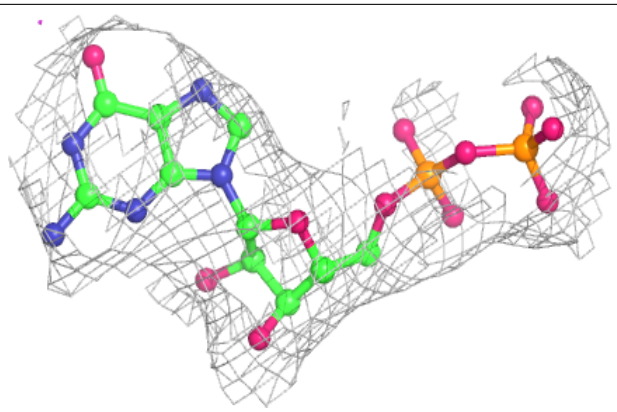


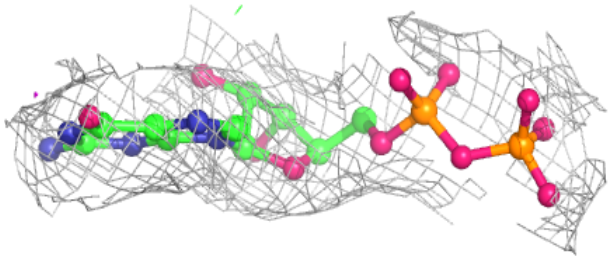


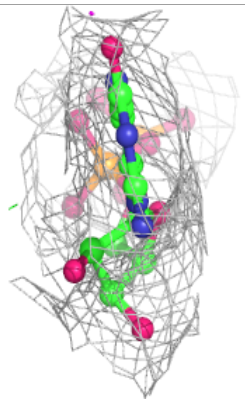


Electron density around GDP D 9001:

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

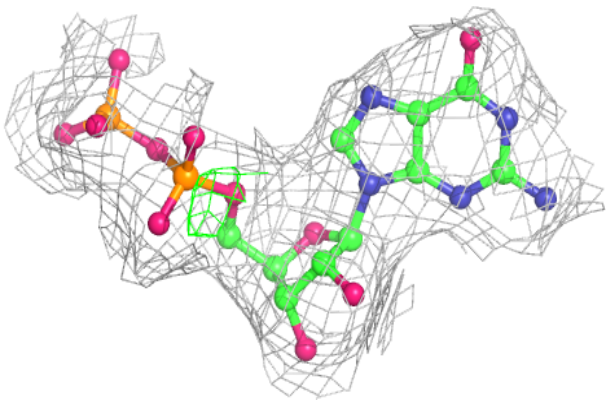


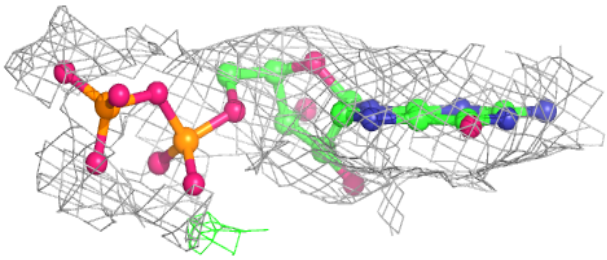


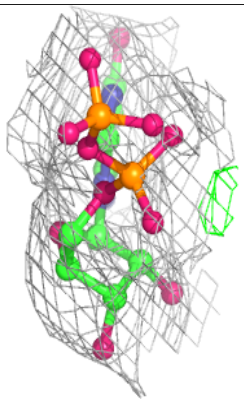


Electron density around GDP B 9001:

$2mF_o$-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.