Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 03:39 PM EST

PDB ID	:	3SJD
Title	:	Crystal structure of S. cerevisiae Get3 with bound ADP-Mg2+ in complex with Get2 cytosolic domain
Authors	:	Reitz, S.; Wild, K.; Sinning, I.
Deposited on	:	2011-06-21
Resolution	:	4.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

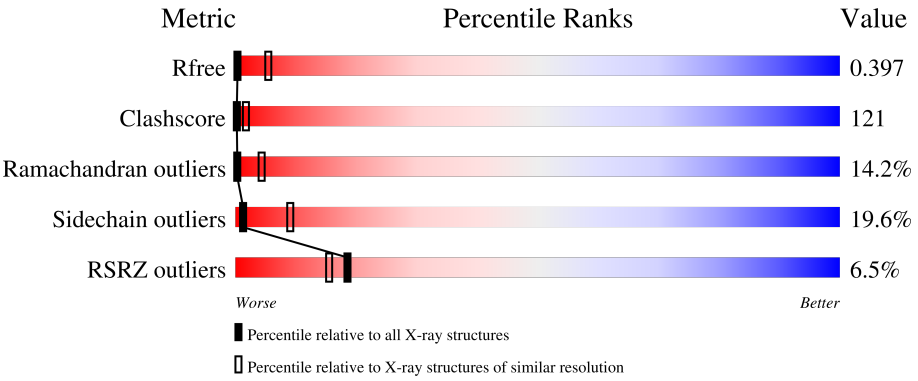
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 4.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)
RSRZ outliers	127900	1113 (5.50-3.70)

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	362	6% 12% 46% 19% • 21%
1	B	362	5% 12% 41% 22% • 23%
1	C	362	5% 14% 44% 20% • 19%
2	D	46	4% 22% 43% 35%
2	E	46	24% 41% 35%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	A	401	-	-	X	-
3	ADP	C	401	-	-	X	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7387 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 ATPase GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2273	1443	375	440	15			
1	B	280	Total	C	N	O	S	0	1	0
			2224	1414	368	427	15			
1	C	292	Total	C	N	O	S	0	0	0
			2310	1460	384	451	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	LEU	-	expression tag	UNP Q12154
A	356	GLU	-	expression tag	UNP Q12154
A	357	HIS	-	expression tag	UNP Q12154
A	358	HIS	-	expression tag	UNP Q12154
A	359	HIS	-	expression tag	UNP Q12154
A	360	HIS	-	expression tag	UNP Q12154
A	361	HIS	-	expression tag	UNP Q12154
A	362	HIS	-	expression tag	UNP Q12154
B	355	LEU	-	expression tag	UNP Q12154
B	356	GLU	-	expression tag	UNP Q12154
B	357	HIS	-	expression tag	UNP Q12154
B	358	HIS	-	expression tag	UNP Q12154
B	359	HIS	-	expression tag	UNP Q12154
B	360	HIS	-	expression tag	UNP Q12154
B	361	HIS	-	expression tag	UNP Q12154
B	362	HIS	-	expression tag	UNP Q12154
C	355	LEU	-	expression tag	UNP Q12154
C	356	GLU	-	expression tag	UNP Q12154
C	357	HIS	-	expression tag	UNP Q12154
C	358	HIS	-	expression tag	UNP Q12154
C	359	HIS	-	expression tag	UNP Q12154
C	360	HIS	-	expression tag	UNP Q12154
C	361	HIS	-	expression tag	UNP Q12154

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Chain	Residue	Modelled	Actual	Comment	Reference
C	362	HIS	-	expression tag	UNP Q12154

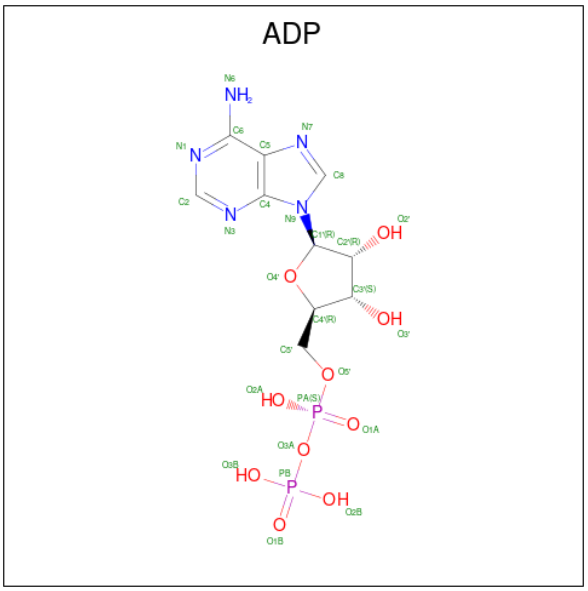
- Molecule 2 is a protein called Golgi to ER traffic protein 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	30	Total	C	N	O	0	0	0
			247	148	55	44			
2	E	30	Total	C	N	O	0	0	0
			247	148	55	44			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	MET	-	expression tag	UNP P40056
D	-8	LYS	-	expression tag	UNP P40056
D	-7	HIS	-	expression tag	UNP P40056
D	-6	HIS	-	expression tag	UNP P40056
D	-5	HIS	-	expression tag	UNP P40056
D	-4	HIS	-	expression tag	UNP P40056
D	-3	HIS	-	expression tag	UNP P40056
D	-2	HIS	-	expression tag	UNP P40056
D	-1	PRO	-	expression tag	UNP P40056
D	0	MET	-	expression tag	UNP P40056
D	1	GLY	-	expression tag	UNP P40056
D	36	TRP	-	expression tag	UNP P40056
E	-9	MET	-	expression tag	UNP P40056
E	-8	LYS	-	expression tag	UNP P40056
E	-7	HIS	-	expression tag	UNP P40056
E	-6	HIS	-	expression tag	UNP P40056
E	-5	HIS	-	expression tag	UNP P40056
E	-4	HIS	-	expression tag	UNP P40056
E	-3	HIS	-	expression tag	UNP P40056
E	-2	HIS	-	expression tag	UNP P40056
E	-1	PRO	-	expression tag	UNP P40056
E	0	MET	-	expression tag	UNP P40056
E	1	GLY	-	expression tag	UNP P40056
E	36	TRP	-	expression tag	UNP P40056

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 27 10 5 10 2	0	0
3	B	1	Total C N O P 27 10 5 10 2	0	0
3	C	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

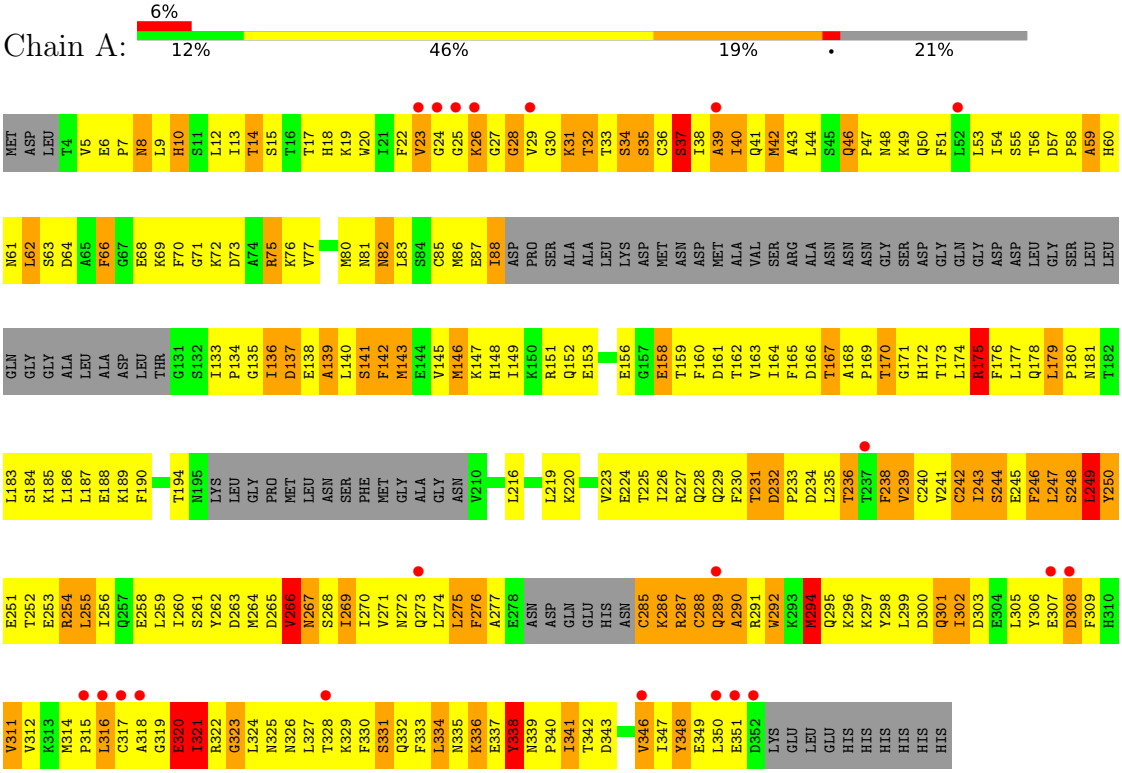
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Zn 1 1	0	0
5	C	1	Total Zn 1 1	0	0

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.

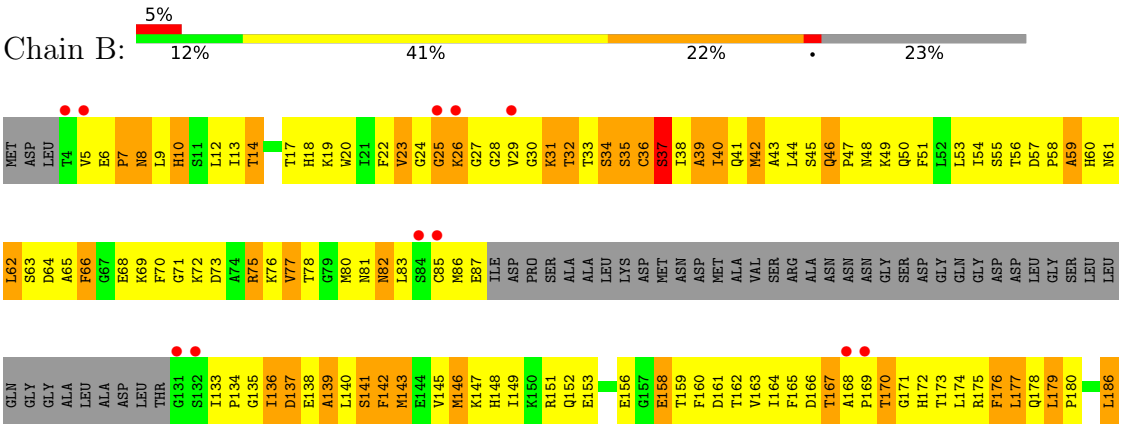
• Molecule 1: ATPase GET3

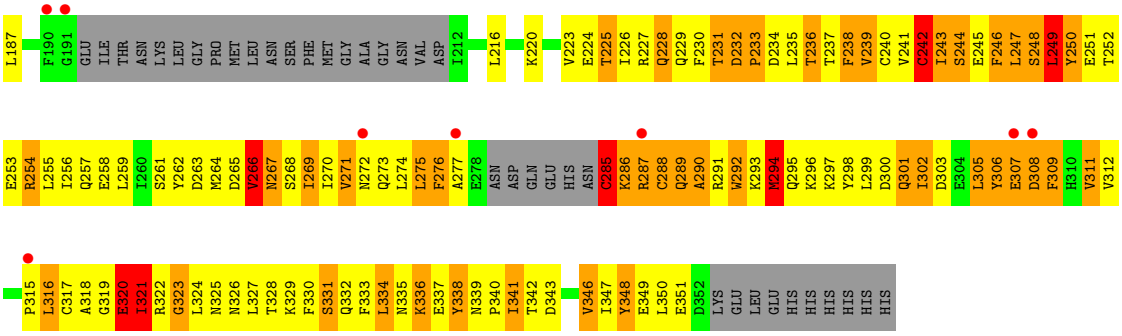
Chain A:



• Molecule 1: ATPase GET3

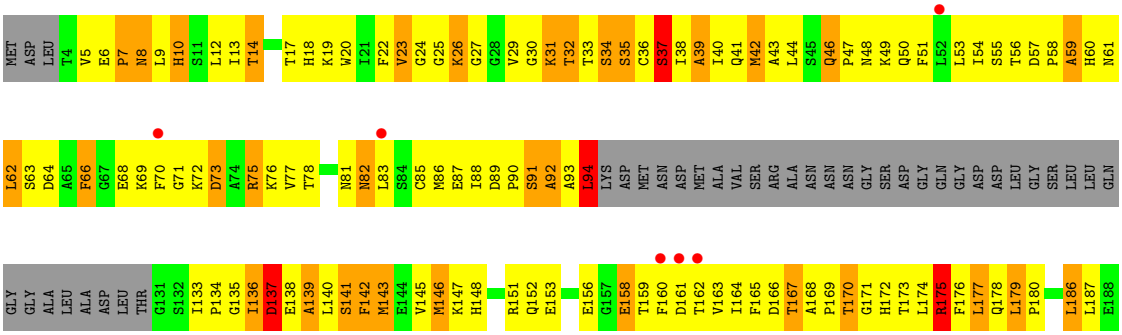
Chain B:

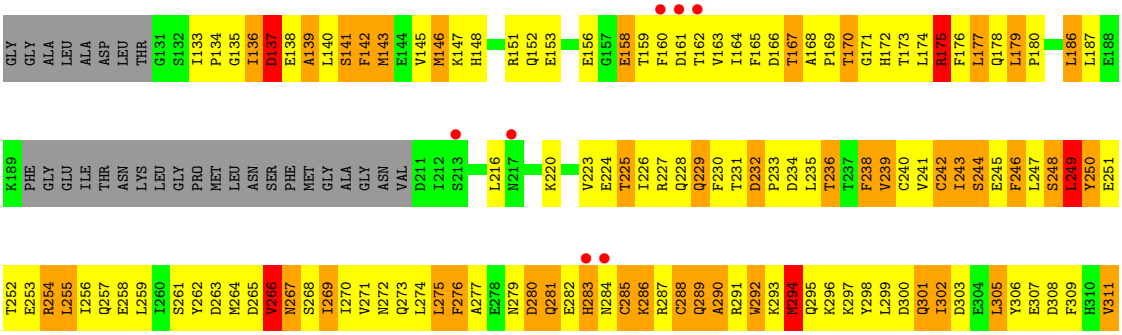


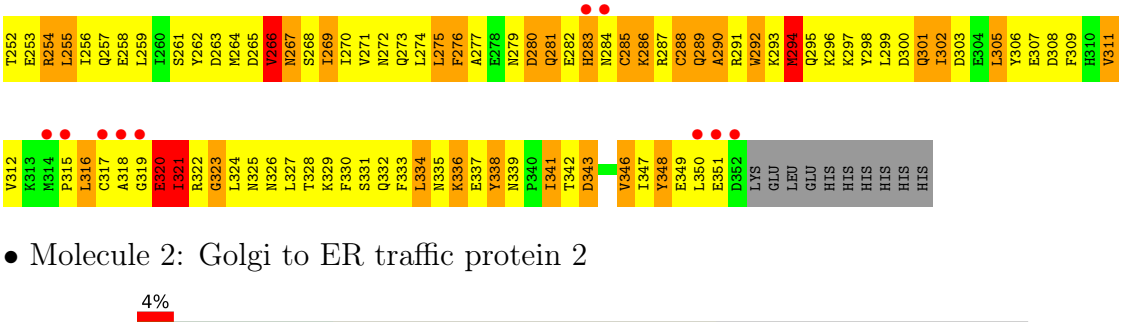


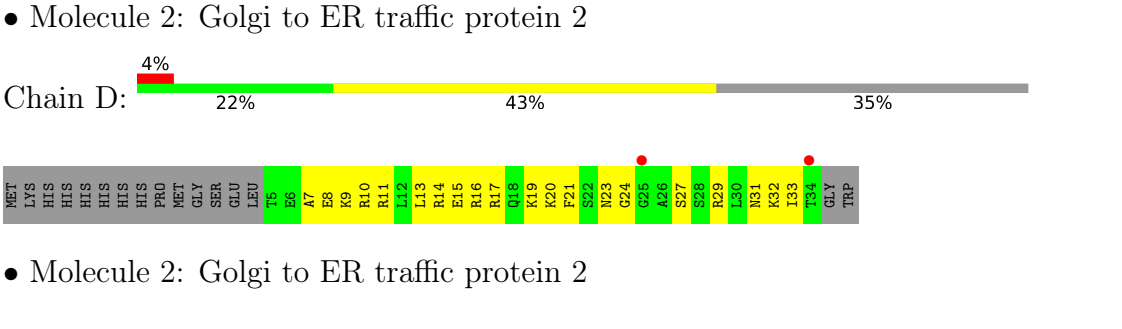
• Molecule 1: ATPase GET3

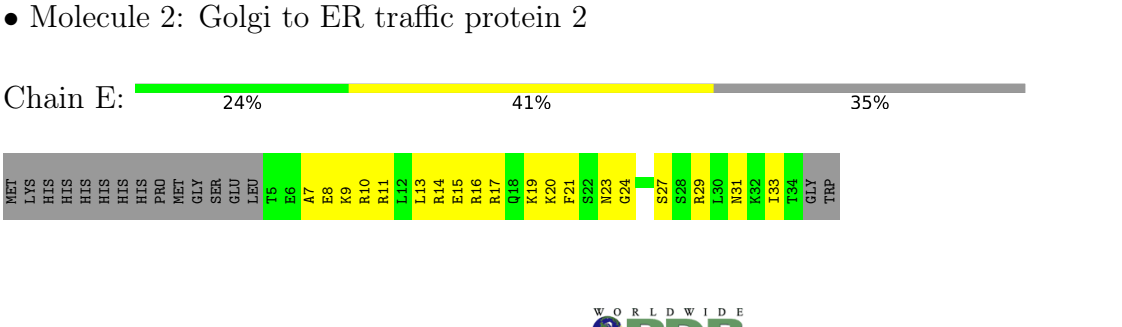
Chain C:











• Molecule 2: Golgi to ER traffic protein 2

Chain D:

• Molecule 2: Golgi to ER traffic protein 2

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	149.64Å 209.75Å 133.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.23 – 4.60 63.34 – 4.60	Depositor EDS
% Data completeness (in resolution range)	94.6 (56.23-4.60) 94.8 (63.34-4.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 4.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.323 , 0.388 0.334 , 0.397	Depositor DCC
R_{free} test set	570 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	248.9	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 472.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	7387	wwPDB-VP
Average B, all atoms (Å^2)	344.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.56	0/2310	0.77	2/3113 (0.1%)
1	B	0.66	3/2264 (0.1%)	0.92	7/3048 (0.2%)
1	C	0.64	1/2349 (0.0%)	0.81	1/3169 (0.0%)
2	D	0.21	0/247	0.44	0/323
2	E	0.21	0/247	0.44	0/323
All	All	0.60	4/7417 (0.1%)	0.82	10/9976 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	36	CYS	CB-SG	-6.89	1.70	1.82
1	B	242	CYS	CB-SG	-5.83	1.72	1.81
1	C	266	VAL	CA-CB	-5.50	1.43	1.54
1	B	285	CYS	CB-SG	5.31	1.91	1.82

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	228	GLN	C-N-CA	-16.50	80.45	121.70
1	B	228	GLN	CA-C-N	-10.77	93.50	117.20
1	B	228	GLN	O-C-N	10.53	139.55	122.70
1	B	308	ASP	N-CA-CB	-8.14	95.95	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	308	ASP	N-CA-C	6.98	129.84	111.00
1	B	306	TYR	CB-CA-C	6.43	123.26	110.40
1	C	94	LEU	CA-CB-CG	5.80	128.65	115.30
1	A	266	VAL	CB-CA-C	-5.24	101.44	111.40
1	A	28	GLY	N-CA-C	-5.18	100.14	113.10
1	B	266	VAL	CB-CA-C	-5.12	101.68	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	THR	Mainchain

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	2273	0	2264	577	0
1	B	2224	0	2220	595	0
1	C	2310	0	2287	592	0
2	D	247	0	261	59	0
2	E	247	0	263	43	0
3	A	27	0	12	11	0
3	B	27	0	12	8	0
3	C	27	0	12	10	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	1	0
All	All	7387	0	7331	1783	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 121.

All (1783) 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:B:228:GLN:HE22	1:B:229:GLN:CG	1.19	1.55
1:A:179:LEU:HD21	1:A:219:LEU:CD2	1.01	1.47
1:A:179:LEU:CD2	1:A:219:LEU:HD21	0.98	1.45
1:B:228:GLN:NE2	1:B:229:GLN:CB	1.78	1.45
1:B:178:GLN:OE1	1:B:262:TYR:CE1	1.72	1.42
1:C:308:ASP:CG	2:D:16:ARG:NH2	1.71	1.41
1:C:187:LEU:CD1	1:C:216:LEU:HD13	1.51	1.40
1:B:187:LEU:CD1	1:B:216:LEU:HD13	1.51	1.39
1:C:178:GLN:OE1	1:C:262:TYR:CE1	1.74	1.38
1:A:174:LEU:HG	1:A:262:TYR:CE2	1.56	1.38
1:C:308:ASP:OD1	2:D:16:ARG:NH2	1.56	1.32
1:A:174:LEU:HG	1:A:262:TYR:CD2	1.65	1.31
1:C:308:ASP:OD2	2:D:16:ARG:NH2	1.59	1.30
1:A:30:GLY:HA2	3:A:401:ADP:O3A	1.32	1.29
1:C:30:GLY:HA2	3:C:401:ADP:O3A	1.32	1.27
1:B:187:LEU:HD21	1:B:216:LEU:CD1	1.66	1.25
1:A:228:GLN:NE2	1:A:229:GLN:HG3	1.49	1.25
1:C:179:LEU:HD12	1:C:179:LEU:O	1.37	1.24
1:C:187:LEU:HD21	1:C:216:LEU:CD1	1.66	1.24
1:A:230:PHE:CZ	1:A:264:MET:HE2	1.73	1.23
1:A:230:PHE:CE2	1:A:264:MET:HE2	1.71	1.23
1:B:178:GLN:OE1	1:B:262:TYR:HE1	0.94	1.23
1:A:227:ARG:CD	1:A:231:THR:OG1	1.88	1.21
1:C:229:GLN:HE22	1:C:235:LEU:CD1	1.53	1.21
1:B:134:PRO:O	1:B:179:LEU:CD2	1.88	1.21
1:C:229:GLN:NE2	1:C:235:LEU:CD1	2.04	1.21
1:A:227:ARG:HD2	1:A:231:THR:OG1	1.41	1.20
1:B:179:LEU:HD12	1:B:179:LEU:O	1.37	1.20
1:A:174:LEU:CG	1:A:262:TYR:CD2	2.24	1.18
1:B:228:GLN:NE2	1:B:229:GLN:HB2	1.58	1.18
1:A:230:PHE:CZ	1:A:264:MET:CE	2.26	1.18
1:B:228:GLN:NE2	1:B:229:GLN:HG3	1.58	1.18
1:B:177:LEU:HD23	1:B:178:GLN:N	1.58	1.17
1:C:29:VAL:HG13	1:C:243:ILE:HG23	1.20	1.17
1:A:285:CYS:SG	1:B:285:CYS:SG	2.42	1.17
1:B:228:GLN:NE2	1:B:229:GLN:CG	2.00	1.17
1:A:29:VAL:HG13	1:A:243:ILE:HG23	1.19	1.16
1:B:228:GLN:NE2	1:B:229:GLN:CA	2.07	1.16
1:B:138:GLU:HB3	1:B:173:THR:O	1.42	1.16
1:C:229:GLN:NE2	1:C:235:LEU:HD13	1.55	1.15
1:B:177:LEU:HD23	1:B:178:GLN:H	1.01	1.15
1:C:178:GLN:HB2	1:C:262:TYR:CD1	1.81	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:PHE:CE2	1:B:174:LEU:CD1	2.31	1.14
1:C:229:GLN:HE22	1:C:235:LEU:HD13	1.01	1.14
1:B:139:ALA:N	1:B:176:PHE:CD2	2.16	1.14
1:C:178:GLN:OE1	1:C:262:TYR:HE1	1.10	1.14
1:B:29:VAL:HG13	1:B:243:ILE:HG23	1.19	1.13
1:B:135:GLY:HA3	1:B:179:LEU:HD23	1.17	1.13
1:C:253:GLU:OE2	2:D:29:ARG:NH2	1.81	1.13
1:C:230:PHE:O	1:C:264:MET:CE	1.97	1.13
1:B:187:LEU:HD11	1:B:216:LEU:HD13	1.13	1.12
1:A:174:LEU:CD2	1:A:262:TYR:CD2	2.32	1.12
1:B:175:ARG:NE	1:B:258:GLU:OE2	1.82	1.12
1:B:22:PHE:CE2	1:B:174:LEU:HD13	1.85	1.12
1:B:233:PRO:HG2	2:D:32:LYS:HD2	1.24	1.11
1:B:187:LEU:HD11	1:B:216:LEU:CD1	1.79	1.11
1:C:227:ARG:HH22	1:C:263:ASP:CB	1.63	1.11
2:E:14:ARG:HG2	2:E:17:ARG:NH2	1.66	1.10
1:B:177:LEU:O	1:B:180:PRO:HD2	1.51	1.10
1:B:233:PRO:HG2	2:D:32:LYS:CD	1.58	1.10
1:B:30:GLY:HA2	3:B:401:ADP:O3A	1.50	1.10
1:C:135:GLY:HA3	1:C:179:LEU:HD23	1.24	1.10
1:C:187:LEU:HD11	1:C:216:LEU:CD1	1.79	1.10
2:D:14:ARG:HG2	2:D:17:ARG:HH22	1.15	1.09
1:B:134:PRO:O	1:B:179:LEU:HD21	1.40	1.09
2:D:14:ARG:HG2	2:D:17:ARG:NH2	1.66	1.09
1:C:177:LEU:O	1:C:180:PRO:HD2	1.52	1.08
1:A:174:LEU:CG	1:A:262:TYR:CE2	2.36	1.07
1:C:187:LEU:HD11	1:C:216:LEU:HD13	1.13	1.07
1:B:230:PHE:HA	1:B:236:THR:HG21	1.38	1.06
1:C:229:GLN:HA	1:C:229:GLN:HE21	1.17	1.06
1:B:135:GLY:CA	1:B:179:LEU:HD23	1.85	1.06
1:C:187:LEU:CD2	1:C:216:LEU:CD1	2.34	1.06
1:B:187:LEU:CD2	1:B:216:LEU:CD1	2.33	1.06
1:C:228:GLN:HE22	1:C:229:GLN:HG2	1.14	1.06
1:B:228:GLN:HE22	1:B:229:GLN:CB	1.55	1.05
1:C:23:VAL:O	1:C:167:THR:HG23	1.54	1.05
1:B:139:ALA:N	1:B:176:PHE:CE2	2.25	1.05
1:C:20:TRP:NE1	1:C:229:GLN:OE1	1.90	1.04
1:C:265:ASP:OD2	2:D:14:ARG:NH1	1.91	1.04
2:E:14:ARG:HG2	2:E:17:ARG:HH22	1.15	1.03
1:A:227:ARG:NE	1:A:231:THR:OG1	1.90	1.03
1:B:175:ARG:HA	1:B:262:TYR:CE2	1.94	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:HIS:HB2	1:C:174:LEU:HG	1.04	1.03
1:C:177:LEU:HD23	1:C:178:GLN:H	1.18	1.03
1:A:223:VAL:O	1:A:227:ARG:CB	2.07	1.02
1:B:228:GLN:NE2	1:B:229:GLN:N	2.07	1.02
1:C:228:GLN:NE2	1:C:229:GLN:HG2	1.75	1.02
1:A:253:GLU:OE2	2:E:29:ARG:NH2	1.92	1.01
1:C:175:ARG:HA	1:C:262:TYR:OH	1.60	1.01
1:B:177:LEU:C	1:B:180:PRO:HD2	1.79	1.01
1:A:175:ARG:HA	1:A:262:TYR:OH	1.61	1.01
1:C:172:HIS:CB	1:C:174:LEU:HG	1.90	1.01
1:B:139:ALA:HA	1:B:176:PHE:CE2	1.94	1.01
1:B:321:ILE:O	1:B:321:ILE:HD13	1.60	1.01
1:C:177:LEU:HD23	1:C:178:GLN:N	1.76	1.00
1:B:138:GLU:C	1:B:176:PHE:CE2	2.35	1.00
1:B:187:LEU:HD21	1:B:216:LEU:HD11	1.00	1.00
1:A:174:LEU:HD21	1:A:262:TYR:CD2	1.96	1.00
1:B:29:VAL:HG11	1:B:242:CYS:HA	1.44	1.00
1:C:308:ASP:OD2	2:D:16:ARG:CZ	2.10	1.00
1:C:187:LEU:HD21	1:C:216:LEU:HD11	1.01	0.99
1:C:187:LEU:CD2	1:C:216:LEU:HD11	1.93	0.99
1:A:230:PHE:CE1	1:A:264:MET:CE	2.46	0.99
1:B:224:GLU:O	1:B:228:GLN:HG3	1.63	0.98
1:C:308:ASP:HB3	2:D:17:ARG:HH11	1.28	0.98
1:C:177:LEU:H	1:C:177:LEU:HD22	1.28	0.98
1:C:285:CYS:SG	1:C:288:CYS:SG	2.61	0.98
1:B:140:LEU:HD22	1:B:140:LEU:H	1.29	0.98
1:B:177:LEU:CD2	1:B:178:GLN:H	1.76	0.98
1:C:225:THR:O	1:C:229:GLN:HB2	1.64	0.98
1:A:223:VAL:O	1:A:227:ARG:N	1.96	0.97
1:C:227:ARG:HH22	1:C:263:ASP:HB2	1.27	0.97
1:C:243:ILE:HD13	1:C:243:ILE:H	1.28	0.97
1:B:228:GLN:HE22	1:B:229:GLN:HG3	0.81	0.97
1:A:23:VAL:O	1:A:167:THR:HG23	1.61	0.97
1:A:179:LEU:CD2	1:A:219:LEU:CD2	1.82	0.97
1:B:243:ILE:HD13	1:B:243:ILE:H	1.28	0.96
1:A:342:THR:HG23	1:A:343:ASP:H	1.30	0.96
1:C:224:GLU:O	1:C:228:GLN:HG3	1.63	0.96
1:B:134:PRO:C	1:B:179:LEU:CD2	2.32	0.96
1:A:140:LEU:HD22	1:A:140:LEU:H	1.28	0.96
1:B:139:ALA:CA	1:B:176:PHE:CE2	2.48	0.96
1:C:140:LEU:H	1:C:140:LEU:HD22	1.27	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:THR:O	1:A:235:LEU:HA	1.66	0.95
1:A:174:LEU:CG	1:A:262:TYR:HD2	1.69	0.95
1:C:43:ALA:HA	1:C:51:PHE:HE2	1.32	0.95
1:B:228:GLN:HE21	1:B:229:GLN:HB2	1.12	0.95
1:C:228:GLN:NE2	1:C:229:GLN:CA	2.30	0.95
1:C:29:VAL:HG11	1:C:242:CYS:HA	1.46	0.95
1:B:175:ARG:HG3	1:B:258:GLU:OE2	1.67	0.95
1:B:22:PHE:HE2	1:B:174:LEU:HD13	1.25	0.94
1:A:227:ARG:O	1:A:231:THR:N	1.99	0.94
1:A:179:LEU:HB3	1:A:180:PRO:HD3	1.47	0.94
1:A:308:ASP:OD2	2:E:17:ARG:HG2	1.66	0.94
1:B:187:LEU:CD2	1:B:216:LEU:HD11	1.93	0.94
1:C:177:LEU:C	1:C:180:PRO:HD2	1.86	0.94
1:C:177:LEU:HD22	1:C:177:LEU:N	1.80	0.94
1:B:342:THR:HG23	1:B:343:ASP:H	1.32	0.93
1:A:228:GLN:NE2	1:A:229:GLN:CG	2.30	0.93
1:C:172:HIS:HB2	1:C:174:LEU:CG	1.98	0.93
1:C:17:THR:O	1:C:235:LEU:HA	1.66	0.93
1:A:29:VAL:HG11	1:A:242:CYS:HA	1.49	0.93
1:A:286:LYS:HD3	1:A:286:LYS:N	1.82	0.92
1:B:228:GLN:CG	1:B:229:GLN:N	2.30	0.92
1:C:342:THR:HG23	1:C:343:ASP:H	1.29	0.92
1:A:179:LEU:CG	1:A:219:LEU:HD21	1.99	0.92
1:B:138:GLU:C	1:B:176:PHE:HE2	1.69	0.92
1:C:53:LEU:HD13	1:C:164:ILE:HG22	1.50	0.92
1:A:179:LEU:CD2	1:A:219:LEU:CG	2.46	0.92
1:B:187:LEU:CD1	1:B:216:LEU:CD1	2.42	0.92
1:B:178:GLN:HB2	1:B:262:TYR:CD1	2.05	0.92
1:C:228:GLN:HE22	1:C:229:GLN:CG	1.81	0.92
1:C:286:LYS:HD3	1:C:286:LYS:N	1.84	0.92
1:C:43:ALA:HA	1:C:51:PHE:CE2	2.03	0.92
2:E:17:ARG:O	2:E:21:PHE:HD2	1.53	0.92
1:A:227:ARG:HD2	1:A:231:THR:HG1	1.17	0.92
1:C:227:ARG:HH22	1:C:263:ASP:HB3	1.35	0.92
1:C:229:GLN:NE2	1:C:235:LEU:HD12	1.82	0.92
1:A:243:ILE:H	1:A:243:ILE:HD13	1.34	0.92
1:B:227:ARG:HH22	1:B:263:ASP:HB2	1.32	0.92
1:C:228:GLN:NE2	1:C:229:GLN:N	2.18	0.92
1:B:286:LYS:N	1:B:286:LYS:HD3	1.83	0.91
1:A:179:LEU:HD21	1:A:219:LEU:CG	2.00	0.91
1:C:309:PHE:CZ	2:D:17:ARG:HD2	2.04	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:GLN:NE2	1:C:229:GLN:CB	2.34	0.91
1:C:133:ILE:HG23	1:C:134:PRO:HD2	1.52	0.91
1:C:321:ILE:O	1:C:321:ILE:HD13	1.70	0.91
1:B:29:VAL:HG11	1:B:242:CYS:CA	2.00	0.90
1:C:285:CYS:O	1:C:288:CYS:HB2	1.71	0.90
1:B:17:THR:O	1:B:235:LEU:HA	1.72	0.90
1:B:308:ASP:HB2	2:D:27:SER:OG	1.71	0.90
1:A:174:LEU:CD2	1:A:262:TYR:HD2	1.73	0.90
1:A:308:ASP:HB2	2:E:17:ARG:HH11	1.33	0.90
1:C:176:PHE:O	1:C:180:PRO:HD3	1.71	0.90
1:B:308:ASP:HB2	2:D:27:SER:CB	2.01	0.90
1:A:308:ASP:CG	2:E:16:ARG:NH2	2.25	0.90
2:D:17:ARG:O	2:D:21:PHE:HD2	1.53	0.90
1:B:228:GLN:HG3	1:B:229:GLN:H	1.37	0.90
1:B:29:VAL:HG13	1:B:243:ILE:CG2	2.03	0.89
1:B:23:VAL:O	1:B:167:THR:HG23	1.71	0.89
1:A:230:PHE:CE1	1:A:264:MET:HE3	2.08	0.89
1:C:29:VAL:HG13	1:C:243:ILE:CG2	2.03	0.89
1:C:228:GLN:NE2	1:C:229:GLN:CG	2.36	0.89
1:C:229:GLN:O	1:C:236:THR:HG21	1.73	0.89
1:A:230:PHE:CZ	1:A:264:MET:HE3	2.06	0.88
1:B:37:SER:OG	1:B:331:SER:HB3	1.72	0.88
2:E:17:ARG:O	2:E:21:PHE:CD2	2.26	0.88
1:C:22:PHE:CE1	1:C:165:PHE:CD1	2.62	0.88
1:C:230:PHE:O	1:C:264:MET:HE2	1.72	0.88
1:C:187:LEU:CD2	1:C:216:LEU:HD13	2.00	0.88
1:A:174:LEU:HG	1:A:262:TYR:HE2	1.35	0.88
2:D:17:ARG:O	2:D:21:PHE:CD2	2.26	0.88
1:A:43:ALA:HA	1:A:51:PHE:HE2	1.38	0.87
1:A:285:CYS:O	1:A:288:CYS:HB2	1.73	0.87
1:B:22:PHE:CE2	1:B:174:LEU:HD11	2.10	0.87
1:B:138:GLU:HB2	1:B:176:PHE:HD2	1.39	0.87
1:A:43:ALA:HA	1:A:51:PHE:CE2	2.09	0.87
1:C:187:LEU:CD1	1:C:216:LEU:CD1	2.42	0.87
1:B:187:LEU:CD2	1:B:216:LEU:HD13	2.00	0.86
1:C:228:GLN:HE21	1:C:229:GLN:CB	1.87	0.86
1:A:321:ILE:HD13	1:A:321:ILE:O	1.74	0.86
1:C:135:GLY:CA	1:C:179:LEU:HD23	2.06	0.86
2:E:20:LYS:O	2:E:24:GLY:N	2.08	0.86
1:B:29:VAL:HG22	1:B:243:ILE:HD12	1.56	0.86
1:A:53:LEU:HD13	1:A:164:ILE:HG22	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ILE:HG23	1:B:134:PRO:HD2	1.56	0.86
1:B:20:TRP:O	1:B:236:THR:HA	1.75	0.86
1:C:224:GLU:O	1:C:228:GLN:CG	2.24	0.86
1:C:306:TYR:HA	1:C:309:PHE:CD2	2.11	0.86
1:A:306:TYR:HD1	1:A:309:PHE:CD1	1.94	0.86
1:B:306:TYR:HD1	1:B:309:PHE:CD1	1.93	0.86
1:C:37:SER:OG	1:C:331:SER:HB3	1.75	0.86
1:A:174:LEU:HD21	1:A:262:TYR:HD2	1.33	0.85
1:B:176:PHE:O	1:B:179:LEU:HB3	1.74	0.85
1:B:39:ALA:HB2	1:B:164:ILE:HD12	1.57	0.85
1:A:37:SER:OG	1:A:331:SER:HB3	1.74	0.85
1:B:187:LEU:HD11	1:B:216:LEU:CG	2.05	0.85
1:B:246:PHE:N	1:B:298:TYR:HE2	1.73	0.85
1:A:319:GLY:HA3	1:B:294:MET:HG3	1.57	0.85
1:C:230:PHE:O	1:C:264:MET:HE1	1.76	0.85
1:B:187:LEU:CG	1:B:216:LEU:HD13	2.07	0.85
1:C:187:LEU:HD11	1:C:216:LEU:CG	2.05	0.85
2:D:20:LYS:O	2:D:24:GLY:N	2.08	0.85
1:C:29:VAL:HG22	1:C:243:ILE:HD12	1.58	0.84
1:B:224:GLU:O	1:B:228:GLN:CG	2.24	0.84
1:A:179:LEU:HD23	1:A:219:LEU:CD2	2.06	0.84
1:A:228:GLN:HE22	1:A:229:GLN:CG	1.89	0.84
1:B:43:ALA:HA	1:B:51:PHE:CE2	2.12	0.84
1:B:233:PRO:HB3	1:B:265:ASP:OD2	1.77	0.84
1:C:187:LEU:CG	1:C:216:LEU:HD13	2.07	0.84
1:C:229:GLN:NE2	1:C:229:GLN:HA	1.92	0.84
1:B:177:LEU:HD22	1:B:177:LEU:N	1.91	0.84
1:B:31:LYS:HA	1:B:34:SER:OG	1.78	0.84
1:B:29:VAL:HG22	1:B:243:ILE:CD1	2.07	0.84
1:B:227:ARG:HH22	1:B:263:ASP:CB	1.90	0.84
1:C:29:VAL:HG22	1:C:243:ILE:CD1	2.07	0.84
1:A:133:ILE:HG23	1:A:134:PRO:HD2	1.58	0.84
1:C:246:PHE:N	1:C:298:TYR:HE2	1.76	0.83
1:B:308:ASP:CB	2:D:27:SER:CB	2.55	0.83
1:C:333:PHE:HZ	1:C:343:ASP:HB3	1.42	0.83
1:A:177:LEU:HD12	1:A:262:TYR:HB3	1.61	0.83
1:C:305:LEU:HD23	1:C:306:TYR:CE2	2.14	0.83
1:C:306:TYR:CA	1:C:309:PHE:HD2	1.92	0.83
1:A:75:ARG:HD3	1:A:76:LYS:O	1.78	0.83
1:A:228:GLN:HE22	1:A:229:GLN:HG3	1.41	0.83
1:B:333:PHE:CD2	1:B:338:TYR:HB2	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:PHE:N	1:A:298:TYR:HE2	1.76	0.83
1:A:308:ASP:N	1:A:308:ASP:OD1	2.10	0.83
1:B:43:ALA:HA	1:B:51:PHE:HE2	1.44	0.83
1:B:228:GLN:CG	1:B:229:GLN:H	1.88	0.83
1:A:29:VAL:HG13	1:A:243:ILE:CG2	2.06	0.82
1:C:178:GLN:HB2	1:C:262:TYR:CE1	2.14	0.82
1:C:43:ALA:HB1	1:C:82:ASN:ND2	1.94	0.82
1:B:228:GLN:CD	1:B:229:GLN:N	2.33	0.82
1:C:133:ILE:HG23	1:C:134:PRO:CD	2.09	0.82
1:C:177:LEU:CD2	1:C:178:GLN:H	1.91	0.82
1:C:305:LEU:HD11	2:D:29:ARG:HD2	1.61	0.82
1:A:223:VAL:O	1:A:227:ARG:HB2	1.79	0.82
1:B:178:GLN:HB2	1:B:262:TYR:CE1	2.15	0.82
1:C:136:ILE:HG22	1:C:137:ASP:N	1.94	0.82
1:B:285:CYS:O	1:B:288:CYS:HB2	1.79	0.82
1:A:39:ALA:HB2	1:A:164:ILE:HD12	1.61	0.82
1:A:168:ALA:HB1	1:A:170:THR:HG23	1.61	0.82
1:A:43:ALA:HB1	1:A:82:ASN:ND2	1.95	0.81
1:B:175:ARG:CG	1:B:258:GLU:OE2	2.28	0.81
1:C:20:TRP:O	1:C:236:THR:HA	1.79	0.81
1:A:22:PHE:CE1	1:A:165:PHE:CD1	2.68	0.81
1:B:168:ALA:HB1	1:B:170:THR:HG23	1.61	0.81
1:B:228:GLN:HE21	1:B:229:GLN:N	1.76	0.81
1:C:8:ASN:O	1:C:9:LEU:HD23	1.80	0.81
1:C:178:GLN:OE1	1:C:262:TYR:CD1	2.33	0.81
1:C:233:PRO:HB3	1:C:265:ASP:OD2	1.80	0.81
1:C:22:PHE:HE1	1:C:165:PHE:CD1	1.99	0.81
1:C:179:LEU:HD12	1:C:179:LEU:C	2.01	0.81
1:A:233:PRO:HB3	1:A:265:ASP:OD2	1.80	0.81
1:A:333:PHE:CD2	1:A:338:TYR:HB2	2.14	0.81
1:B:326:ASN:OD1	1:B:350:LEU:HG	1.80	0.81
1:C:333:PHE:CD2	1:C:338:TYR:HB2	2.16	0.81
1:C:305:LEU:HG	1:C:305:LEU:O	1.80	0.81
1:A:29:VAL:HG22	1:A:243:ILE:HD12	1.63	0.81
1:C:50:GLN:HE22	1:C:82:ASN:HA	1.44	0.81
1:B:135:GLY:HA3	1:B:179:LEU:CD2	2.06	0.80
1:C:187:LEU:HD13	1:C:216:LEU:HD13	1.63	0.80
2:D:19:LYS:O	2:D:23:ASN:CB	2.30	0.80
1:A:20:TRP:O	1:A:236:THR:HA	1.81	0.80
1:B:187:LEU:HD13	1:B:216:LEU:HD13	1.63	0.80
1:B:179:LEU:HD12	1:B:179:LEU:C	2.01	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:PHE:CG	1:A:338:TYR:HB2	2.16	0.80
1:C:134:PRO:O	1:C:179:LEU:HD21	1.81	0.80
1:B:177:LEU:O	1:B:180:PRO:CD	2.29	0.80
1:C:177:LEU:O	1:C:180:PRO:CD	2.28	0.80
1:C:306:TYR:HA	1:C:309:PHE:HD2	1.46	0.80
1:A:333:PHE:HZ	1:A:343:ASP:HB3	1.45	0.80
1:C:245:GLU:C	1:C:298:TYR:HE2	1.85	0.80
1:B:53:LEU:HD13	1:B:164:ILE:HG22	1.63	0.80
1:B:136:ILE:HG22	1:B:137:ASP:N	1.97	0.80
1:C:291:ARG:O	1:C:294:MET:HB2	1.82	0.80
1:B:46:GLN:N	1:B:47:PRO:HD3	1.97	0.79
1:A:245:GLU:HA	1:A:298:TYR:CE2	2.16	0.79
1:C:246:PHE:C	1:C:246:PHE:HD1	1.85	0.79
1:B:245:GLU:HA	1:B:298:TYR:CE2	2.17	0.79
1:C:245:GLU:HA	1:C:298:TYR:CE2	2.17	0.79
2:E:19:LYS:O	2:E:23:ASN:CB	2.30	0.79
1:C:228:GLN:HE21	1:C:229:GLN:N	1.78	0.79
1:A:291:ARG:O	1:A:294:MET:HB2	1.82	0.79
1:C:39:ALA:HB2	1:C:164:ILE:HD12	1.65	0.79
1:A:133:ILE:HG23	1:A:134:PRO:CD	2.13	0.79
1:B:176:PHE:O	1:B:180:PRO:CD	2.31	0.79
1:B:133:ILE:HG23	1:B:134:PRO:CD	2.13	0.79
1:A:245:GLU:C	1:A:298:TYR:HE2	1.87	0.78
1:B:22:PHE:CE1	1:B:165:PHE:CD1	2.70	0.78
1:A:19:LYS:O	1:A:163:VAL:HG12	1.84	0.78
1:C:284:ASN:HB3	1:C:289:GLN:OE1	1.83	0.78
1:A:308:ASP:O	2:E:17:ARG:NH1	2.17	0.78
1:C:29:VAL:HG11	1:C:242:CYS:CA	2.13	0.78
1:C:50:GLN:NE2	1:C:82:ASN:HA	1.97	0.78
1:B:19:LYS:O	1:B:163:VAL:HG12	1.83	0.78
1:C:176:PHE:O	1:C:180:PRO:CD	2.32	0.78
1:A:8:ASN:O	1:A:9:LEU:HD23	1.83	0.77
1:C:231:THR:O	1:C:233:PRO:HD3	1.84	0.77
1:A:30:GLY:HA2	3:A:401:ADP:PB	2.24	0.77
1:A:174:LEU:CD2	1:A:262:TYR:CE2	2.66	0.77
1:B:333:PHE:CG	1:B:338:TYR:HB2	2.20	0.77
1:B:142:PHE:O	1:B:145:VAL:N	2.17	0.77
1:C:134:PRO:O	1:C:179:LEU:CD2	2.33	0.77
1:A:179:LEU:HD23	1:A:219:LEU:CG	2.13	0.77
1:A:230:PHE:HA	1:A:236:THR:HG21	1.66	0.77
1:B:30:GLY:O	1:B:241:VAL:HG11	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ASP:OD2	2:E:17:ARG:CG	2.33	0.76
1:B:342:THR:HG23	1:B:343:ASP:N	2.00	0.76
1:C:168:ALA:HB1	1:C:170:THR:HG23	1.66	0.76
1:C:327:LEU:O	1:C:330:PHE:HB3	1.84	0.76
1:A:51:PHE:CD1	1:A:162:THR:HB	2.21	0.76
1:B:138:GLU:HB2	1:B:176:PHE:CD2	2.20	0.76
1:A:315:PRO:HG3	1:A:338:TYR:CD2	2.20	0.76
1:C:75:ARG:HD3	1:C:76:LYS:O	1.84	0.76
1:B:51:PHE:HD1	1:B:162:THR:HB	1.51	0.76
1:B:308:ASP:HB3	2:D:27:SER:HB3	1.65	0.76
1:A:29:VAL:HG11	1:A:242:CYS:CA	2.16	0.76
1:C:31:LYS:HA	1:C:34:SER:OG	1.86	0.76
1:A:29:VAL:HG22	1:A:243:ILE:CD1	2.14	0.76
1:C:333:PHE:CG	1:C:338:TYR:HB2	2.20	0.76
1:A:136:ILE:HG22	1:A:137:ASP:N	2.00	0.76
1:B:43:ALA:HB1	1:B:82:ASN:ND2	2.00	0.76
1:C:244:SER:O	1:C:245:GLU:HG3	1.86	0.76
1:C:229:GLN:O	1:C:236:THR:CG2	2.34	0.76
1:B:175:ARG:CD	1:B:258:GLU:OE2	2.33	0.76
1:B:274:LEU:HA	1:B:295:GLN:HE22	1.51	0.76
1:C:19:LYS:O	1:C:163:VAL:HG12	1.86	0.75
1:B:176:PHE:O	1:B:179:LEU:N	2.19	0.75
1:A:327:LEU:O	1:A:330:PHE:HB3	1.85	0.75
1:B:233:PRO:CG	2:D:32:LYS:HD2	2.09	0.75
1:C:342:THR:HG23	1:C:343:ASP:N	2.01	0.75
1:B:333:PHE:HZ	1:B:343:ASP:HB3	1.52	0.75
1:B:139:ALA:CA	1:B:176:PHE:CD2	2.69	0.75
1:B:139:ALA:HA	1:B:176:PHE:CZ	2.21	0.75
1:B:291:ARG:O	1:B:294:MET:HB2	1.86	0.75
1:A:342:THR:HG23	1:A:343:ASP:N	2.00	0.75
1:B:327:LEU:O	1:B:330:PHE:HB3	1.86	0.75
1:C:246:PHE:C	1:C:246:PHE:CD1	2.56	0.75
1:C:177:LEU:N	1:C:177:LEU:CD2	2.49	0.74
1:A:51:PHE:HD1	1:A:162:THR:HB	1.50	0.74
1:B:138:GLU:CB	1:B:176:PHE:CD2	2.70	0.74
1:C:178:GLN:NE2	1:C:261:SER:OG	2.20	0.74
1:C:273:GLN:HA	1:C:316:LEU:HB2	1.69	0.74
1:A:172:HIS:O	1:A:172:HIS:CD2	2.40	0.74
1:C:227:ARG:NH2	1:C:263:ASP:CB	2.47	0.74
1:C:274:LEU:HA	1:C:295:GLN:HE22	1.50	0.74
1:B:24:GLY:HA2	1:B:31:LYS:CD	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PHE:O	1:A:145:VAL:N	2.20	0.74
1:B:8:ASN:O	1:B:9:LEU:HD23	1.88	0.74
1:A:38:ILE:HG22	1:A:164:ILE:CD1	2.18	0.74
1:C:51:PHE:HD1	1:C:162:THR:HB	1.52	0.73
1:B:274:LEU:HA	1:B:295:GLN:NE2	2.03	0.73
1:B:24:GLY:HA2	1:B:31:LYS:HD2	1.71	0.73
1:C:53:LEU:HD13	1:C:164:ILE:CG2	2.17	0.73
1:B:246:PHE:N	1:B:298:TYR:CE2	2.55	0.73
1:C:31:LYS:O	1:C:34:SER:HB2	1.88	0.73
1:A:273:GLN:HA	1:A:316:LEU:HB2	1.69	0.73
1:B:51:PHE:CD1	1:B:162:THR:HB	2.23	0.73
1:B:266:VAL:HG22	1:B:266:VAL:O	1.87	0.73
1:C:22:PHE:CE1	1:C:165:PHE:CG	2.77	0.73
1:C:172:HIS:CD2	1:C:172:HIS:O	2.42	0.73
1:C:239:VAL:HG13	1:C:268:SER:HB2	1.71	0.73
1:A:46:GLN:N	1:A:47:PRO:HD3	2.04	0.72
1:A:223:VAL:O	1:A:227:ARG:HB3	1.88	0.72
1:B:322:ARG:O	1:B:326:ASN:HB2	1.89	0.72
1:C:178:GLN:CB	1:C:262:TYR:CE1	2.72	0.72
1:C:322:ARG:O	1:C:326:ASN:HB2	1.88	0.72
1:A:322:ARG:O	1:A:326:ASN:HB2	1.89	0.72
1:B:172:HIS:CD2	1:B:172:HIS:O	2.42	0.72
1:C:46:GLN:N	1:C:47:PRO:HD3	2.04	0.72
1:C:22:PHE:HE1	1:C:165:PHE:CG	2.07	0.72
1:C:274:LEU:HA	1:C:295:GLN:NE2	2.02	0.72
1:A:50:GLN:NE2	1:A:82:ASN:HA	2.04	0.72
1:A:244:SER:O	1:A:245:GLU:HG3	1.89	0.72
1:A:12:LEU:HD13	1:A:18:HIS:HD2	1.53	0.72
1:C:246:PHE:N	1:C:298:TYR:CE2	2.58	0.72
1:C:252:THR:O	1:C:255:LEU:HB3	1.88	0.72
1:A:22:PHE:HE1	1:A:165:PHE:CD1	2.07	0.72
1:C:174:LEU:O	1:C:176:PHE:N	2.22	0.72
1:B:231:THR:O	1:B:233:PRO:HD3	1.90	0.72
1:C:142:PHE:O	1:C:145:VAL:N	2.22	0.72
1:A:241:VAL:HG13	1:A:270:ILE:HG22	1.72	0.72
1:C:308:ASP:HB2	2:D:17:ARG:HD3	1.71	0.72
1:C:315:PRO:HG3	1:C:338:TYR:CD2	2.24	0.72
1:A:174:LEU:O	1:A:176:PHE:N	2.22	0.71
1:A:287:ARG:HD3	1:B:348:TYR:CZ	2.25	0.71
1:B:134:PRO:C	1:B:179:LEU:HD22	2.08	0.71
1:C:12:LEU:HD13	1:C:18:HIS:HD2	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:VAL:HG13	1:C:270:ILE:HG22	1.71	0.71
1:A:176:PHE:O	1:A:179:LEU:HB2	1.88	0.71
1:B:273:GLN:HA	1:B:316:LEU:HB2	1.70	0.71
1:B:315:PRO:HG3	1:B:338:TYR:CD2	2.23	0.71
1:A:226:ILE:O	1:A:230:PHE:CB	2.38	0.71
1:C:51:PHE:CD1	1:C:162:THR:HB	2.24	0.71
1:A:59:ALA:HB2	1:B:251:GLU:OE1	1.90	0.71
1:A:246:PHE:N	1:A:298:TYR:CE2	2.58	0.71
1:B:39:ALA:CB	1:B:164:ILE:HD12	2.20	0.71
1:A:172:HIS:CD2	1:A:174:LEU:HB3	2.26	0.71
1:A:253:GLU:OE2	2:E:29:ARG:CZ	2.39	0.71
1:A:174:LEU:CG	1:A:262:TYR:HE2	1.96	0.71
1:A:300:ASP:O	1:A:301:GLN:C	2.27	0.71
1:A:348:TYR:CZ	1:B:287:ARG:HD3	2.26	0.71
1:C:227:ARG:NH2	1:C:263:ASP:HB2	2.03	0.71
1:A:253:GLU:OE2	2:E:29:ARG:NH1	2.24	0.71
1:A:326:ASN:OD1	1:A:350:LEU:HG	1.90	0.71
1:B:49:LYS:HB2	1:B:51:PHE:CZ	2.25	0.71
1:C:172:HIS:CD2	1:C:174:LEU:HB2	2.25	0.70
1:B:163:VAL:HG22	1:B:165:PHE:HE2	1.54	0.70
1:A:39:ALA:CB	1:A:164:ILE:HD12	2.21	0.70
1:A:320:GLU:OE1	1:A:320:GLU:HA	1.91	0.70
1:C:228:GLN:HE21	1:C:229:GLN:HB2	1.55	0.70
1:A:246:PHE:C	1:A:246:PHE:HD1	1.94	0.70
1:B:133:ILE:HG22	1:B:136:ILE:HG12	1.72	0.70
1:B:245:GLU:HA	1:B:298:TYR:HE2	1.57	0.70
1:B:245:GLU:C	1:B:298:TYR:HE2	1.93	0.70
1:C:138:GLU:O	1:C:141:SER:HB3	1.92	0.70
1:C:245:GLU:CA	1:C:298:TYR:HE2	2.05	0.70
1:C:305:LEU:CD1	2:D:29:ARG:HD2	2.20	0.70
1:A:245:GLU:CA	1:A:298:TYR:HE2	2.05	0.70
1:B:246:PHE:HD1	1:B:246:PHE:C	1.93	0.70
1:B:275:LEU:HB2	1:B:295:GLN:OE1	1.91	0.70
1:C:292:TRP:O	1:C:292:TRP:HE3	1.74	0.70
1:A:59:ALA:CB	1:B:251:GLU:OE1	2.40	0.70
1:B:22:PHE:HE1	1:B:165:PHE:CD1	2.09	0.70
1:B:305:LEU:O	1:B:305:LEU:HG	1.90	0.70
2:E:20:LYS:O	2:E:24:GLY:HA3	1.92	0.70
1:B:38:ILE:HG22	1:B:164:ILE:CD1	2.22	0.70
1:C:280:ASP:OD2	1:C:283:HIS:HB2	1.92	0.70
1:A:179:LEU:HD23	1:A:219:LEU:HG	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:TRP:HE3	1:A:292:TRP:O	1.75	0.69
1:B:36:CYS:O	1:B:38:ILE:N	2.24	0.69
1:B:50:GLN:NE2	1:B:82:ASN:HA	2.07	0.69
1:A:274:LEU:HA	1:A:295:GLN:HE22	1.56	0.69
1:B:12:LEU:HD13	1:B:18:HIS:HD2	1.57	0.69
1:B:57:ASP:OD2	1:B:59:ALA:HB3	1.92	0.69
1:B:138:GLU:O	1:B:176:PHE:HE2	1.75	0.69
1:B:175:ARG:HE	1:B:258:GLU:CD	1.95	0.69
1:C:280:ASP:CG	1:C:283:HIS:HB2	2.12	0.69
1:C:326:ASN:OD1	1:C:350:LEU:HG	1.92	0.69
1:A:31:LYS:H	3:A:401:ADP:PB	2.16	0.69
1:A:36:CYS:O	1:A:38:ILE:N	2.26	0.69
1:A:38:ILE:HG22	1:A:164:ILE:HD11	1.75	0.69
1:B:75:ARG:HD3	1:B:76:LYS:O	1.92	0.69
1:B:230:PHE:CA	1:B:236:THR:HG21	2.17	0.69
2:D:19:LYS:O	2:D:23:ASN:N	2.25	0.69
2:D:20:LYS:O	2:D:24:GLY:HA3	1.92	0.69
1:B:292:TRP:O	1:B:292:TRP:HE3	1.76	0.69
1:B:298:TYR:O	1:B:302:ILE:HD12	1.93	0.69
1:C:34:SER:O	1:C:36:CYS:N	2.25	0.69
1:B:289:GLN:O	1:B:292:TRP:HB3	1.93	0.69
1:C:298:TYR:O	1:C:302:ILE:HD12	1.93	0.69
2:E:19:LYS:O	2:E:23:ASN:HB2	1.92	0.69
1:A:34:SER:O	1:A:36:CYS:N	2.26	0.69
1:A:133:ILE:HG22	1:A:136:ILE:HG12	1.75	0.69
1:C:136:ILE:HG22	1:C:137:ASP:H	1.57	0.69
1:A:298:TYR:O	1:A:302:ILE:HD12	1.93	0.68
1:C:306:TYR:CA	1:C:309:PHE:CD2	2.73	0.68
2:E:19:LYS:O	2:E:23:ASN:CG	2.32	0.68
1:B:177:LEU:CD2	1:B:178:GLN:N	2.42	0.68
1:C:176:PHE:O	1:C:179:LEU:HB3	1.93	0.68
1:C:300:ASP:O	1:C:301:GLN:C	2.31	0.68
1:A:292:TRP:O	1:A:292:TRP:CE3	2.47	0.68
1:A:22:PHE:CE1	1:A:165:PHE:CG	2.81	0.68
1:C:10:HIS:HB2	1:C:335:ASN:OD1	1.94	0.68
1:B:8:ASN:OD1	1:B:10:HIS:N	2.26	0.68
1:C:48:ASN:O	1:C:49:LYS:HD3	1.94	0.68
1:C:230:PHE:HA	1:C:236:THR:HG21	1.76	0.68
1:A:252:THR:O	1:A:255:LEU:HB3	1.94	0.68
1:B:300:ASP:O	1:B:301:GLN:C	2.31	0.68
2:D:20:LYS:O	2:D:24:GLY:CA	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LYS:HB2	1:B:241:VAL:HB	1.76	0.68
1:B:176:PHE:O	1:B:180:PRO:HD3	1.94	0.68
1:A:274:LEU:HA	1:A:295:GLN:NE2	2.09	0.68
1:B:138:GLU:O	1:B:141:SER:HB3	1.93	0.68
1:B:254:ARG:HG3	1:B:254:ARG:NH1	2.09	0.68
2:E:19:LYS:O	2:E:23:ASN:N	2.25	0.68
2:D:19:LYS:O	2:D:23:ASN:HB2	1.92	0.67
1:B:305:LEU:HD23	1:B:306:TYR:CE2	2.28	0.67
2:D:19:LYS:O	2:D:23:ASN:CG	2.32	0.67
1:C:320:GLU:OE1	1:C:320:GLU:HA	1.93	0.67
1:B:38:ILE:HG22	1:B:164:ILE:HD11	1.76	0.67
1:C:38:ILE:HG22	1:C:164:ILE:CD1	2.24	0.67
2:E:20:LYS:O	2:E:24:GLY:CA	2.42	0.67
2:E:29:ARG:O	2:E:33:ILE:HG13	1.95	0.67
1:A:315:PRO:HG3	1:A:338:TYR:CG	2.30	0.67
1:C:30:GLY:HA2	3:C:401:ADP:PB	2.34	0.67
1:C:178:GLN:CB	1:C:262:TYR:CD1	2.71	0.67
1:A:227:ARG:HA	1:A:230:PHE:HB3	1.77	0.67
1:C:292:TRP:O	1:C:292:TRP:CE3	2.47	0.67
1:C:226:ILE:HG23	1:C:230:PHE:CD2	2.29	0.67
1:C:308:ASP:O	2:D:17:ARG:NH1	2.28	0.67
1:A:50:GLN:HE22	1:A:82:ASN:HA	1.60	0.67
1:C:88:ILE:O	1:C:90:PRO:HD3	1.95	0.67
2:D:16:ARG:O	2:D:20:LYS:HG2	1.95	0.67
1:A:275:LEU:HB2	1:A:295:GLN:OE1	1.95	0.67
1:C:289:GLN:O	1:C:292:TRP:HB3	1.95	0.67
1:A:247:LEU:HD22	1:B:64:ASP:CG	2.16	0.66
1:A:317:CYS:O	3:A:401:ADP:H2	1.77	0.66
1:C:38:ILE:HG22	1:C:164:ILE:HD11	1.75	0.66
1:C:229:GLN:HE21	1:C:235:LEU:HD12	1.60	0.66
1:C:305:LEU:O	1:C:305:LEU:CG	2.40	0.66
1:B:134:PRO:O	1:B:179:LEU:HD23	1.93	0.66
1:B:254:ARG:HG3	1:B:254:ARG:HH11	1.61	0.66
1:C:254:ARG:HG3	1:C:254:ARG:NH1	2.10	0.66
1:A:48:ASN:O	1:A:49:LYS:HD3	1.96	0.66
1:C:39:ALA:CB	1:C:164:ILE:HD12	2.25	0.66
1:C:133:ILE:HG22	1:C:136:ILE:HG12	1.76	0.66
1:B:270:ILE:HG22	1:B:270:ILE:O	1.95	0.66
1:A:31:LYS:HA	1:A:34:SER:OG	1.95	0.66
1:B:163:VAL:HG22	1:B:165:PHE:CE2	2.31	0.66
1:B:232:ASP:OD2	1:B:234:ASP:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:THR:CG2	1:A:343:ASP:H	2.06	0.66
1:C:6:GLU:HB3	1:C:8:ASN:ND2	2.11	0.66
2:E:16:ARG:O	2:E:20:LYS:HG2	1.95	0.66
1:A:174:LEU:CD2	1:A:259:LEU:HD23	2.26	0.66
2:D:29:ARG:O	2:D:33:ILE:HG13	1.95	0.66
1:A:22:PHE:HE1	1:A:165:PHE:CG	2.14	0.65
1:B:187:LEU:HD11	1:B:216:LEU:CD2	2.26	0.65
1:C:266:VAL:O	1:C:266:VAL:HG22	1.96	0.65
1:A:320:GLU:HG2	1:B:294:MET:CE	2.26	0.65
1:B:60:HIS:CD2	1:B:69:LYS:NZ	2.65	0.65
1:B:245:GLU:CA	1:B:298:TYR:HE2	2.09	0.65
1:A:245:GLU:CA	1:A:298:TYR:CE2	2.79	0.65
1:B:34:SER:O	1:B:36:CYS:N	2.29	0.65
1:C:245:GLU:CA	1:C:298:TYR:CE2	2.79	0.65
1:A:333:PHE:CZ	1:A:343:ASP:HB3	2.31	0.65
1:B:228:GLN:HE21	1:B:229:GLN:CB	1.68	0.65
1:B:246:PHE:C	1:B:246:PHE:CD1	2.68	0.65
1:B:252:THR:O	1:B:255:LEU:HB3	1.95	0.65
1:C:12:LEU:CD1	1:C:18:HIS:HD2	2.10	0.65
1:C:24:GLY:HA2	1:C:31:LYS:CD	2.26	0.65
1:A:228:GLN:CD	1:A:229:GLN:N	2.50	0.65
1:B:320:GLU:OE1	1:B:320:GLU:HA	1.97	0.65
1:A:246:PHE:C	1:A:246:PHE:CD1	2.67	0.65
1:B:342:THR:CG2	1:B:343:ASP:H	2.09	0.65
1:C:8:ASN:N	1:C:312:VAL:HG22	2.12	0.65
1:C:187:LEU:HD11	1:C:216:LEU:CD2	2.26	0.65
1:C:347:ILE:C	1:C:349:GLU:H	1.99	0.65
1:B:138:GLU:CB	1:B:176:PHE:HD2	2.05	0.65
1:B:175:ARG:HA	1:B:262:TYR:CZ	2.31	0.65
2:E:11:ARG:O	2:E:15:GLU:HG3	1.97	0.65
1:A:6:GLU:HB3	1:A:8:ASN:ND2	2.12	0.64
1:A:70:PHE:CE1	1:A:85:CYS:HB3	2.32	0.64
1:B:177:LEU:CD2	1:B:177:LEU:N	2.60	0.64
1:C:163:VAL:HG22	1:C:165:PHE:HE2	1.62	0.64
1:C:254:ARG:HG3	1:C:254:ARG:HH11	1.62	0.64
2:D:11:ARG:O	2:D:15:GLU:HG3	1.97	0.64
1:A:30:GLY:HA2	3:A:401:ADP:PA	2.37	0.64
1:A:289:GLN:O	1:A:292:TRP:HB3	1.97	0.64
1:B:31:LYS:O	1:B:34:SER:HB2	1.97	0.64
1:B:244:SER:O	1:B:245:GLU:HG3	1.96	0.64
1:A:53:LEU:HD13	1:A:164:ILE:CG2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLN:CD	1:A:229:GLN:HG3	2.16	0.64
1:B:168:ALA:CB	1:B:170:THR:HG23	2.27	0.64
1:A:223:VAL:O	1:A:227:ARG:CA	2.45	0.64
1:A:30:GLY:O	1:A:241:VAL:HG11	1.98	0.64
1:A:47:PRO:HA	1:A:82:ASN:HD22	1.62	0.64
1:A:75:ARG:HD2	1:A:75:ARG:O	1.98	0.64
1:B:347:ILE:HD13	1:B:347:ILE:N	2.12	0.64
1:C:20:TRP:CE2	1:C:229:GLN:OE1	2.50	0.64
1:C:31:LYS:H	3:C:401:ADP:PB	2.21	0.64
1:B:40:ILE:HG22	1:B:41:GLN:N	2.11	0.64
1:B:324:LEU:HD12	1:B:324:LEU:O	1.98	0.64
2:D:14:ARG:CG	2:D:17:ARG:NH2	2.55	0.64
1:A:12:LEU:CD1	1:A:18:HIS:HD2	2.11	0.64
1:A:138:GLU:O	1:A:141:SER:HB3	1.96	0.64
1:C:77:VAL:HG23	1:C:83:LEU:O	1.98	0.64
1:A:245:GLU:HA	1:A:298:TYR:HE2	1.58	0.64
1:A:266:VAL:O	1:A:266:VAL:HG22	1.98	0.64
1:B:178:GLN:CB	1:B:262:TYR:CE1	2.81	0.64
1:A:227:ARG:CZ	1:A:231:THR:OG1	2.45	0.64
1:A:228:GLN:OE1	1:A:229:GLN:N	2.30	0.64
1:A:291:ARG:HH11	1:A:291:ARG:HG2	1.64	0.64
1:B:292:TRP:O	1:B:292:TRP:CE3	2.50	0.64
1:B:339:ASN:OD1	1:B:339:ASN:C	2.37	0.64
1:C:47:PRO:HA	1:C:82:ASN:HD22	1.62	0.64
1:C:49:LYS:HB2	1:C:51:PHE:CZ	2.33	0.64
1:B:54:ILE:HG22	1:B:86:MET:HB3	1.79	0.63
1:C:140:LEU:HA	1:C:143:MET:HB2	1.80	0.63
1:C:284:ASN:OD1	1:C:288:CYS:CB	2.46	0.63
1:A:10:HIS:HB2	1:A:335:ASN:OD1	1.97	0.63
1:A:179:LEU:CG	1:A:219:LEU:CD2	2.69	0.63
1:A:49:LYS:HB2	1:A:51:PHE:CZ	2.33	0.63
1:A:253:GLU:CD	2:E:29:ARG:HH12	2.02	0.63
1:B:339:ASN:OD1	1:B:341:ILE:HG13	1.99	0.63
1:B:18:HIS:ND1	1:B:234:ASP:O	2.31	0.63
1:A:57:ASP:OD2	1:A:59:ALA:HB3	1.99	0.63
1:B:311:VAL:HG22	1:B:311:VAL:O	1.98	0.63
1:C:288:CYS:SG	5:C:363:ZN:ZN	1.85	0.63
1:B:225:THR:O	1:B:228:GLN:NE2	2.30	0.63
1:C:53:LEU:CD1	1:C:164:ILE:HG22	2.27	0.63
1:C:279:ASN:O	1:C:280:ASP:HB3	1.98	0.63
1:B:135:GLY:CA	1:B:179:LEU:CD2	2.71	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:PHE:O	1:B:179:LEU:CB	2.47	0.63
1:C:227:ARG:O	1:C:231:THR:N	2.32	0.63
1:C:30:GLY:HA2	3:C:401:ADP:PA	2.38	0.63
1:C:225:THR:O	1:C:228:GLN:NE2	2.30	0.63
1:C:315:PRO:HG3	1:C:338:TYR:CG	2.33	0.63
1:B:22:PHE:CE1	1:B:165:PHE:CG	2.87	0.62
1:B:53:LEU:HD13	1:B:164:ILE:CG2	2.29	0.62
1:B:187:LEU:HD11	1:B:216:LEU:HD22	1.81	0.62
1:B:228:GLN:HE21	1:B:229:GLN:H	1.47	0.62
1:C:266:VAL:O	1:C:266:VAL:HG13	1.99	0.62
1:B:242:CYS:HB2	1:B:252:THR:OG1	1.98	0.62
1:A:348:TYR:CZ	1:B:287:ARG:HG2	2.34	0.62
1:A:18:HIS:HA	1:A:235:LEU:HA	1.82	0.62
1:A:239:VAL:HG13	1:A:268:SER:HB2	1.79	0.62
1:B:48:ASN:O	1:B:49:LYS:HD3	1.99	0.62
1:C:270:ILE:HG22	1:C:270:ILE:O	1.99	0.62
1:C:8:ASN:H	1:C:312:VAL:HG22	1.63	0.62
1:C:18:HIS:O	1:C:162:THR:HG23	1.99	0.62
1:C:36:CYS:O	1:C:38:ILE:N	2.32	0.62
1:C:238:PHE:CZ	1:C:259:LEU:HD11	2.34	0.62
1:A:28:GLY:HA3	1:B:28:GLY:HA3	1.82	0.62
1:B:60:HIS:HD2	1:B:69:LYS:NZ	1.96	0.62
1:B:223:VAL:HA	1:B:226:ILE:HB	1.82	0.62
1:B:347:ILE:C	1:B:349:GLU:H	2.03	0.62
1:C:228:GLN:HE21	1:C:229:GLN:CA	2.02	0.62
2:E:14:ARG:HA	2:E:17:ARG:CZ	2.30	0.62
1:C:133:ILE:CG2	1:C:134:PRO:HD2	2.28	0.62
1:B:12:LEU:CD1	1:B:18:HIS:HD2	2.13	0.62
1:C:339:ASN:HB3	1:C:342:THR:CG2	2.30	0.62
1:B:10:HIS:HB2	1:B:335:ASN:OD1	2.00	0.62
1:B:152:GLN:O	1:B:156:GLU:HB2	2.00	0.61
1:C:342:THR:CG2	1:C:343:ASP:H	2.06	0.61
1:A:50:GLN:N	1:A:161:ASP:OD2	2.33	0.61
1:B:251:GLU:O	1:B:254:ARG:HB2	2.00	0.61
1:C:60:HIS:HD2	1:C:69:LYS:NZ	1.98	0.61
1:C:187:LEU:HD11	1:C:216:LEU:HD22	1.81	0.61
1:A:178:GLN:HE21	1:A:262:TYR:HE1	1.47	0.61
1:A:12:LEU:HD12	1:A:12:LEU:O	2.00	0.61
1:A:39:ALA:CA	1:A:164:ILE:HD12	2.30	0.61
2:D:14:ARG:HA	2:D:17:ARG:CZ	2.30	0.61
1:B:245:GLU:CA	1:B:298:TYR:CE2	2.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:VAL:CG2	1:B:165:PHE:HE2	2.13	0.61
1:C:60:HIS:CD2	1:C:69:LYS:NZ	2.69	0.61
1:C:333:PHE:CZ	1:C:343:ASP:HB3	2.29	0.61
1:A:31:LYS:N	3:A:401:ADP:O3B	2.34	0.61
1:A:339:ASN:C	1:A:339:ASN:OD1	2.39	0.61
1:C:177:LEU:HD21	1:C:262:TYR:CD2	2.35	0.61
1:C:254:ARG:O	1:C:255:LEU:C	2.38	0.61
1:A:40:ILE:HG22	1:A:41:GLN:N	2.15	0.61
1:A:347:ILE:C	1:A:349:GLU:H	2.04	0.61
1:C:24:GLY:HA2	1:C:31:LYS:HD2	1.82	0.61
1:C:245:GLU:HA	1:C:298:TYR:HE2	1.60	0.61
1:C:18:HIS:HA	1:C:235:LEU:HA	1.82	0.61
1:A:232:ASP:OD2	1:A:234:ASP:HB2	2.00	0.60
1:A:306:TYR:CD1	1:A:309:PHE:CD1	2.84	0.60
1:C:223:VAL:HA	1:C:226:ILE:HB	1.82	0.60
1:A:179:LEU:HB3	1:A:180:PRO:CD	2.26	0.60
1:B:339:ASN:HB3	1:B:342:THR:CG2	2.31	0.60
1:A:254:ARG:HG3	1:A:254:ARG:HH11	1.66	0.60
1:A:300:ASP:O	1:A:302:ILE:N	2.35	0.60
1:A:254:ARG:HG3	1:A:254:ARG:NH1	2.14	0.60
1:C:139:ALA:O	1:C:140:LEU:C	2.39	0.60
1:C:291:ARG:HG2	1:C:291:ARG:HH11	1.66	0.60
1:C:306:TYR:CD1	1:C:309:PHE:CD2	2.89	0.60
1:A:138:GLU:HB3	1:A:173:THR:HB	1.83	0.60
1:C:19:LYS:C	1:C:20:TRP:CD1	2.75	0.60
1:C:275:LEU:HB2	1:C:295:GLN:OE1	2.00	0.60
1:C:317:CYS:O	3:C:401:ADP:H2	1.84	0.60
1:A:18:HIS:ND1	1:A:234:ASP:O	2.33	0.60
1:A:168:ALA:CB	1:A:170:THR:HG23	2.30	0.60
1:A:251:GLU:O	1:A:254:ARG:HB2	2.02	0.60
1:B:296:LYS:C	1:B:298:TYR:N	2.54	0.60
1:B:136:ILE:HG22	1:B:137:ASP:H	1.66	0.60
1:C:227:ARG:HD2	1:C:231:THR:OG1	2.02	0.60
1:C:305:LEU:O	1:C:306:TYR:CD2	2.55	0.60
1:B:228:GLN:O	1:B:229:GLN:O	2.02	0.60
1:C:164:ILE:HG22	1:C:164:ILE:O	2.01	0.60
1:C:227:ARG:NH2	1:C:263:ASP:HB3	2.10	0.60
1:A:18:HIS:O	1:A:162:THR:HG23	2.02	0.60
1:A:64:ASP:CG	1:B:247:LEU:HD22	2.22	0.60
1:A:179:LEU:HG	1:A:183:LEU:CD1	2.32	0.60
1:C:134:PRO:C	1:C:179:LEU:CD2	2.70	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:GLN:HG3	1:C:333:PHE:N	2.17	0.60
1:B:50:GLN:HE22	1:B:82:ASN:HA	1.64	0.60
1:B:239:VAL:HG13	1:B:268:SER:HB2	1.84	0.60
1:A:24:GLY:HA2	1:A:31:LYS:CD	2.33	0.59
1:B:22:PHE:HE1	1:B:165:PHE:CG	2.20	0.59
1:B:305:LEU:O	1:B:305:LEU:CG	2.50	0.59
1:C:141:SER:O	1:C:145:VAL:HG23	2.02	0.59
1:C:339:ASN:C	1:C:339:ASN:OD1	2.40	0.59
1:B:18:HIS:HA	1:B:235:LEU:HA	1.84	0.59
1:B:63:SER:HB3	1:B:69:LYS:HA	1.83	0.59
1:C:8:ASN:OD1	1:C:10:HIS:N	2.34	0.59
1:C:39:ALA:CA	1:C:164:ILE:HD12	2.33	0.59
1:A:8:ASN:OD1	1:A:10:HIS:N	2.35	0.59
1:B:19:LYS:C	1:B:20:TRP:CD1	2.76	0.59
1:B:254:ARG:O	1:B:255:LEU:C	2.39	0.59
1:A:9:LEU:O	1:A:13:ILE:HG13	2.02	0.59
1:A:181:ASN:O	1:A:184:SER:N	2.20	0.59
1:B:50:GLN:N	1:B:161:ASP:OD2	2.35	0.59
1:B:70:PHE:CE1	1:B:85:CYS:HB3	2.38	0.59
1:C:93:ALA:O	1:C:94:LEU:O	2.20	0.59
1:A:31:LYS:O	1:A:34:SER:HB2	2.01	0.59
1:A:258:GLU:O	1:A:261:SER:HB3	2.03	0.59
1:A:296:LYS:C	1:A:298:TYR:N	2.56	0.59
1:B:228:GLN:NE2	1:B:229:GLN:H	1.96	0.59
1:C:50:GLN:HE22	1:C:82:ASN:CA	2.14	0.59
1:C:177:LEU:CD2	1:C:178:GLN:N	2.58	0.59
1:C:178:GLN:HB2	1:C:262:TYR:HD1	1.57	0.59
1:A:152:GLN:O	1:A:156:GLU:HB2	2.03	0.59
1:C:135:GLY:O	1:C:136:ILE:O	2.20	0.59
1:C:138:GLU:HB3	1:C:173:THR:HB	1.84	0.59
1:C:242:CYS:HB2	1:C:252:THR:OG1	2.02	0.59
1:A:179:LEU:HG	1:A:183:LEU:HD12	1.85	0.59
1:A:185:LYS:O	1:A:188:GLU:HG2	2.03	0.59
1:A:226:ILE:O	1:A:230:PHE:N	2.33	0.59
1:A:228:GLN:OE1	1:A:228:GLN:C	2.41	0.59
1:B:315:PRO:HG3	1:B:338:TYR:CG	2.37	0.59
1:C:22:PHE:CD1	1:C:165:PHE:HB2	2.37	0.59
1:C:54:ILE:HG22	1:C:86:MET:HB3	1.84	0.59
1:C:251:GLU:O	1:C:254:ARG:HB2	2.03	0.59
1:A:17:THR:O	1:A:235:LEU:HD23	2.03	0.58
1:A:60:HIS:HD2	1:A:69:LYS:NZ	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LEU:HD12	1:B:12:LEU:O	2.03	0.58
1:B:39:ALA:CA	1:B:164:ILE:HD12	2.31	0.58
1:B:178:GLN:OE1	1:B:262:TYR:CD1	2.49	0.58
1:C:30:GLY:O	1:C:241:VAL:HG11	2.03	0.58
1:C:140:LEU:HD22	1:C:140:LEU:N	2.09	0.58
1:B:37:SER:HG	1:B:330:PHE:HD2	1.50	0.58
1:C:40:ILE:HG22	1:C:41:GLN:N	2.18	0.58
1:B:291:ARG:HG2	1:B:291:ARG:HH11	1.68	0.58
1:B:332:GLN:HG3	1:B:333:PHE:N	2.16	0.58
1:A:227:ARG:NH2	1:A:263:ASP:CB	2.66	0.58
1:C:228:GLN:HE21	1:C:229:GLN:H	1.46	0.58
1:A:60:HIS:CD2	1:A:69:LYS:NZ	2.72	0.58
1:A:175:ARG:HB2	1:A:175:ARG:CZ	2.34	0.58
1:A:306:TYR:HB3	1:A:309:PHE:HB2	1.86	0.58
1:A:311:VAL:O	1:A:311:VAL:HG22	2.03	0.58
1:B:141:SER:O	1:B:145:VAL:HG23	2.04	0.58
1:C:152:GLN:O	1:C:156:GLU:HB2	2.04	0.58
1:C:163:VAL:CG2	1:C:165:PHE:HE2	2.16	0.58
1:C:275:LEU:HD22	1:C:292:TRP:CA	2.33	0.58
1:B:22:PHE:CD2	1:B:174:LEU:CD1	2.83	0.58
1:B:30:GLY:HA2	3:B:401:ADP:PB	2.43	0.58
1:C:153:GLU:OE2	1:C:160:PHE:HB2	2.04	0.58
1:A:348:TYR:OH	1:B:287:ARG:HG2	2.04	0.58
1:B:266:VAL:O	1:B:266:VAL:HG13	2.04	0.58
1:A:140:LEU:HA	1:A:143:MET:HB2	1.85	0.58
1:B:140:LEU:HA	1:B:143:MET:HB2	1.84	0.58
1:A:242:CYS:HB2	1:A:252:THR:OG1	2.03	0.58
1:C:12:LEU:HD12	1:C:12:LEU:O	2.04	0.58
1:C:22:PHE:HD1	1:C:165:PHE:HB2	1.69	0.58
1:C:172:HIS:CG	1:C:174:LEU:HD12	2.38	0.57
1:C:269:ILE:O	1:C:269:ILE:HG22	2.02	0.57
1:B:49:LYS:CB	1:B:51:PHE:CZ	2.87	0.57
1:C:333:PHE:CE2	1:C:338:TYR:HD2	2.22	0.57
1:A:153:GLU:OE2	1:A:160:PHE:HB2	2.04	0.57
1:A:227:ARG:HH22	1:A:263:ASP:CB	2.16	0.57
1:A:339:ASN:HB3	1:A:342:THR:CG2	2.34	0.57
1:B:31:LYS:HA	1:B:34:SER:CB	2.33	0.57
1:B:225:THR:O	1:B:229:GLN:HB2	2.05	0.57
1:B:243:ILE:HD13	1:B:243:ILE:N	2.09	0.57
1:A:272:ASN:OD1	1:A:273:GLN:N	2.38	0.57
1:B:176:PHE:O	1:B:180:PRO:HD2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:VAL:HG22	1:C:165:PHE:CE2	2.39	0.57
1:A:8:ASN:N	1:A:312:VAL:HG22	2.20	0.57
1:B:135:GLY:N	1:B:179:LEU:CD2	2.67	0.57
1:B:230:PHE:HB3	1:B:264:MET:CE	2.34	0.57
1:C:246:PHE:HD1	1:C:246:PHE:O	1.86	0.57
1:C:308:ASP:CB	2:D:17:ARG:HD3	2.33	0.57
1:A:31:LYS:HB2	1:A:241:VAL:HB	1.85	0.57
1:A:141:SER:O	1:A:145:VAL:HG23	2.04	0.57
1:A:174:LEU:HD22	1:A:259:LEU:HD23	1.86	0.57
1:C:339:ASN:HB3	1:C:342:THR:HG22	1.87	0.57
2:D:10:ARG:HD2	2:D:14:ARG:HH21	1.70	0.57
1:A:163:VAL:HG22	1:A:165:PHE:HE2	1.69	0.57
1:A:176:PHE:O	1:A:179:LEU:CB	2.52	0.57
1:B:175:ARG:CA	1:B:262:TYR:CE2	2.80	0.57
1:A:63:SER:HB3	1:A:69:LYS:HA	1.87	0.57
1:A:140:LEU:HD22	1:A:140:LEU:N	2.11	0.57
1:A:243:ILE:HD13	1:A:243:ILE:N	2.13	0.57
1:B:306:TYR:O	1:B:307:GLU:C	2.42	0.57
1:B:306:TYR:CD1	1:B:309:PHE:CD1	2.85	0.57
1:C:175:ARG:CZ	1:C:175:ARG:HB2	2.34	0.57
1:A:142:PHE:O	1:A:143:MET:C	2.42	0.57
1:B:230:PHE:O	1:B:264:MET:HE3	2.05	0.57
1:B:243:ILE:H	1:B:243:ILE:CD1	2.09	0.57
1:C:18:HIS:ND1	1:C:234:ASP:O	2.37	0.57
1:B:142:PHE:O	1:B:143:MET:C	2.43	0.57
1:C:243:ILE:HD13	1:C:243:ILE:N	2.08	0.57
1:A:140:LEU:O	1:A:141:SER:C	2.44	0.56
1:C:50:GLN:N	1:C:161:ASP:OD2	2.37	0.56
1:A:75:ARG:CD	1:A:76:LYS:O	2.51	0.56
1:A:136:ILE:HG22	1:A:137:ASP:H	1.70	0.56
1:A:324:LEU:HD12	1:A:324:LEU:O	2.05	0.56
1:A:332:GLN:HG3	1:A:333:PHE:N	2.20	0.56
1:C:17:THR:O	1:C:235:LEU:HD23	2.06	0.56
1:C:31:LYS:HA	1:C:34:SER:CB	2.35	0.56
1:C:175:ARG:HA	1:C:262:TYR:CZ	2.41	0.56
1:C:232:ASP:OD2	1:C:234:ASP:HB2	2.05	0.56
1:C:296:LYS:C	1:C:298:TYR:N	2.57	0.56
1:C:300:ASP:O	1:C:302:ILE:N	2.38	0.56
1:A:315:PRO:HB3	1:A:338:TYR:CE1	2.40	0.56
1:C:43:ALA:CA	1:C:51:PHE:CE2	2.82	0.56
1:A:320:GLU:HG3	1:A:322:ARG:HH12	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:O	1:B:141:SER:C	2.44	0.56
1:B:153:GLU:OE2	1:B:160:PHE:HB2	2.06	0.56
1:C:26:LYS:HD3	1:C:251:GLU:OE1	2.05	0.56
1:C:142:PHE:O	1:C:143:MET:C	2.44	0.56
1:C:232:ASP:OD1	1:C:232:ASP:O	2.23	0.56
1:A:258:GLU:HA	1:A:261:SER:HB3	1.88	0.56
1:A:275:LEU:HD22	1:A:292:TRP:CA	2.36	0.56
1:B:20:TRP:HB2	1:B:236:THR:HB	1.86	0.56
1:B:42:MET:CE	1:B:162:THR:HG21	2.35	0.56
1:C:70:PHE:CE1	1:C:85:CYS:HB3	2.40	0.56
1:C:238:PHE:CE2	1:C:259:LEU:HD21	2.41	0.56
1:C:339:ASN:OD1	1:C:341:ILE:HG13	2.05	0.56
2:E:10:ARG:HD2	2:E:14:ARG:HH21	1.70	0.56
1:A:31:LYS:O	1:A:31:LYS:HG2	2.05	0.56
1:A:164:ILE:HG22	1:A:164:ILE:O	2.06	0.56
1:A:319:GLY:O	1:A:320:GLU:O	2.23	0.56
1:A:305:LEU:O	1:A:306:TYR:CD2	2.59	0.56
1:B:164:ILE:HG22	1:B:164:ILE:O	2.05	0.56
1:A:230:PHE:CD2	1:A:264:MET:HE2	2.34	0.56
1:A:266:VAL:O	1:A:266:VAL:HG13	2.06	0.56
1:B:232:ASP:CG	1:B:234:ASP:H	2.09	0.56
1:B:318:ALA:H	1:B:351:GLU:CD	2.09	0.56
1:A:12:LEU:HD13	1:A:18:HIS:CD2	2.38	0.56
1:A:54:ILE:HG22	1:A:86:MET:HB3	1.87	0.56
1:A:226:ILE:O	1:A:230:PHE:HB3	2.05	0.56
1:B:275:LEU:HD22	1:B:292:TRP:CA	2.36	0.56
1:C:136:ILE:O	1:C:137:ASP:C	2.45	0.56
1:A:39:ALA:HB2	1:A:164:ILE:CD1	2.34	0.56
1:C:75:ARG:HD2	1:C:75:ARG:O	2.05	0.56
1:C:255:LEU:HD11	1:C:259:LEU:HD11	1.88	0.56
1:C:258:GLU:O	1:C:261:SER:HB3	2.06	0.56
1:A:139:ALA:O	1:A:140:LEU:C	2.45	0.55
1:A:178:GLN:NE2	1:A:262:TYR:HE1	2.02	0.55
1:A:254:ARG:O	1:A:255:LEU:C	2.43	0.55
1:C:220:LYS:HG2	1:C:224:GLU:OE1	2.06	0.55
1:A:220:LYS:HG2	1:A:224:GLU:OE1	2.06	0.55
1:B:139:ALA:N	1:B:176:PHE:HD2	1.92	0.55
2:E:14:ARG:CG	2:E:17:ARG:HH22	2.05	0.55
1:A:174:LEU:CD1	1:A:262:TYR:HD2	2.18	0.55
1:B:60:HIS:CD2	1:B:69:LYS:HZ1	2.25	0.55
1:B:230:PHE:HB3	1:B:264:MET:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ASP:O	1:B:302:ILE:N	2.39	0.55
1:C:275:LEU:O	1:C:276:PHE:HB2	2.06	0.55
1:C:347:ILE:O	1:C:349:GLU:N	2.39	0.55
1:C:177:LEU:HD21	1:C:262:TYR:CG	2.41	0.55
1:C:275:LEU:HD22	1:C:292:TRP:HA	1.88	0.55
1:B:220:LYS:HG2	1:B:224:GLU:OE1	2.07	0.55
1:C:140:LEU:H	1:C:140:LEU:CD2	2.08	0.55
1:C:245:GLU:C	1:C:298:TYR:CE2	2.75	0.55
1:A:77:VAL:HG23	1:A:83:LEU:O	2.07	0.55
1:B:58:PRO:O	1:B:60:HIS:N	2.39	0.55
1:B:286:LYS:HD3	1:B:286:LYS:H	1.68	0.55
1:B:296:LYS:C	1:B:298:TYR:H	2.09	0.55
1:C:140:LEU:O	1:C:141:SER:C	2.44	0.55
1:C:226:ILE:HG23	1:C:230:PHE:CE2	2.41	0.55
1:A:178:GLN:HA	1:A:181:ASN:ND2	2.21	0.55
1:A:285:CYS:N	1:B:285:CYS:SG	2.80	0.55
1:C:31:LYS:HB2	1:C:241:VAL:HB	1.89	0.55
1:C:229:GLN:NE2	1:C:229:GLN:CA	2.67	0.55
1:C:272:ASN:OD1	1:C:273:GLN:N	2.39	0.55
1:C:347:ILE:HD13	1:C:347:ILE:N	2.21	0.55
1:A:8:ASN:OD1	1:A:10:HIS:HB3	2.06	0.55
1:A:12:LEU:C	1:A:14:THR:N	2.59	0.55
1:B:233:PRO:CG	2:D:32:LYS:CD	2.40	0.55
1:B:254:ARG:HH11	1:B:254:ARG:CG	2.19	0.55
1:C:230:PHE:O	1:C:264:MET:SD	2.64	0.55
1:A:24:GLY:HA2	1:A:31:LYS:HD2	1.89	0.55
1:A:75:ARG:HD2	1:A:75:ARG:C	2.26	0.55
1:A:322:ARG:NH1	1:B:246:PHE:CD2	2.75	0.55
1:B:71:GLY:O	1:B:73:ASP:N	2.40	0.55
1:C:227:ARG:NH1	1:C:262:TYR:O	2.39	0.55
1:A:22:PHE:CD1	1:A:165:PHE:HB2	2.42	0.55
1:B:26:LYS:HD3	1:B:251:GLU:OE1	2.07	0.55
1:B:32:THR:OG1	3:B:401:ADP:PA	2.64	0.55
1:B:75:ARG:O	1:B:75:ARG:HD2	2.06	0.55
1:A:333:PHE:CE2	1:A:338:TYR:HD2	2.24	0.54
1:B:133:ILE:CG2	1:B:134:PRO:HD2	2.33	0.54
1:B:333:PHE:CZ	1:B:343:ASP:HB3	2.38	0.54
1:A:19:LYS:C	1:A:20:TRP:CD1	2.81	0.54
1:B:63:SER:HB3	1:B:68:GLU:O	2.07	0.54
1:B:139:ALA:O	1:B:140:LEU:C	2.45	0.54
1:C:63:SER:HB3	1:C:69:LYS:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLY:O	1:C:138:GLU:HB2	2.08	0.54
1:C:168:ALA:CB	1:C:170:THR:HG23	2.35	0.54
1:C:227:ARG:CZ	1:C:231:THR:HG23	2.37	0.54
1:C:311:VAL:O	1:C:311:VAL:HG22	2.07	0.54
1:C:136:ILE:CG2	1:C:137:ASP:N	2.63	0.54
1:B:295:GLN:O	1:B:299:LEU:HG	2.07	0.54
1:B:339:ASN:HB3	1:B:342:THR:HG22	1.87	0.54
1:C:280:ASP:OD2	1:C:283:HIS:N	2.40	0.54
1:A:38:ILE:HG22	1:A:164:ILE:HD13	1.90	0.54
1:A:163:VAL:HG22	1:A:165:PHE:CE2	2.43	0.54
1:B:228:GLN:CD	1:B:229:GLN:HG3	2.27	0.54
1:A:32:THR:N	3:A:401:ADP:O2B	2.41	0.54
1:B:258:GLU:O	1:B:261:SER:HB3	2.07	0.54
1:C:306:TYR:HB3	1:C:309:PHE:HB2	1.90	0.54
1:A:319:GLY:O	1:A:320:GLU:C	2.45	0.54
1:C:12:LEU:HD13	1:C:18:HIS:CD2	2.40	0.54
1:C:306:TYR:HD1	1:C:309:PHE:CD2	2.24	0.54
1:A:64:ASP:C	1:A:66:PHE:H	2.10	0.54
1:B:12:LEU:C	1:B:14:THR:N	2.60	0.54
1:B:18:HIS:O	1:B:162:THR:HG23	2.07	0.54
1:B:31:LYS:H	3:B:401:ADP:PB	2.30	0.54
1:A:224:GLU:HA	1:A:227:ARG:HB3	1.89	0.54
1:A:287:ARG:HG2	1:B:348:TYR:CE1	2.43	0.54
1:B:64:ASP:C	1:B:66:PHE:H	2.11	0.54
1:C:145:VAL:O	1:C:146:MET:C	2.46	0.54
1:C:243:ILE:HD13	1:C:248:SER:OG	2.08	0.54
1:C:328:THR:O	1:C:330:PHE:N	2.41	0.54
1:A:133:ILE:CG2	1:A:134:PRO:HD2	2.34	0.54
1:A:135:GLY:O	1:A:138:GLU:HB2	2.08	0.54
1:C:32:THR:OG1	3:C:401:ADP:PA	2.66	0.54
1:C:339:ASN:CG	1:C:342:THR:HG22	2.28	0.54
2:E:14:ARG:CG	2:E:17:ARG:NH2	2.55	0.54
1:A:348:TYR:CE2	1:B:287:ARG:HD3	2.42	0.53
1:C:170:THR:O	1:C:170:THR:OG1	2.25	0.53
1:C:224:GLU:HA	1:C:227:ARG:HB3	1.90	0.53
1:A:318:ALA:H	1:A:351:GLU:CD	2.11	0.53
1:B:285:CYS:O	1:B:288:CYS:CB	2.55	0.53
1:C:254:ARG:HH11	1:C:254:ARG:CG	2.21	0.53
1:A:139:ALA:O	1:A:142:PHE:HB3	2.09	0.53
1:B:228:GLN:CD	1:B:229:GLN:CA	2.73	0.53
1:B:259:LEU:O	1:B:262:TYR:N	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:LYS:O	1:B:298:TYR:N	2.42	0.53
1:C:177:LEU:O	1:C:180:PRO:CG	2.55	0.53
1:A:339:ASN:HB3	1:A:342:THR:HG22	1.90	0.53
1:B:136:ILE:CG2	1:B:137:ASP:N	2.66	0.53
1:A:174:LEU:HD23	1:A:262:TYR:CE2	2.43	0.53
1:A:347:ILE:HD13	1:A:347:ILE:N	2.23	0.53
1:C:138:GLU:CB	1:C:173:THR:HB	2.38	0.53
1:C:139:ALA:O	1:C:142:PHE:HB3	2.08	0.53
1:A:275:LEU:HD22	1:A:292:TRP:HA	1.91	0.53
1:B:29:VAL:HG11	1:B:242:CYS:N	2.23	0.53
1:B:306:TYR:HB3	1:B:309:PHE:HB2	1.91	0.53
1:C:324:LEU:HD12	1:C:324:LEU:O	2.09	0.53
1:A:232:ASP:OD1	1:A:232:ASP:O	2.26	0.53
1:A:247:LEU:HD22	1:B:64:ASP:OD1	2.08	0.53
1:A:285:CYS:SG	1:B:285:CYS:N	2.82	0.53
1:B:350:LEU:HD12	1:B:350:LEU:N	2.23	0.53
1:C:46:GLN:N	1:C:47:PRO:CD	2.72	0.53
1:C:277:ALA:HB3	1:C:292:TRP:HD1	1.73	0.53
1:A:322:ARG:NH1	1:B:246:PHE:CB	2.72	0.53
1:A:348:TYR:CE1	1:B:287:ARG:HG2	2.43	0.53
1:B:227:ARG:NH2	1:B:263:ASP:HB2	2.14	0.53
1:C:308:ASP:HB3	2:D:17:ARG:NH1	2.10	0.53
1:C:309:PHE:CE2	2:D:17:ARG:HD2	2.42	0.53
1:A:175:ARG:HA	1:A:262:TYR:CZ	2.44	0.53
1:A:227:ARG:NH2	1:A:263:ASP:HB2	2.23	0.53
1:B:30:GLY:HA2	3:B:401:ADP:PA	2.46	0.53
1:B:224:GLU:HA	1:B:227:ARG:HB3	1.90	0.53
1:B:232:ASP:OD1	1:B:235:LEU:HG	2.09	0.53
1:B:243:ILE:HD13	1:B:248:SER:OG	2.09	0.53
1:C:57:ASP:OD2	1:C:59:ALA:HB3	2.09	0.53
1:C:318:ALA:H	1:C:351:GLU:CD	2.12	0.53
1:A:295:GLN:O	1:A:299:LEU:HG	2.09	0.52
1:B:275:LEU:HD22	1:B:292:TRP:HA	1.91	0.52
1:A:296:LYS:O	1:A:298:TYR:N	2.42	0.52
1:B:9:LEU:O	1:B:13:ILE:HG13	2.09	0.52
1:B:13:ILE:HD13	1:B:41:GLN:HB3	1.91	0.52
1:B:47:PRO:HA	1:B:82:ASN:HD22	1.74	0.52
1:B:139:ALA:O	1:B:142:PHE:HB3	2.08	0.52
1:B:140:LEU:HD22	1:B:140:LEU:N	2.11	0.52
1:C:178:GLN:CD	1:C:261:SER:HG	2.12	0.52
1:C:295:GLN:O	1:C:299:LEU:HG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:GLU:HG3	1:C:322:ARG:HH12	1.74	0.52
2:D:14:ARG:CG	2:D:17:ARG:HH22	2.05	0.52
1:A:226:ILE:O	1:A:230:PHE:HB2	2.08	0.52
1:B:29:VAL:O	1:B:272:ASN:ND2	2.42	0.52
1:B:34:SER:OG	1:B:241:VAL:HG21	2.09	0.52
1:A:26:LYS:HD3	1:A:251:GLU:OE1	2.10	0.52
1:A:31:LYS:C	1:A:31:LYS:HZ2	2.13	0.52
1:A:43:ALA:CA	1:A:51:PHE:CE2	2.88	0.52
1:B:140:LEU:H	1:B:140:LEU:CD2	2.10	0.52
1:B:176:PHE:O	1:B:179:LEU:CA	2.57	0.52
1:A:183:LEU:HD22	1:A:216:LEU:CD2	2.40	0.52
1:B:12:LEU:O	1:B:14:THR:N	2.42	0.52
1:C:19:LYS:C	1:C:20:TRP:CG	2.82	0.52
1:A:286:LYS:HD3	1:A:286:LYS:H	1.71	0.52
1:A:20:TRP:HB2	1:A:236:THR:HB	1.92	0.52
1:B:8:ASN:OD1	1:B:10:HIS:HB3	2.10	0.52
1:B:308:ASP:CB	2:D:27:SER:OG	2.51	0.52
1:B:328:THR:O	1:B:330:PHE:N	2.43	0.52
1:A:57:ASP:HB2	1:A:169:PRO:HD3	1.91	0.52
1:A:238:PHE:CD1	1:A:238:PHE:C	2.83	0.52
1:A:249:LEU:O	1:A:250:TYR:C	2.47	0.52
1:B:12:LEU:C	1:B:14:THR:H	2.13	0.52
1:B:31:LYS:HA	1:B:241:VAL:HG21	1.90	0.52
1:C:12:LEU:C	1:C:14:THR:N	2.61	0.52
1:C:230:PHE:HB3	1:C:264:MET:HE2	1.91	0.52
1:C:277:ALA:HB3	1:C:292:TRP:CD1	2.45	0.52
1:C:306:TYR:O	1:C:309:PHE:N	2.38	0.52
2:E:9:LYS:O	2:E:13:LEU:HG	2.10	0.52
1:A:37:SER:HG	1:A:330:PHE:HD2	1.57	0.52
1:A:181:ASN:C	1:A:183:LEU:N	2.62	0.52
1:A:232:ASP:CG	1:A:234:ASP:H	2.13	0.52
1:A:270:ILE:HG22	1:A:270:ILE:O	2.08	0.52
1:B:12:LEU:HD13	1:B:18:HIS:CD2	2.42	0.52
1:A:31:LYS:HA	1:A:34:SER:CB	2.40	0.52
1:A:147:LYS:O	1:A:151:ARG:HG3	2.09	0.52
1:C:306:TYR:C	1:C:309:PHE:HD2	2.13	0.52
1:A:177:LEU:CD1	1:A:230:PHE:HE2	2.23	0.51
1:B:242:CYS:O	1:B:242:CYS:SG	2.67	0.51
1:B:31:LYS:O	1:B:31:LYS:HG2	2.08	0.51
1:B:135:GLY:N	1:B:179:LEU:HD23	2.21	0.51
1:B:315:PRO:HB3	1:B:338:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:PHE:CE2	1:B:338:TYR:HD2	2.28	0.51
1:C:75:ARG:CD	1:C:76:LYS:O	2.58	0.51
1:B:8:ASN:N	1:B:312:VAL:HG22	2.26	0.51
1:A:29:VAL:O	1:A:272:ASN:ND2	2.43	0.51
1:A:138:GLU:CB	1:A:173:THR:HB	2.40	0.51
1:A:320:GLU:OE1	1:A:320:GLU:CA	2.57	0.51
1:B:24:GLY:HA2	1:B:31:LYS:HD3	1.92	0.51
1:B:177:LEU:O	1:B:180:PRO:CG	2.58	0.51
1:C:37:SER:HG	1:C:330:PHE:HD2	1.58	0.51
1:C:228:GLN:NE2	1:C:229:GLN:HA	2.21	0.51
1:A:8:ASN:H	1:A:312:VAL:HG22	1.74	0.51
1:A:46:GLN:N	1:A:47:PRO:CD	2.73	0.51
1:B:241:VAL:HG13	1:B:270:ILE:HG22	1.92	0.51
1:B:308:ASP:OD1	1:B:308:ASP:N	2.44	0.51
1:B:333:PHE:CE2	1:B:338:TYR:HB2	2.46	0.51
1:C:63:SER:HB3	1:C:68:GLU:O	2.11	0.51
1:C:238:PHE:CD1	1:C:238:PHE:C	2.84	0.51
1:C:277:ALA:HB1	1:C:289:GLN:HG3	1.92	0.51
2:D:9:LYS:O	2:D:13:LEU:HG	2.10	0.51
1:A:38:ILE:C	1:A:40:ILE:H	2.14	0.51
1:A:135:GLY:HA2	1:A:175:ARG:HG2	1.93	0.51
1:A:296:LYS:HA	1:A:299:LEU:HG	1.93	0.51
1:A:302:ILE:O	1:A:303:ASP:C	2.49	0.51
1:A:306:TYR:O	1:A:309:PHE:HB2	2.11	0.51
1:B:6:GLU:HB3	1:B:8:ASN:ND2	2.25	0.51
1:B:22:PHE:CZ	1:B:174:LEU:HD11	2.46	0.51
1:B:50:GLN:O	1:B:161:ASP:N	2.37	0.51
1:B:147:LYS:O	1:B:151:ARG:HG3	2.10	0.51
1:C:299:LEU:O	1:C:302:ILE:HB	2.11	0.51
1:A:63:SER:HB3	1:A:68:GLU:O	2.11	0.51
1:A:177:LEU:CD1	1:A:230:PHE:CE2	2.94	0.51
1:A:275:LEU:O	1:A:276:PHE:HB2	2.11	0.51
1:B:19:LYS:C	1:B:20:TRP:CG	2.83	0.51
1:B:275:LEU:O	1:B:276:PHE:HB2	2.11	0.51
1:C:49:LYS:HD2	1:C:161:ASP:CG	2.31	0.51
1:C:306:TYR:CB	1:C:309:PHE:CD2	2.94	0.51
1:B:44:LEU:O	1:B:47:PRO:HG3	2.11	0.51
1:B:50:GLN:CD	1:B:82:ASN:HA	2.31	0.51
1:B:77:VAL:HG23	1:B:83:LEU:O	2.10	0.51
1:C:64:ASP:C	1:C:66:PHE:H	2.14	0.51
1:C:259:LEU:O	1:C:262:TYR:N	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:ILE:C	1:C:349:GLU:N	2.64	0.51
1:A:71:GLY:O	1:A:73:ASP:N	2.43	0.51
1:A:163:VAL:CG2	1:A:165:PHE:HE2	2.24	0.51
1:A:153:GLU:HG2	1:A:160:PHE:CD2	2.46	0.51
1:A:254:ARG:HH11	1:A:254:ARG:CG	2.24	0.51
1:A:350:LEU:HD12	1:A:350:LEU:N	2.26	0.51
1:B:135:GLY:O	1:B:138:GLU:HB2	2.10	0.51
1:C:135:GLY:O	1:C:136:ILE:C	2.49	0.51
1:C:284:ASN:OD1	1:C:288:CYS:HB2	2.10	0.51
1:C:305:LEU:C	1:C:306:TYR:CD2	2.84	0.51
1:A:13:ILE:HD13	1:A:41:GLN:HB3	1.92	0.50
1:A:76:LYS:HD2	1:A:82:ASN:N	2.25	0.50
1:A:148:HIS:HA	1:A:151:ARG:HD2	1.93	0.50
1:A:247:LEU:CD2	1:B:64:ASP:CG	2.78	0.50
1:B:145:VAL:O	1:B:146:MET:C	2.49	0.50
1:B:326:ASN:O	1:B:350:LEU:HD21	2.11	0.50
1:B:347:ILE:O	1:B:349:GLU:N	2.44	0.50
1:C:13:ILE:HD13	1:C:41:GLN:HB3	1.93	0.50
1:C:153:GLU:HG2	1:C:160:PHE:CD2	2.46	0.50
1:C:339:ASN:CB	1:C:342:THR:HG22	2.41	0.50
1:A:308:ASP:HB2	2:E:17:ARG:NH1	2.16	0.50
1:B:153:GLU:HG2	1:B:160:PHE:CD2	2.46	0.50
1:B:174:LEU:O	1:B:177:LEU:CD1	2.59	0.50
1:B:238:PHE:CZ	1:B:259:LEU:HD11	2.46	0.50
1:C:133:ILE:CG2	1:C:134:PRO:CD	2.87	0.50
2:D:10:ARG:O	2:D:14:ARG:HG3	2.12	0.50
1:A:39:ALA:HA	1:A:164:ILE:HD12	1.92	0.50
1:A:49:LYS:HD2	1:A:161:ASP:CG	2.32	0.50
1:A:320:GLU:HG2	1:B:294:MET:HE1	1.93	0.50
1:A:322:ARG:HH12	1:B:246:PHE:CB	2.24	0.50
1:C:9:LEU:O	1:C:13:ILE:HG13	2.11	0.50
1:A:49:LYS:CB	1:A:51:PHE:CZ	2.94	0.50
1:B:22:PHE:CD1	1:B:165:PHE:HB2	2.47	0.50
1:C:71:GLY:O	1:C:73:ASP:N	2.45	0.50
1:C:258:GLU:HA	1:C:261:SER:HB3	1.94	0.50
1:A:58:PRO:O	1:A:60:HIS:N	2.44	0.50
1:A:190:PHE:O	1:A:194:THR:HG23	2.11	0.50
1:A:291:ARG:HG2	1:A:291:ARG:NH1	2.26	0.50
1:B:17:THR:O	1:B:235:LEU:HD23	2.11	0.50
1:B:49:LYS:HB2	1:B:51:PHE:CE2	2.45	0.50
1:B:258:GLU:HA	1:B:261:SER:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:VAL:CG1	1:B:274:LEU:HD21	2.41	0.50
1:C:156:GLU:CG	1:C:158:GLU:HG3	2.42	0.50
2:D:8:GLU:O	2:D:11:ARG:N	2.44	0.50
2:E:8:GLU:O	2:E:11:ARG:N	2.44	0.50
1:A:61:ASN:O	1:A:64:ASP:HB3	2.12	0.50
1:A:136:ILE:O	1:A:137:ASP:C	2.50	0.50
1:A:277:ALA:HB3	1:A:292:TRP:HD1	1.76	0.50
1:B:46:GLN:N	1:B:47:PRO:CD	2.67	0.50
1:B:138:GLU:HB3	1:B:176:PHE:CD2	2.47	0.50
1:C:230:PHE:HB3	1:C:264:MET:CE	2.42	0.50
1:C:350:LEU:N	1:C:350:LEU:HD12	2.27	0.50
1:B:39:ALA:HB2	1:B:164:ILE:CD1	2.36	0.50
1:B:246:PHE:HB2	1:B:298:TYR:OH	2.12	0.50
1:B:319:GLY:O	1:B:320:GLU:C	2.51	0.50
1:B:346:VAL:O	1:B:349:GLU:HB3	2.11	0.50
1:C:241:VAL:HG13	1:C:270:ILE:CG2	2.41	0.50
1:A:9:LEU:C	1:A:13:ILE:HG13	2.32	0.50
1:A:183:LEU:HD22	1:A:216:LEU:HD22	1.94	0.50
1:A:277:ALA:HB1	1:A:289:GLN:HG3	1.94	0.50
1:B:42:MET:SD	1:B:162:THR:HG21	2.51	0.50
1:B:305:LEU:O	1:B:306:TYR:CD2	2.64	0.50
1:B:326:ASN:CG	1:B:350:LEU:HG	2.31	0.50
1:B:327:LEU:O	1:B:328:THR:C	2.49	0.50
1:C:291:ARG:HG2	1:C:291:ARG:NH1	2.27	0.50
2:E:10:ARG:O	2:E:14:ARG:HG3	2.12	0.50
1:A:50:GLN:CD	1:A:82:ASN:HA	2.32	0.50
1:A:228:GLN:HE22	1:A:229:GLN:HG2	1.72	0.50
1:B:37:SER:O	1:B:41:GLN:HG2	2.11	0.50
1:B:321:ILE:O	1:B:321:ILE:CD1	2.48	0.50
1:C:31:LYS:N	3:C:401:ADP:O3B	2.45	0.50
1:C:242:CYS:O	1:C:242:CYS:SG	2.67	0.50
1:C:315:PRO:HB3	1:C:338:TYR:CE1	2.47	0.50
1:A:170:THR:O	1:A:170:THR:OG1	2.30	0.49
1:B:38:ILE:C	1:B:40:ILE:H	2.16	0.49
1:C:24:GLY:HA2	1:C:31:LYS:HD3	1.94	0.49
1:A:317:CYS:O	3:A:401:ADP:C2	2.63	0.49
1:A:308:ASP:CB	2:E:16:ARG:NH2	2.76	0.49
1:A:321:ILE:HD13	1:A:321:ILE:C	2.33	0.49
1:B:272:ASN:OD1	1:B:273:GLN:N	2.46	0.49
1:B:298:TYR:O	1:B:299:LEU:C	2.49	0.49
1:C:174:LEU:HD13	1:C:259:LEU:CD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:GLU:OE1	1:C:320:GLU:CA	2.59	0.49
1:A:346:VAL:O	1:A:349:GLU:HB3	2.12	0.49
1:C:284:ASN:OD1	1:C:288:CYS:HB3	2.11	0.49
2:E:7:ALA:O	2:E:10:ARG:N	2.45	0.49
1:A:12:LEU:C	1:A:14:THR:H	2.14	0.49
1:A:142:PHE:O	1:A:145:VAL:HG23	2.12	0.49
1:A:245:GLU:C	1:A:298:TYR:CE2	2.77	0.49
1:B:31:LYS:HZ2	1:B:31:LYS:C	2.16	0.49
1:B:136:ILE:O	1:B:137:ASP:C	2.49	0.49
1:C:12:LEU:C	1:C:14:THR:H	2.15	0.49
1:C:47:PRO:C	1:C:49:LYS:H	2.16	0.49
1:C:178:GLN:CD	1:C:261:SER:OG	2.50	0.49
1:A:156:GLU:CG	1:A:158:GLU:HG3	2.42	0.49
1:B:9:LEU:O	1:B:12:LEU:N	2.45	0.49
1:B:82:ASN:OD1	1:B:82:ASN:N	2.45	0.49
1:B:230:PHE:O	1:B:264:MET:CE	2.61	0.49
1:C:39:ALA:HA	1:C:164:ILE:HD12	1.94	0.49
1:C:60:HIS:HD2	1:C:69:LYS:HZ1	1.59	0.49
1:C:174:LEU:O	1:C:175:ARG:C	2.51	0.49
1:C:179:LEU:C	1:C:179:LEU:CD1	2.75	0.49
1:C:226:ILE:O	1:C:230:PHE:N	2.37	0.49
2:D:17:ARG:HB3	2:D:21:PHE:HE2	1.77	0.49
2:E:17:ARG:HB3	2:E:21:PHE:HE2	1.77	0.49
1:A:136:ILE:HD13	1:A:136:ILE:N	2.27	0.49
1:A:145:VAL:O	1:A:146:MET:C	2.50	0.49
1:C:90:PRO:O	1:C:91:SER:C	2.51	0.49
1:A:229:GLN:O	1:A:235:LEU:HD12	2.12	0.49
1:B:38:ILE:O	1:B:40:ILE:N	2.46	0.49
1:B:76:LYS:HD2	1:B:82:ASN:N	2.27	0.49
1:B:145:VAL:O	1:B:149:ILE:HG13	2.12	0.49
1:B:318:ALA:N	1:B:351:GLU:HG2	2.27	0.49
1:C:49:LYS:CB	1:C:51:PHE:CZ	2.95	0.49
1:C:135:GLY:HA2	1:C:175:ARG:HG2	1.94	0.49
1:C:143:MET:O	1:C:146:MET:HB2	2.13	0.49
1:A:296:LYS:C	1:A:298:TYR:H	2.14	0.49
1:A:299:LEU:O	1:A:302:ILE:HB	2.13	0.49
1:A:306:TYR:O	1:A:307:GLU:C	2.50	0.49
1:B:138:GLU:C	1:B:176:PHE:CD2	2.71	0.49
1:C:296:LYS:O	1:C:298:TYR:N	2.46	0.49
1:C:346:VAL:O	1:C:349:GLU:HB3	2.12	0.49
2:D:14:ARG:HA	2:D:17:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:14:ARG:HA	2:E:17:ARG:NH2	2.27	0.49
1:A:177:LEU:HD11	1:A:230:PHE:CE2	2.48	0.49
1:B:49:LYS:HD2	1:B:161:ASP:CG	2.33	0.49
1:B:152:GLN:O	1:B:156:GLU:CB	2.61	0.49
1:C:298:TYR:O	1:C:299:LEU:C	2.49	0.49
1:C:306:TYR:O	1:C:307:GLU:C	2.51	0.49
1:A:227:ARG:CZ	1:A:231:THR:CG2	2.91	0.48
1:C:8:ASN:OD1	1:C:10:HIS:HB3	2.13	0.48
1:C:50:GLN:HG3	1:C:158:GLU:OE1	2.13	0.48
1:C:275:LEU:O	1:C:276:PHE:CB	2.61	0.48
1:C:305:LEU:HD11	2:D:29:ARG:CD	2.36	0.48
1:C:318:ALA:N	1:C:351:GLU:HG2	2.27	0.48
1:A:34:SER:OG	1:A:241:VAL:HG21	2.13	0.48
1:A:42:MET:CE	1:A:162:THR:HG21	2.43	0.48
1:A:238:PHE:CZ	1:A:259:LEU:HD11	2.47	0.48
1:B:254:ARG:NH1	1:B:254:ARG:CG	2.76	0.48
1:C:283:HIS:CE1	1:C:348:TYR:OH	2.66	0.48
1:A:225:THR:O	1:A:228:GLN:HG3	2.13	0.48
1:A:347:ILE:O	1:A:349:GLU:N	2.46	0.48
1:B:232:ASP:OD1	1:B:232:ASP:O	2.31	0.48
1:C:326:ASN:O	1:C:350:LEU:HD21	2.13	0.48
1:A:46:GLN:O	1:A:49:LYS:N	2.47	0.48
1:A:165:PHE:N	1:A:165:PHE:CD2	2.82	0.48
1:B:165:PHE:HD2	1:B:165:PHE:N	2.11	0.48
1:B:245:GLU:C	1:B:298:TYR:CE2	2.82	0.48
1:B:319:GLY:O	1:B:320:GLU:O	2.31	0.48
1:C:302:ILE:O	1:C:303:ASP:C	2.52	0.48
1:A:277:ALA:HB3	1:A:292:TRP:CD1	2.48	0.48
1:A:308:ASP:HB3	2:E:16:ARG:HH21	1.79	0.48
1:B:18:HIS:HD1	1:B:234:ASP:C	2.17	0.48
1:B:148:HIS:HA	1:B:151:ARG:HD2	1.96	0.48
1:C:75:ARG:HD2	1:C:75:ARG:C	2.34	0.48
1:C:296:LYS:HA	1:C:299:LEU:HG	1.94	0.48
1:A:55:SER:HB3	1:A:62:LEU:HD11	1.96	0.48
1:A:271:VAL:CG1	1:A:274:LEU:HD21	2.44	0.48
1:B:338:TYR:CD1	1:B:338:TYR:C	2.87	0.48
1:B:339:ASN:CG	1:B:342:THR:HG22	2.33	0.48
1:C:61:ASN:O	1:C:64:ASP:HB3	2.14	0.48
1:C:136:ILE:HD13	1:C:136:ILE:N	2.28	0.48
1:A:181:ASN:C	1:A:183:LEU:H	2.16	0.48
1:A:339:ASN:CG	1:A:342:THR:HG22	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:GLU:HG3	1:B:322:ARG:HH12	1.78	0.48
2:D:7:ALA:O	2:D:10:ARG:N	2.45	0.48
1:B:75:ARG:HD2	1:B:75:ARG:C	2.34	0.48
1:C:8:ASN:O	1:C:9:LEU:CD2	2.58	0.48
1:C:139:ALA:O	1:C:142:PHE:N	2.47	0.48
1:A:179:LEU:CD2	1:A:219:LEU:CD1	2.92	0.48
1:A:227:ARG:CD	1:A:231:THR:HG1	1.92	0.48
1:B:136:ILE:HD13	1:B:136:ILE:N	2.29	0.48
1:C:19:LYS:O	1:C:20:TRP:CG	2.67	0.48
1:C:253:GLU:OE2	2:D:29:ARG:CZ	2.56	0.48
1:C:317:CYS:O	3:C:401:ADP:C2	2.67	0.48
1:A:174:LEU:HD22	1:A:259:LEU:CD2	2.44	0.48
1:A:38:ILE:C	1:A:40:ILE:N	2.68	0.47
1:A:165:PHE:N	1:A:165:PHE:HD2	2.12	0.47
1:A:177:LEU:HD13	1:A:230:PHE:HE2	1.79	0.47
1:A:230:PHE:CD1	1:A:264:MET:CE	2.96	0.47
1:A:290:ALA:O	1:A:291:ARG:C	2.53	0.47
1:A:318:ALA:HA	1:B:291:ARG:HD3	1.96	0.47
1:A:347:ILE:C	1:A:349:GLU:N	2.67	0.47
1:B:277:ALA:HB1	1:B:289:GLN:HG3	1.97	0.47
1:B:299:LEU:O	1:B:302:ILE:HB	2.14	0.47
1:B:339:ASN:CB	1:B:342:THR:HG22	2.43	0.47
1:C:165:PHE:N	1:C:165:PHE:HD2	2.12	0.47
1:C:296:LYS:C	1:C:298:TYR:H	2.16	0.47
1:C:308:ASP:CB	2:D:17:ARG:HH11	2.14	0.47
1:A:322:ARG:CZ	1:B:246:PHE:CD2	2.98	0.47
1:C:23:VAL:C	1:C:167:THR:HG23	2.28	0.47
1:C:232:ASP:CG	1:C:234:ASP:H	2.16	0.47
1:C:336:LYS:O	1:C:337:GLU:C	2.52	0.47
1:A:29:VAL:O	1:A:29:VAL:HG12	2.15	0.47
1:A:135:GLY:O	1:A:136:ILE:C	2.52	0.47
1:B:238:PHE:CE2	1:B:259:LEU:HD21	2.49	0.47
1:C:46:GLN:O	1:C:49:LYS:N	2.48	0.47
1:C:178:GLN:CD	1:C:262:TYR:HE1	2.04	0.47
1:A:322:ARG:HH12	1:B:246:PHE:HB3	1.80	0.47
1:A:333:PHE:CE1	1:A:338:TYR:HA	2.49	0.47
1:B:50:GLN:HE22	1:B:82:ASN:CA	2.28	0.47
1:C:18:HIS:HA	1:C:235:LEU:CA	2.45	0.47
1:C:187:LEU:CG	1:C:216:LEU:CD1	2.79	0.47
1:C:243:ILE:H	1:C:243:ILE:CD1	2.09	0.47
1:A:172:HIS:C	1:A:174:LEU:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ARG:NH2	1:A:263:ASP:O	2.47	0.47
1:C:319:GLY:O	1:C:320:GLU:O	2.32	0.47
1:A:174:LEU:CD1	1:A:262:TYR:CD2	2.95	0.47
1:A:179:LEU:CD1	1:A:183:LEU:HD11	2.43	0.47
1:A:318:ALA:N	1:A:351:GLU:HG2	2.29	0.47
1:B:245:GLU:O	1:B:246:PHE:C	2.52	0.47
1:B:347:ILE:C	1:B:349:GLU:N	2.66	0.47
1:A:22:PHE:HD1	1:A:165:PHE:HB2	1.77	0.47
1:A:28:GLY:HA3	1:B:28:GLY:CA	2.44	0.47
1:A:32:THR:HG21	1:A:61:ASN:HB2	1.96	0.47
1:A:32:THR:HG23	1:A:61:ASN:ND2	2.30	0.47
1:A:242:CYS:O	1:A:271:VAL:HA	2.15	0.47
1:A:275:LEU:O	1:A:276:PHE:CB	2.63	0.47
1:B:22:PHE:HD1	1:B:165:PHE:HB2	1.80	0.47
1:B:175:ARG:CA	1:B:262:TYR:CZ	2.94	0.47
1:B:179:LEU:C	1:B:179:LEU:CD1	2.75	0.47
1:B:296:LYS:HA	1:B:299:LEU:HG	1.96	0.47
1:C:38:ILE:C	1:C:40:ILE:H	2.17	0.47
1:C:38:ILE:O	1:C:40:ILE:N	2.47	0.47
1:C:40:ILE:O	1:C:44:LEU:HD13	2.15	0.47
1:C:58:PRO:O	1:C:60:HIS:N	2.48	0.47
1:C:60:HIS:CD2	1:C:69:LYS:HZ1	2.32	0.47
1:C:281:GLN:O	1:C:283:HIS:N	2.47	0.47
1:C:341:ILE:HG13	1:C:341:ILE:H	1.21	0.47
1:B:165:PHE:N	1:B:165:PHE:CD2	2.82	0.47
1:C:39:ALA:HB2	1:C:164:ILE:CD1	2.41	0.47
1:C:54:ILE:HD12	1:C:88:ILE:HD11	1.96	0.47
1:C:135:GLY:HA3	1:C:179:LEU:CD2	2.17	0.47
1:A:53:LEU:CD1	1:A:164:ILE:HG22	2.35	0.47
1:A:145:VAL:O	1:A:149:ILE:HG13	2.13	0.47
1:A:238:PHE:CE2	1:A:259:LEU:HD21	2.50	0.47
1:B:291:ARG:HG2	1:B:291:ARG:NH1	2.30	0.47
1:C:12:LEU:O	1:C:14:THR:N	2.48	0.47
1:C:172:HIS:NE2	1:C:258:GLU:OE2	2.46	0.47
1:C:272:ASN:O	1:C:273:GLN:C	2.52	0.47
1:A:37:SER:OG	1:A:331:SER:CB	2.57	0.47
1:A:179:LEU:O	1:A:183:LEU:HD12	2.15	0.47
1:A:273:GLN:O	1:A:295:GLN:NE2	2.44	0.47
1:B:135:GLY:O	1:B:136:ILE:C	2.53	0.47
1:B:302:ILE:O	1:B:303:ASP:C	2.53	0.47
1:C:32:THR:HG23	1:C:61:ASN:ND2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLN:HE22	1:A:82:ASN:CA	2.26	0.46
1:A:298:TYR:O	1:A:299:LEU:C	2.54	0.46
1:B:57:ASP:HA	1:B:58:PRO:HD2	1.70	0.46
1:B:142:PHE:O	1:B:145:VAL:HG23	2.14	0.46
1:B:255:LEU:O	1:B:256:ILE:C	2.54	0.46
1:B:265:ASP:CG	2:D:32:LYS:CE	2.84	0.46
1:C:167:THR:O	1:C:168:ALA:C	2.53	0.46
1:A:139:ALA:O	1:A:142:PHE:N	2.48	0.46
1:A:174:LEU:O	1:A:175:ARG:C	2.52	0.46
1:A:339:ASN:OD1	1:A:341:ILE:HG13	2.16	0.46
1:A:339:ASN:CB	1:A:342:THR:HG22	2.45	0.46
1:B:55:SER:HB3	1:B:62:LEU:HD11	1.97	0.46
1:B:61:ASN:O	1:B:64:ASP:HB3	2.15	0.46
1:B:156:GLU:CG	1:B:158:GLU:HG3	2.46	0.46
1:B:170:THR:O	1:B:170:THR:OG1	2.31	0.46
1:B:317:CYS:O	3:B:401:ADP:H2	1.98	0.46
1:C:10:HIS:HA	1:C:13:ILE:HG13	1.96	0.46
1:C:273:GLN:O	1:C:295:GLN:NE2	2.44	0.46
1:B:174:LEU:O	1:B:177:LEU:HD13	2.15	0.46
1:B:187:LEU:HD23	1:B:187:LEU:HA	1.79	0.46
1:C:76:LYS:HD2	1:C:82:ASN:N	2.31	0.46
1:C:187:LEU:HD11	1:C:216:LEU:CB	2.45	0.46
1:C:267:ASN:C	1:C:268:SER:HG	2.18	0.46
1:C:291:ARG:O	1:C:292:TRP:C	2.53	0.46
1:A:242:CYS:O	1:A:242:CYS:SG	2.70	0.46
1:A:305:LEU:O	1:A:306:TYR:CG	2.69	0.46
1:B:31:LYS:NZ	1:B:166:ASP:OD2	2.49	0.46
1:C:36:CYS:C	1:C:38:ILE:N	2.68	0.46
1:C:172:HIS:O	1:C:172:HIS:CG	2.69	0.46
1:B:45:SER:O	1:B:46:GLN:CG	2.63	0.46
1:B:143:MET:O	1:B:146:MET:HB2	2.14	0.46
1:C:19:LYS:HB2	1:C:20:TRP:CD1	2.50	0.46
1:C:31:LYS:C	1:C:34:SER:HB2	2.36	0.46
1:C:152:GLN:O	1:C:156:GLU:CB	2.63	0.46
1:C:319:GLY:O	1:C:320:GLU:C	2.53	0.46
1:A:331:SER:O	1:A:334:LEU:HB2	2.15	0.46
1:B:38:ILE:HG22	1:B:164:ILE:HD13	1.96	0.46
1:B:167:THR:O	1:B:168:ALA:C	2.54	0.46
1:C:142:PHE:HZ	1:C:230:PHE:HZ	1.63	0.46
1:A:34:SER:C	1:A:36:CYS:N	2.69	0.46
1:B:229:GLN:HG2	1:B:235:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:GLU:OE1	1:B:320:GLU:CA	2.62	0.46
1:C:31:LYS:C	1:C:31:LYS:HZ2	2.19	0.46
1:C:55:SER:HB3	1:C:62:LEU:HD11	1.97	0.46
1:C:229:GLN:HE21	1:C:235:LEU:CD1	2.12	0.46
1:C:232:ASP:OD1	1:C:235:LEU:HG	2.16	0.46
1:C:288:CYS:O	1:C:289:GLN:C	2.54	0.46
1:A:47:PRO:C	1:A:49:LYS:H	2.18	0.46
1:A:76:LYS:HD2	1:A:81:ASN:C	2.36	0.46
1:A:135:GLY:O	1:A:136:ILE:O	2.33	0.46
1:A:152:GLN:O	1:A:156:GLU:CB	2.64	0.46
1:A:232:ASP:OD1	1:A:235:LEU:HG	2.16	0.46
1:A:238:PHE:C	1:A:238:PHE:HD1	2.19	0.46
1:A:243:ILE:HD13	1:A:248:SER:OG	2.15	0.46
1:A:248:SER:O	1:A:249:LEU:C	2.54	0.46
1:A:255:LEU:HD11	1:A:259:LEU:HD11	1.97	0.46
1:A:323:GLY:O	1:A:324:LEU:C	2.53	0.46
1:B:77:VAL:CG1	1:B:78:THR:N	2.79	0.46
1:B:269:ILE:HG22	1:B:269:ILE:O	2.15	0.46
1:C:76:LYS:HD2	1:C:81:ASN:C	2.36	0.46
1:C:290:ALA:O	1:C:291:ARG:C	2.54	0.46
1:C:323:GLY:O	1:C:324:LEU:C	2.54	0.46
1:A:31:LYS:NZ	1:A:166:ASP:CG	2.69	0.46
1:A:143:MET:O	1:A:146:MET:HB2	2.16	0.46
1:A:168:ALA:C	1:A:170:THR:N	2.69	0.46
1:A:252:THR:O	1:A:253:GLU:C	2.54	0.46
1:A:272:ASN:CG	1:A:273:GLN:HG3	2.36	0.46
1:B:7:PRO:O	1:B:7:PRO:HG2	2.16	0.46
1:B:44:LEU:HD12	1:B:80:MET:HE1	1.98	0.46
1:C:226:ILE:CG2	1:C:230:PHE:CD2	2.97	0.46
1:C:254:ARG:O	1:C:257:GLN:N	2.49	0.46
1:C:294:MET:O	1:C:295:GLN:C	2.54	0.46
1:C:295:GLN:O	1:C:298:TYR:HB2	2.16	0.46
1:A:12:LEU:O	1:A:14:THR:N	2.49	0.46
1:A:227:ARG:NH2	1:A:262:TYR:O	2.48	0.46
1:A:230:PHE:CE2	1:A:264:MET:CE	2.62	0.46
1:A:245:GLU:HG2	1:A:294:MET:SD	2.56	0.46
1:A:287:ARG:HD3	1:B:348:TYR:CE2	2.51	0.46
1:A:336:LYS:O	1:A:337:GLU:C	2.52	0.46
1:B:173:THR:O	1:B:176:PHE:CE2	2.69	0.46
1:B:272:ASN:O	1:B:273:GLN:C	2.52	0.46
1:C:31:LYS:O	1:C:31:LYS:HG2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:TYR:O	1:C:301:GLN:HB2	2.15	0.46
1:B:36:CYS:C	1:B:38:ILE:N	2.69	0.45
1:B:46:GLN:O	1:B:49:LYS:N	2.49	0.45
1:B:187:LEU:HD11	1:B:216:LEU:CB	2.45	0.45
1:C:42:MET:CE	1:C:162:THR:HG21	2.46	0.45
1:C:147:LYS:O	1:C:151:ARG:HG3	2.16	0.45
1:C:165:PHE:N	1:C:165:PHE:CD2	2.84	0.45
1:A:19:LYS:C	1:A:20:TRP:CG	2.89	0.45
1:A:295:GLN:O	1:A:298:TYR:HB2	2.15	0.45
1:B:57:ASP:HB2	1:B:169:PRO:HD3	1.98	0.45
1:B:298:TYR:HA	1:B:301:GLN:HG2	1.97	0.45
1:C:34:SER:OG	1:C:241:VAL:HG21	2.17	0.45
1:C:176:PHE:CD1	1:C:177:LEU:N	2.85	0.45
1:C:239:VAL:HG13	1:C:268:SER:CB	2.45	0.45
1:C:338:TYR:CD1	1:C:338:TYR:C	2.89	0.45
1:A:227:ARG:NH2	1:A:263:ASP:HB3	2.30	0.45
1:A:298:TYR:HA	1:A:301:GLN:HG2	1.99	0.45
1:B:37:SER:OG	1:B:331:SER:CB	2.53	0.45
1:B:41:GLN:OE1	1:B:331:SER:CB	2.65	0.45
1:C:10:HIS:CA	1:C:13:ILE:HG13	2.46	0.45
1:C:57:ASP:HB2	1:C:169:PRO:HD3	1.98	0.45
1:A:50:GLN:O	1:A:161:ASP:N	2.37	0.45
1:A:259:LEU:O	1:A:262:TYR:N	2.36	0.45
1:A:269:ILE:O	1:A:269:ILE:HG22	2.16	0.45
1:C:333:PHE:CE2	1:C:338:TYR:HB2	2.51	0.45
1:A:30:GLY:CA	3:A:401:ADP:PB	3.00	0.45
1:B:168:ALA:O	1:B:171:GLY:N	2.49	0.45
1:B:177:LEU:HD22	1:B:177:LEU:H	1.76	0.45
1:C:283:HIS:CE1	1:C:348:TYR:HH	2.35	0.45
1:C:327:LEU:O	1:C:328:THR:C	2.53	0.45
1:A:60:HIS:HD2	1:A:69:LYS:HZ1	1.65	0.45
1:A:265:ASP:OD1	2:E:14:ARG:HD3	2.15	0.45
1:C:32:THR:HG21	1:C:61:ASN:HB2	1.97	0.45
1:C:50:GLN:CD	1:C:82:ASN:HA	2.35	0.45
1:C:274:LEU:CA	1:C:295:GLN:HE22	2.25	0.45
1:A:243:ILE:H	1:A:243:ILE:CD1	2.17	0.45
1:A:244:SER:C	1:A:298:TYR:HD2	2.19	0.45
1:A:296:LYS:O	1:A:297:LYS:C	2.54	0.45
1:B:50:GLN:OE1	1:B:82:ASN:HA	2.17	0.45
1:B:139:ALA:O	1:B:142:PHE:N	2.49	0.45
1:B:172:HIS:O	1:B:172:HIS:CG	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:PHE:C	1:B:238:PHE:CD1	2.90	0.45
1:B:275:LEU:O	1:B:276:PHE:CB	2.64	0.45
1:C:9:LEU:C	1:C:13:ILE:HG13	2.36	0.45
1:C:38:ILE:C	1:C:40:ILE:N	2.70	0.45
1:C:91:SER:O	1:C:92:ALA:C	2.54	0.45
1:C:248:SER:O	1:C:249:LEU:C	2.55	0.45
1:C:306:TYR:HD1	1:C:309:PHE:CG	2.35	0.45
1:A:37:SER:O	1:A:41:GLN:HG2	2.17	0.45
1:A:179:LEU:CD2	1:A:219:LEU:HD11	2.47	0.45
1:A:181:ASN:O	1:A:183:LEU:N	2.49	0.45
1:A:224:GLU:O	1:A:228:GLN:N	2.39	0.45
1:A:305:LEU:C	1:A:306:TYR:CD2	2.91	0.45
1:B:43:ALA:CA	1:B:51:PHE:CE2	2.92	0.45
1:C:82:ASN:N	1:C:82:ASN:OD1	2.50	0.45
1:C:331:SER:O	1:C:334:LEU:HB2	2.17	0.45
1:A:10:HIS:ND1	1:A:10:HIS:C	2.70	0.45
1:A:168:ALA:O	1:A:171:GLY:N	2.49	0.45
1:A:241:VAL:HG13	1:A:270:ILE:CG2	2.44	0.45
1:A:306:TYR:O	1:A:309:PHE:N	2.44	0.45
1:B:31:LYS:NZ	1:B:166:ASP:CG	2.70	0.45
1:B:134:PRO:O	1:B:136:ILE:N	2.43	0.45
1:B:248:SER:O	1:B:249:LEU:C	2.55	0.45
1:C:32:THR:N	3:C:401:ADP:O2B	2.50	0.45
1:A:38:ILE:HG22	1:A:39:ALA:N	2.33	0.44
1:A:82:ASN:N	1:A:82:ASN:OD1	2.51	0.44
1:B:34:SER:CB	1:B:241:VAL:HG21	2.47	0.44
1:B:60:HIS:HD2	1:B:69:LYS:HZ1	1.61	0.44
1:C:245:GLU:HG2	1:C:294:MET:SD	2.57	0.44
1:C:255:LEU:O	1:C:256:ILE:C	2.53	0.44
1:C:306:TYR:HA	1:C:309:PHE:CE2	2.50	0.44
1:C:328:THR:C	1:C:330:PHE:H	2.20	0.44
1:A:172:HIS:O	1:A:172:HIS:CG	2.69	0.44
1:A:172:HIS:NE2	1:A:258:GLU:OE2	2.50	0.44
1:B:62:LEU:HB2	1:B:87:GLU:OE1	2.17	0.44
1:B:333:PHE:CE1	1:B:338:TYR:HA	2.52	0.44
1:C:142:PHE:CZ	1:C:230:PHE:CZ	3.05	0.44
1:A:36:CYS:O	1:A:37:SER:C	2.55	0.44
1:B:53:LEU:CD1	1:B:164:ILE:HG22	2.41	0.44
1:B:135:GLY:CA	1:B:176:PHE:HB3	2.48	0.44
1:B:172:HIS:NE2	1:B:258:GLU:OE2	2.47	0.44
1:C:50:GLN:O	1:C:161:ASP:N	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:LEU:HD23	1:C:187:LEU:N	2.32	0.44
1:C:243:ILE:HD11	1:C:248:SER:HB2	1.99	0.44
1:B:186:LEU:HD23	1:B:187:LEU:N	2.32	0.44
1:B:245:GLU:HG2	1:B:294:MET:SD	2.57	0.44
1:C:9:LEU:O	1:C:12:LEU:N	2.48	0.44
1:C:34:SER:CB	1:C:241:VAL:HG21	2.48	0.44
1:C:172:HIS:CB	1:C:174:LEU:CG	2.74	0.44
1:C:249:LEU:O	1:C:250:TYR:C	2.56	0.44
1:C:292:TRP:CE3	1:C:292:TRP:C	2.90	0.44
1:C:293:LYS:O	1:C:294:MET:C	2.55	0.44
2:E:10:ARG:HD2	2:E:14:ARG:NH2	2.32	0.44
1:A:36:CYS:C	1:A:38:ILE:N	2.69	0.44
1:A:38:ILE:O	1:A:40:ILE:N	2.51	0.44
1:A:326:ASN:O	1:A:350:LEU:HD21	2.17	0.44
1:B:12:LEU:O	1:B:13:ILE:C	2.56	0.44
1:B:39:ALA:HA	1:B:164:ILE:HD12	1.98	0.44
1:B:76:LYS:HD2	1:B:81:ASN:C	2.36	0.44
1:B:178:GLN:NE2	1:B:261:SER:OG	2.51	0.44
1:B:178:GLN:CD	1:B:262:TYR:HE1	1.95	0.44
1:B:297:LYS:O	1:B:301:GLN:HG2	2.17	0.44
1:B:305:LEU:O	1:B:306:TYR:CG	2.70	0.44
1:C:7:PRO:O	1:C:8:ASN:HB3	2.17	0.44
1:C:228:GLN:CD	1:C:229:GLN:N	2.70	0.44
1:C:277:ALA:CB	1:C:289:GLN:HG3	2.48	0.44
1:C:280:ASP:OD1	1:C:283:HIS:HB2	2.17	0.44
1:B:9:LEU:C	1:B:13:ILE:HG13	2.38	0.44
1:B:32:THR:O	1:B:35:SER:HB2	2.17	0.44
1:B:38:ILE:HG22	1:B:39:ALA:N	2.32	0.44
1:B:39:ALA:O	1:B:83:LEU:HD22	2.16	0.44
1:C:9:LEU:O	1:C:13:ILE:N	2.45	0.44
1:A:18:HIS:HA	1:A:235:LEU:CA	2.46	0.44
1:A:37:SER:CB	1:A:331:SER:HB3	2.47	0.44
1:A:49:LYS:HB2	1:A:51:PHE:CE2	2.52	0.44
1:A:348:TYR:CZ	1:B:287:ARG:CD	2.98	0.44
1:B:255:LEU:HD11	1:B:259:LEU:HD11	1.99	0.44
1:B:291:ARG:O	1:B:292:TRP:C	2.54	0.44
1:A:134:PRO:O	1:A:136:ILE:N	2.44	0.44
1:A:140:LEU:H	1:A:140:LEU:CD2	2.09	0.44
1:A:245:GLU:O	1:A:246:PHE:C	2.55	0.44
1:A:322:ARG:NH1	1:B:246:PHE:HB3	2.33	0.44
1:B:24:GLY:CA	1:B:31:LYS:CD	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ILE:C	1:B:40:ILE:N	2.70	0.44
1:B:47:PRO:C	1:B:49:LYS:H	2.21	0.44
1:B:250:TYR:O	1:B:253:GLU:HB3	2.18	0.44
1:C:20:TRP:HB2	1:C:236:THR:HB	1.99	0.44
1:C:22:PHE:HE1	1:C:165:PHE:CE1	2.35	0.44
1:C:34:SER:C	1:C:36:CYS:N	2.70	0.44
2:D:10:ARG:HD2	2:D:14:ARG:NH2	2.32	0.44
1:A:136:ILE:CG2	1:A:137:ASP:N	2.68	0.44
1:A:177:LEU:HD13	1:A:227:ARG:NH1	2.33	0.44
1:B:133:ILE:CG2	1:B:134:PRO:CD	2.91	0.44
1:B:228:GLN:HG3	1:B:229:GLN:N	2.07	0.44
1:B:274:LEU:CA	1:B:295:GLN:HE22	2.26	0.44
1:C:87:GLU:C	1:C:88:ILE:HG23	2.38	0.44
1:C:243:ILE:CD1	1:C:248:SER:HB2	2.47	0.44
1:C:305:LEU:HD23	1:C:306:TYR:CZ	2.52	0.44
1:A:50:GLN:HG3	1:A:158:GLU:OE1	2.18	0.43
1:A:61:ASN:N	1:A:61:ASN:OD1	2.46	0.43
1:A:64:ASP:C	1:A:66:PHE:N	2.71	0.43
1:A:272:ASN:O	1:A:273:GLN:C	2.55	0.43
1:B:35:SER:CB	1:B:166:ASP:OD1	2.66	0.43
1:C:36:CYS:O	1:C:37:SER:C	2.56	0.43
1:C:286:LYS:HD3	1:C:286:LYS:H	1.73	0.43
1:A:267:ASN:C	1:A:268:SER:HG	2.20	0.43
1:A:328:THR:O	1:A:330:PHE:N	2.51	0.43
1:B:244:SER:C	1:B:298:TYR:HD2	2.21	0.43
1:C:29:VAL:O	1:C:272:ASN:ND2	2.51	0.43
1:A:27:GLY:C	1:A:29:VAL:H	2.21	0.43
1:B:296:LYS:O	1:B:297:LYS:C	2.57	0.43
1:B:339:ASN:HD21	1:B:341:ILE:HD12	1.83	0.43
1:C:172:HIS:C	1:C:174:LEU:H	2.19	0.43
1:C:238:PHE:C	1:C:238:PHE:HD1	2.21	0.43
1:A:348:TYR:OH	1:B:287:ARG:CG	2.66	0.43
1:B:41:GLN:OE1	1:B:331:SER:HB2	2.18	0.43
1:C:19:LYS:N	1:C:235:LEU:O	2.51	0.43
1:C:49:LYS:HB2	1:C:51:PHE:CE2	2.53	0.43
1:C:57:ASP:HA	1:C:58:PRO:HD2	1.73	0.43
1:C:174:LEU:CD1	1:C:259:LEU:HD21	2.48	0.43
2:D:17:ARG:C	2:D:21:PHE:HD2	2.17	0.43
1:A:33:THR:O	1:A:36:CYS:HB2	2.19	0.43
1:B:31:LYS:NZ	1:B:32:THR:HA	2.33	0.43
1:C:156:GLU:HG2	1:C:158:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:CYS:O	1:C:288:CYS:CB	2.56	0.43
1:A:30:GLY:CA	3:A:401:ADP:O3B	2.66	0.43
1:A:163:VAL:O	1:A:163:VAL:HG13	2.19	0.43
1:A:297:LYS:O	1:A:301:GLN:HG2	2.19	0.43
1:B:43:ALA:O	1:B:44:LEU:C	2.56	0.43
1:B:233:PRO:HG3	1:B:265:ASP:HB2	2.00	0.43
1:B:273:GLN:O	1:B:295:GLN:NE2	2.45	0.43
1:B:336:LYS:O	1:B:337:GLU:C	2.55	0.43
1:C:133:ILE:CG2	1:C:134:PRO:N	2.82	0.43
1:C:142:PHE:CZ	1:C:230:PHE:HZ	2.36	0.43
2:E:7:ALA:O	2:E:8:GLU:C	2.57	0.43
1:A:34:SER:CB	1:A:241:VAL:HG21	2.47	0.43
1:A:73:ASP:HA	1:A:86:MET:SD	2.59	0.43
1:A:156:GLU:HG2	1:A:158:GLU:HG3	2.00	0.43
1:A:322:ARG:O	1:A:326:ASN:CB	2.65	0.43
1:B:10:HIS:HA	1:B:13:ILE:HG13	2.00	0.43
1:B:133:ILE:CG2	1:B:134:PRO:N	2.82	0.43
1:B:241:VAL:O	1:B:242:CYS:HB3	2.17	0.43
1:B:321:ILE:HD13	1:B:321:ILE:C	2.34	0.43
1:C:77:VAL:CG1	1:C:78:THR:N	2.82	0.43
1:A:75:ARG:CD	1:A:75:ARG:C	2.87	0.43
1:A:239:VAL:HG13	1:A:268:SER:CB	2.47	0.43
1:A:294:MET:CE	1:B:320:GLU:HG2	2.48	0.43
1:A:339:ASN:HA	1:A:340:PRO:HD3	1.93	0.43
1:B:31:LYS:HB2	1:B:241:VAL:CB	2.46	0.43
1:B:33:THR:O	1:B:36:CYS:HB2	2.19	0.43
1:B:246:PHE:H	1:B:298:TYR:HE2	1.62	0.43
1:C:246:PHE:HB2	1:C:298:TYR:OH	2.18	0.43
1:A:166:ASP:O	1:A:167:THR:C	2.56	0.43
1:B:29:VAL:CG1	1:B:242:CYS:HA	2.31	0.43
1:B:36:CYS:O	1:B:37:SER:C	2.56	0.43
1:B:331:SER:O	1:B:334:LEU:HB2	2.19	0.43
1:C:168:ALA:O	1:C:171:GLY:N	2.52	0.43
1:C:296:LYS:O	1:C:297:LYS:C	2.57	0.43
1:C:328:THR:C	1:C:330:PHE:N	2.72	0.43
2:E:27:SER:O	2:E:31:ASN:OD1	2.37	0.43
1:B:50:GLN:HG3	1:B:158:GLU:OE1	2.19	0.43
1:B:226:ILE:HG23	1:B:230:PHE:CE2	2.53	0.43
1:B:252:THR:O	1:B:253:GLU:C	2.56	0.43
1:C:148:HIS:HA	1:C:151:ARG:HD2	2.01	0.43
1:C:305:LEU:O	1:C:306:TYR:CG	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:PHE:CZ	1:C:343:ASP:CB	3.00	0.43
2:D:7:ALA:O	2:D:8:GLU:C	2.56	0.43
1:A:9:LEU:HD23	1:A:9:LEU:HA	1.77	0.42
1:A:44:LEU:HD12	1:A:80:MET:HE1	2.00	0.42
1:A:173:THR:O	1:A:174:LEU:C	2.57	0.42
1:A:243:ILE:CD1	1:A:248:SER:HB2	2.49	0.42
1:A:288:CYS:O	1:A:289:GLN:C	2.58	0.42
1:B:9:LEU:O	1:B:13:ILE:N	2.43	0.42
1:B:75:ARG:CD	1:B:76:LYS:O	2.65	0.42
1:B:168:ALA:C	1:B:170:THR:N	2.69	0.42
1:B:277:ALA:HB3	1:B:292:TRP:HD1	1.84	0.42
1:C:138:GLU:HB3	1:C:173:THR:O	2.18	0.42
1:C:308:ASP:HB2	2:D:17:ARG:CD	2.45	0.42
1:A:8:ASN:O	1:A:9:LEU:CD2	2.60	0.42
1:A:189:LYS:HD3	1:A:189:LYS:HA	1.84	0.42
1:A:277:ALA:CB	1:A:289:GLN:HG3	2.49	0.42
1:B:187:LEU:CG	1:B:216:LEU:CD1	2.79	0.42
1:B:265:ASP:HB2	2:D:32:LYS:HE2	2.00	0.42
1:B:323:GLY:O	1:B:324:LEU:C	2.57	0.42
1:B:333:PHE:HD1	1:B:336:LYS:O	2.02	0.42
1:C:9:LEU:HD23	1:C:9:LEU:HA	1.76	0.42
1:C:238:PHE:CE2	1:C:259:LEU:CD2	3.02	0.42
1:C:277:ALA:CB	1:C:284:ASN:ND2	2.82	0.42
2:E:17:ARG:C	2:E:21:PHE:HD2	2.17	0.42
1:B:64:ASP:C	1:B:66:PHE:N	2.73	0.42
1:B:135:GLY:O	1:B:136:ILE:O	2.37	0.42
1:A:136:ILE:CG2	1:A:137:ASP:H	2.31	0.42
1:B:237:THR:OG1	1:B:238:PHE:N	2.53	0.42
1:B:243:ILE:CD1	1:B:248:SER:HB2	2.50	0.42
1:B:296:LYS:HA	1:B:296:LYS:HD3	1.69	0.42
1:C:142:PHE:O	1:C:145:VAL:HG23	2.19	0.42
1:A:10:HIS:HA	1:A:13:ILE:HG13	2.02	0.42
1:A:31:LYS:NZ	1:A:166:ASP:OD2	2.52	0.42
1:B:138:GLU:O	1:B:176:PHE:CE2	2.61	0.42
1:B:277:ALA:HB3	1:B:292:TRP:CD1	2.55	0.42
1:B:296:LYS:HD2	1:B:300:ASP:OD2	2.20	0.42
1:B:328:THR:C	1:B:330:PHE:N	2.73	0.42
1:B:328:THR:C	1:B:330:PHE:H	2.22	0.42
1:C:228:GLN:CG	1:C:229:GLN:N	2.83	0.42
2:D:27:SER:O	2:D:31:ASN:OD1	2.37	0.42
1:B:57:ASP:O	1:B:58:PRO:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ARG:CZ	1:C:231:THR:CG2	2.97	0.42
1:B:50:GLN:HB2	1:B:159:THR:O	2.19	0.42
1:B:175:ARG:C	1:B:177:LEU:HD22	2.40	0.42
1:C:38:ILE:HG22	1:C:164:ILE:HD13	2.01	0.42
1:A:133:ILE:CG2	1:A:134:PRO:CD	2.91	0.42
1:A:179:LEU:O	1:A:183:LEU:HG	2.20	0.42
1:B:29:VAL:O	1:B:29:VAL:HG12	2.20	0.42
1:C:242:CYS:O	1:C:271:VAL:HA	2.20	0.42
1:C:271:VAL:CG1	1:C:274:LEU:HD21	2.50	0.42
1:C:333:PHE:HD1	1:C:333:PHE:HA	1.68	0.42
1:C:334:LEU:HD23	1:C:334:LEU:HA	1.41	0.42
1:A:267:ASN:HD22	1:A:267:ASN:H	1.68	0.42
1:A:330:PHE:O	1:A:332:GLN:N	2.52	0.42
1:B:294:MET:O	1:B:295:GLN:C	2.57	0.42
1:C:321:ILE:O	1:C:321:ILE:CD1	2.56	0.42
1:A:273:GLN:HA	1:A:316:LEU:CD1	2.50	0.42
1:C:22:PHE:CE1	1:C:165:PHE:CE1	3.08	0.42
1:C:243:ILE:CD1	1:C:243:ILE:N	2.77	0.42
1:C:326:ASN:CG	1:C:350:LEU:HG	2.40	0.42
1:A:13:ILE:HD12	1:A:335:ASN:CG	2.41	0.41
1:A:348:TYR:CZ	1:B:287:ARG:CG	3.03	0.41
1:B:177:LEU:C	1:B:180:PRO:CD	2.69	0.41
1:A:31:LYS:HA	1:A:34:SER:HB2	2.02	0.41
1:A:292:TRP:CE3	1:A:292:TRP:C	2.94	0.41
1:A:334:LEU:HD22	1:A:334:LEU:HA	1.65	0.41
1:B:19:LYS:HB2	1:B:20:TRP:CD1	2.55	0.41
1:B:249:LEU:O	1:B:250:TYR:C	2.58	0.41
1:C:63:SER:O	1:C:66:PHE:N	2.46	0.41
1:C:298:TYR:HA	1:C:301:GLN:HG2	2.02	0.41
1:A:28:GLY:CA	1:B:28:GLY:HA3	2.50	0.41
1:A:50:GLN:OE1	1:A:82:ASN:HA	2.20	0.41
1:A:167:THR:O	1:A:168:ALA:C	2.59	0.41
1:A:319:GLY:HA3	1:B:294:MET:CG	2.39	0.41
1:A:334:LEU:HA	1:A:334:LEU:HD23	1.49	0.41
1:B:10:HIS:CA	1:B:13:ILE:HG13	2.50	0.41
1:B:32:THR:N	3:B:401:ADP:O2B	2.52	0.41
1:B:227:ARG:NH1	1:B:262:TYR:O	2.45	0.41
1:B:339:ASN:OD1	1:B:341:ILE:N	2.54	0.41
1:C:169:PRO:C	1:C:171:GLY:H	2.22	0.41
1:C:187:LEU:CD1	1:C:216:LEU:HD22	2.50	0.41
1:A:59:ALA:HB1	1:B:251:GLU:CD	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PHE:CD1	1:A:85:CYS:HB3	2.55	0.41
1:A:298:TYR:O	1:A:301:GLN:HB2	2.20	0.41
1:C:31:LYS:NZ	1:C:32:THR:HA	2.35	0.41
1:C:244:SER:C	1:C:298:TYR:HD2	2.24	0.41
1:C:287:ARG:O	1:C:290:ALA:HB3	2.20	0.41
1:A:31:LYS:NZ	1:A:32:THR:HA	2.35	0.41
1:A:40:ILE:O	1:A:44:LEU:HD13	2.21	0.41
1:A:133:ILE:CG2	1:A:134:PRO:N	2.82	0.41
1:A:138:GLU:HB3	1:A:173:THR:O	2.21	0.41
1:A:179:LEU:CD2	1:A:219:LEU:HD23	2.23	0.41
1:A:250:TYR:O	1:A:253:GLU:HB3	2.20	0.41
1:A:314:MET:CE	1:A:334:LEU:HD23	2.49	0.41
1:B:32:THR:HG23	1:B:61:ASN:ND2	2.35	0.41
1:B:62:LEU:O	1:B:65:ALA:N	2.53	0.41
1:C:12:LEU:CD1	1:C:12:LEU:O	2.68	0.41
1:C:50:GLN:HB2	1:C:159:THR:O	2.20	0.41
1:C:229:GLN:O	1:C:236:THR:HG22	2.19	0.41
2:E:7:ALA:O	2:E:10:ARG:HB3	2.20	0.41
1:A:273:GLN:HA	1:A:316:LEU:HD13	2.03	0.41
1:A:296:LYS:HD2	1:A:300:ASP:OD2	2.20	0.41
1:B:290:ALA:O	1:B:293:LYS:N	2.54	0.41
1:B:350:LEU:N	1:B:350:LEU:CD1	2.83	0.41
1:C:187:LEU:HA	1:C:187:LEU:HD23	1.79	0.41
1:C:273:GLN:HA	1:C:316:LEU:CD1	2.50	0.41
1:C:297:LYS:O	1:C:301:GLN:HG2	2.21	0.41
1:A:178:GLN:HA	1:A:181:ASN:HD21	1.86	0.41
1:A:179:LEU:C	1:A:183:LEU:HD12	2.41	0.41
1:A:326:ASN:CG	1:A:350:LEU:HG	2.39	0.41
1:C:31:LYS:HZ2	1:C:32:THR:HA	1.86	0.41
1:C:137:ASP:N	1:C:137:ASP:OD2	2.51	0.41
1:A:64:ASP:OD2	1:B:246:PHE:CE1	2.74	0.41
1:A:187:LEU:HD23	1:A:187:LEU:HA	1.74	0.41
1:B:178:GLN:CD	1:B:262:TYR:CE1	2.75	0.41
1:B:227:ARG:HH22	1:B:263:ASP:HB3	1.76	0.41
1:B:254:ARG:O	1:B:257:GLN:N	2.54	0.41
1:C:29:VAL:O	1:C:29:VAL:HG12	2.21	0.41
1:A:14:THR:HA	1:A:46:GLN:HE21	1.85	0.41
1:A:32:THR:OG1	3:A:401:ADP:PA	2.78	0.41
1:A:53:LEU:HD12	1:A:164:ILE:O	2.20	0.41
1:A:64:ASP:OD2	1:B:247:LEU:HD22	2.20	0.41
1:A:136:ILE:HD13	1:A:136:ILE:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:HG12	1:A:149:ILE:CD1	2.50	0.41
1:A:338:TYR:CE2	1:A:347:ILE:HD11	2.55	0.41
1:B:228:GLN:NE2	1:B:229:GLN:HA	2.22	0.41
1:B:242:CYS:O	1:B:271:VAL:HA	2.21	0.41
1:B:277:ALA:CB	1:B:289:GLN:HG3	2.50	0.41
1:B:295:GLN:O	1:B:298:TYR:HB2	2.21	0.41
1:C:35:SER:CB	1:C:166:ASP:OD1	2.69	0.41
1:C:296:LYS:HD2	1:C:300:ASP:OD2	2.20	0.41
1:C:306:TYR:CD1	1:C:309:PHE:CE2	3.09	0.41
1:C:333:PHE:HZ	1:C:343:ASP:CB	2.23	0.41
2:D:7:ALA:O	2:D:10:ARG:HB3	2.20	0.41
1:A:39:ALA:CA	1:A:164:ILE:CD1	2.99	0.41
1:A:62:LEU:HB2	1:A:87:GLU:OE1	2.20	0.41
1:A:175:ARG:O	1:A:178:GLN:HG2	2.20	0.41
1:C:19:LYS:HB2	1:C:20:TRP:NE1	2.36	0.41
1:C:273:GLN:HA	1:C:316:LEU:HD13	2.03	0.41
1:C:281:GLN:C	1:C:283:HIS:N	2.75	0.41
1:A:12:LEU:HD12	1:A:15:SER:HB3	2.03	0.40
1:A:169:PRO:C	1:A:171:GLY:H	2.24	0.40
1:B:70:PHE:CD1	1:B:85:CYS:HB3	2.57	0.40
1:B:267:ASN:HD22	1:B:267:ASN:H	1.69	0.40
1:B:292:TRP:CE3	1:B:292:TRP:C	2.95	0.40
1:C:27:GLY:C	1:C:29:VAL:N	2.75	0.40
1:C:36:CYS:O	1:C:39:ALA:N	2.54	0.40
1:C:64:ASP:C	1:C:66:PHE:N	2.74	0.40
1:C:252:THR:O	1:C:253:GLU:C	2.59	0.40
1:A:50:GLN:HB2	1:A:159:THR:O	2.21	0.40
1:A:156:GLU:HG3	1:A:158:GLU:N	2.36	0.40
1:A:224:GLU:O	1:A:228:GLN:HG3	2.21	0.40
1:A:294:MET:O	1:A:295:GLN:C	2.59	0.40
1:A:308:ASP:OD1	2:E:16:ARG:NH2	2.37	0.40
1:B:25:GLY:O	1:B:27:GLY:N	2.54	0.40
1:B:289:GLN:HE21	1:B:289:GLN:HB2	1.55	0.40
1:C:30:GLY:CA	3:C:401:ADP:PB	3.08	0.40
1:C:40:ILE:O	1:C:42:MET:N	2.54	0.40
1:A:12:LEU:CD1	1:A:12:LEU:O	2.66	0.40
1:A:87:GLU:O	1:A:88:ILE:HG23	2.22	0.40
1:A:243:ILE:HD11	1:A:248:SER:HB2	2.04	0.40
1:A:331:SER:O	1:A:332:GLN:C	2.58	0.40
1:B:19:LYS:O	1:B:20:TRP:CG	2.73	0.40
1:B:293:LYS:O	1:B:294:MET:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ASN:HA	1:B:340:PRO:HD3	1.90	0.40
1:C:33:THR:O	1:C:34:SER:C	2.60	0.40
1:C:176:PHE:HA	1:C:179:LEU:HB3	2.04	0.40
1:C:290:ALA:O	1:C:293:LYS:N	2.55	0.40
1:A:34:SER:O	1:A:35:SER:C	2.59	0.40
1:A:259:LEU:O	1:A:260:ILE:C	2.60	0.40
1:A:287:ARG:O	1:A:288:CYS:O	2.40	0.40
1:A:296:LYS:HD3	1:A:299:LEU:HD12	2.03	0.40
1:A:322:ARG:HH22	1:B:246:PHE:HB3	1.86	0.40
1:B:35:SER:O	1:B:53:LEU:HD22	2.21	0.40
1:C:43:ALA:HB2	1:C:51:PHE:HD2	1.87	0.40
1:A:233:PRO:HG3	1:A:265:ASP:HB2	2.03	0.40
1:B:31:LYS:N	3:B:401:ADP:O3B	2.53	0.40
1:B:187:LEU:CD1	1:B:216:LEU:HD22	2.50	0.40
1:C:14:THR:HA	1:C:46:GLN:HE21	1.87	0.40
1:C:31:LYS:HA	1:C:34:SER:HB2	2.02	0.40
1:C:31:LYS:NZ	1:C:166:ASP:CG	2.75	0.40
1:C:136:ILE:HD13	1:C:136:ILE:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	279/362 (77%)	168 (60%)	70 (25%)	41 (15%)	0 4
1	B	273/362 (75%)	163 (60%)	68 (25%)	42 (15%)	0 4
1	C	286/362 (79%)	173 (60%)	68 (24%)	45 (16%)	0 4
2	D	28/46 (61%)	25 (89%)	3 (11%)	0	100 100
2	E	28/46 (61%)	25 (89%)	3 (11%)	0	100 100
All	All	894/1178 (76%)	554 (62%)	212 (24%)	128 (14%)	0 4

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	136	ILE
1	A	142	PHE
1	A	175	ARG
1	A	249	LEU
1	A	288	CYS
1	B	34	SER
1	B	35	SER
1	B	136	ILE
1	B	142	PHE
1	B	249	LEU
1	B	288	CYS
1	C	35	SER
1	C	91	SER
1	C	92	ALA
1	C	136	ILE
1	C	142	PHE
1	C	175	ARG
1	C	249	LEU
1	C	288	CYS
1	A	34	SER
1	A	37	SER
1	A	39	ALA
1	A	62	LEU
1	A	143	MET
1	A	146	MET
1	A	276	PHE
1	A	294	MET
1	A	301	GLN
1	A	320	GLU
1	A	323	GLY
1	A	348	TYR
1	B	37	SER
1	B	39	ALA
1	B	62	LEU
1	B	143	MET
1	B	146	MET
1	B	276	PHE
1	B	294	MET
1	B	301	GLN
1	B	307	GLU
1	B	320	GLU

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Mol	Chain	Res	Type
1	B	325	ASN
1	B	336	LYS
1	B	348	TYR
1	C	8	ASN
1	C	34	SER
1	C	37	SER
1	C	39	ALA
1	C	62	LEU
1	C	139	ALA
1	C	143	MET
1	C	146	MET
1	C	276	PHE
1	C	282	GLU
1	C	294	MET
1	C	320	GLU
1	C	325	ASN
1	C	329	LYS
1	C	348	TYR
1	A	8	ASN
1	A	26	LYS
1	A	59	ALA
1	A	72	LYS
1	A	82	ASN
1	A	139	ALA
1	A	248	SER
1	A	266	VAL
1	A	290	ALA
1	A	325	ASN
1	A	329	LYS
1	B	8	ASN
1	B	26	LYS
1	B	59	ALA
1	B	72[A]	LYS
1	B	72[B]	LYS
1	B	82	ASN
1	B	139	ALA
1	B	266	VAL
1	B	290	ALA
1	B	323	GLY
1	B	329	LYS
1	C	26	LYS
1	C	72	LYS

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Mol	Chain	Res	Type
1	C	82	ASN
1	C	248	SER
1	C	290	ALA
1	C	301	GLN
1	C	323	GLY
1	A	141	SER
1	A	250	TYR
1	A	336	LYS
1	B	141	SER
1	B	242	CYS
1	B	248	SER
1	B	331	SER
1	C	59	ALA
1	C	141	SER
1	C	250	TYR
1	C	281	GLN
1	C	336	LYS
1	A	46	GLN
1	A	179	LEU
1	A	331	SER
1	B	46	GLN
1	B	250	TYR
1	C	7	PRO
1	C	46	GLN
1	C	137	ASP
1	C	255	LEU
1	C	343	ASP
1	A	7	PRO
1	A	255	LEU
1	A	338	TYR
1	C	25	GLY
1	A	25	GLY
1	B	77	VAL
1	C	89	ASP
1	B	7	PRO
1	B	25	GLY
1	B	233	PRO
1	B	302	ILE
1	C	302	ILE
1	A	302	ILE
1	C	266	VAL
1	A	321	ILE

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Mol	Chain	Res	Type
1	C	321	ILE
1	B	321	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	258/317 (81%)	207 (80%)	51 (20%)	1 9
1	B	252/317 (80%)	197 (78%)	55 (22%)	1 6
1	C	262/317 (83%)	207 (79%)	55 (21%)	1 7
2	D	26/40 (65%)	26 (100%)	0	100 100
2	E	26/40 (65%)	26 (100%)	0	100 100
All	All	824/1031 (80%)	663 (80%)	161 (20%)	1 9

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	10	HIS
1	A	14	THR
1	A	23	VAL
1	A	31	LYS
1	A	32	THR
1	A	37	SER
1	A	40	ILE
1	A	42	MET
1	A	56	THR
1	A	66	PHE
1	A	75	ARG
1	A	88	ILE
1	A	137	ASP
1	A	158	GLU
1	A	167	THR
1	A	170	THR

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Mol	Chain	Res	Type
1	A	175	ARG
1	A	186	LEU
1	A	232	ASP
1	A	236	THR
1	A	238	PHE
1	A	239	VAL
1	A	240	CYS
1	A	242	CYS
1	A	243	ILE
1	A	244	SER
1	A	246	PHE
1	A	247	LEU
1	A	249	LEU
1	A	254	ARG
1	A	256	ILE
1	A	266	VAL
1	A	267	ASN
1	A	269	ILE
1	A	275	LEU
1	A	285	CYS
1	A	286	LYS
1	A	287	ARG
1	A	289	GLN
1	A	292	TRP
1	A	294	MET
1	A	308	ASP
1	A	311	VAL
1	A	316	LEU
1	A	320	GLU
1	A	321	ILE
1	A	334	LEU
1	A	338	TYR
1	A	341	ILE
1	A	346	VAL
1	B	5	VAL
1	B	10	HIS
1	B	14	THR
1	B	23	VAL
1	B	31	LYS
1	B	32	THR
1	B	37	SER
1	B	40	ILE

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Mol	Chain	Res	Type
1	B	42	MET
1	B	56	THR
1	B	66	PHE
1	B	75	ARG
1	B	137	ASP
1	B	158	GLU
1	B	167	THR
1	B	170	THR
1	B	176	PHE
1	B	177	LEU
1	B	179	LEU
1	B	186	LEU
1	B	225	THR
1	B	231	THR
1	B	232	ASP
1	B	236	THR
1	B	238	PHE
1	B	239	VAL
1	B	240	CYS
1	B	242	CYS
1	B	243	ILE
1	B	244	SER
1	B	246	PHE
1	B	247	LEU
1	B	249	LEU
1	B	254	ARG
1	B	266	VAL
1	B	267	ASN
1	B	269	ILE
1	B	271	VAL
1	B	275	LEU
1	B	285	CYS
1	B	286	LYS
1	B	287	ARG
1	B	289	GLN
1	B	292	TRP
1	B	294	MET
1	B	305	LEU
1	B	309	PHE
1	B	311	VAL
1	B	316	LEU
1	B	320	GLU

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Mol	Chain	Res	Type
1	B	321	ILE
1	B	334	LEU
1	B	338	TYR
1	B	341	ILE
1	B	346	VAL
1	C	5	VAL
1	C	10	HIS
1	C	14	THR
1	C	23	VAL
1	C	31	LYS
1	C	32	THR
1	C	37	SER
1	C	42	MET
1	C	56	THR
1	C	66	PHE
1	C	73	ASP
1	C	75	ARG
1	C	94	LEU
1	C	137	ASP
1	C	158	GLU
1	C	167	THR
1	C	170	THR
1	C	175	ARG
1	C	177	LEU
1	C	179	LEU
1	C	186	LEU
1	C	225	THR
1	C	229	GLN
1	C	232	ASP
1	C	236	THR
1	C	238	PHE
1	C	239	VAL
1	C	240	CYS
1	C	242	CYS
1	C	243	ILE
1	C	244	SER
1	C	246	PHE
1	C	247	LEU
1	C	249	LEU
1	C	254	ARG
1	C	266	VAL
1	C	267	ASN

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Mol	Chain	Res	Type
1	C	269	ILE
1	C	275	LEU
1	C	280	ASP
1	C	283	HIS
1	C	285	CYS
1	C	286	LYS
1	C	289	GLN
1	C	292	TRP
1	C	294	MET
1	C	305	LEU
1	C	311	VAL
1	C	316	LEU
1	C	320	GLU
1	C	321	ILE
1	C	334	LEU
1	C	338	TYR
1	C	341	ILE
1	C	346	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	60	HIS
1	A	289	GLN
1	B	60	HIS
1	B	178	GLN
1	B	228	GLN
1	B	267	ASN
1	B	289	GLN
1	C	60	HIS
1	C	178	GLN
1	C	228	GLN
1	C	229	GLN
1	C	279	ASN
1	C	289	GLN

5.3.3 RNA

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)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ADP	B	401	4	24,29,29	1.04	1 (4%)	29,45,45	1.63	6 (20%)
3	ADP	A	401	4	24,29,29	1.38	2 (8%)	29,45,45	1.51	5 (17%)
3	ADP	C	401	4	24,29,29	1.37	5 (20%)	29,45,45	1.50	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	401	4	-	0/12/32/32	0/3/3/3
3	ADP	A	401	4	-	0/12/32/32	0/3/3/3
3	ADP	C	401	4	-	0/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ADP	O4'-C1'	4.34	1.47	1.41
3	C	401	ADP	PB-O1B	2.61	1.59	1.50
3	A	401	ADP	PB-O3B	-2.60	1.44	1.54
3	C	401	ADP	PB-O3B	-2.55	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	ADP	O4'-C1'	2.35	1.44	1.41
3	B	401	ADP	PB-O3B	-2.30	1.46	1.54
3	C	401	ADP	C2'-C1'	2.09	1.56	1.53
3	C	401	ADP	C2-N3	2.03	1.35	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	ADP	C1'-N9-C4	-4.13	119.39	126.64
3	C	401	ADP	C1'-N9-C4	-3.93	119.73	126.64
3	B	401	ADP	C1'-N9-C4	-3.79	119.99	126.64
3	B	401	ADP	O2B-PB-O1B	-3.09	98.60	110.68
3	B	401	ADP	PA-O3A-PB	3.02	143.18	132.83
3	B	401	ADP	O3B-PB-O3A	3.01	114.73	104.64
3	B	401	ADP	O3B-PB-O2B	2.71	117.99	107.64
3	A	401	ADP	C4-C5-N7	2.65	112.16	109.40
3	C	401	ADP	O3B-PB-O3A	2.64	113.50	104.64
3	A	401	ADP	PA-O3A-PB	2.59	141.70	132.83
3	C	401	ADP	O3B-PB-O1B	2.53	120.60	110.68
3	A	401	ADP	O3B-PB-O1B	2.40	120.09	110.68
3	C	401	ADP	PA-O3A-PB	2.36	140.91	132.83
3	A	401	ADP	O3B-PB-O2B	2.32	116.52	107.64
3	C	401	ADP	C4-C5-N7	2.31	111.81	109.40
3	B	401	ADP	O3B-PB-O1B	2.17	119.19	110.68
3	C	401	ADP	O2B-PB-O1B	-2.05	102.65	110.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

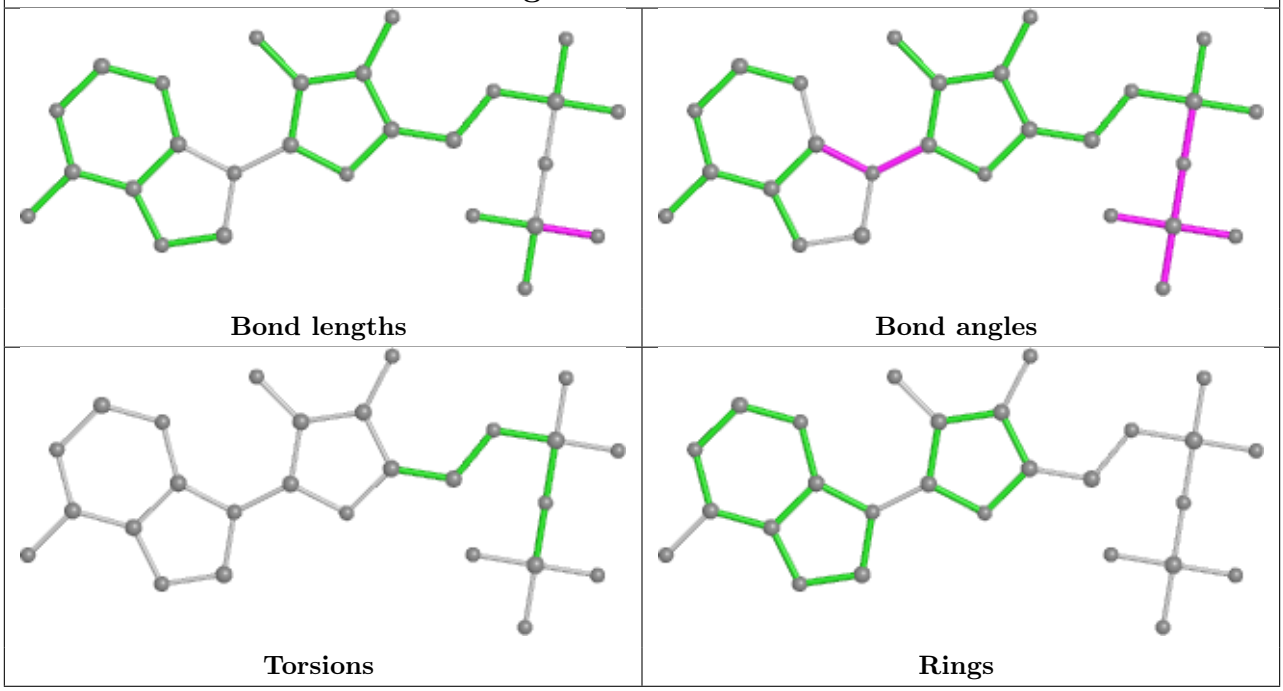
3 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	ADP	8	0
3	A	401	ADP	11	0
3	C	401	ADP	10	0

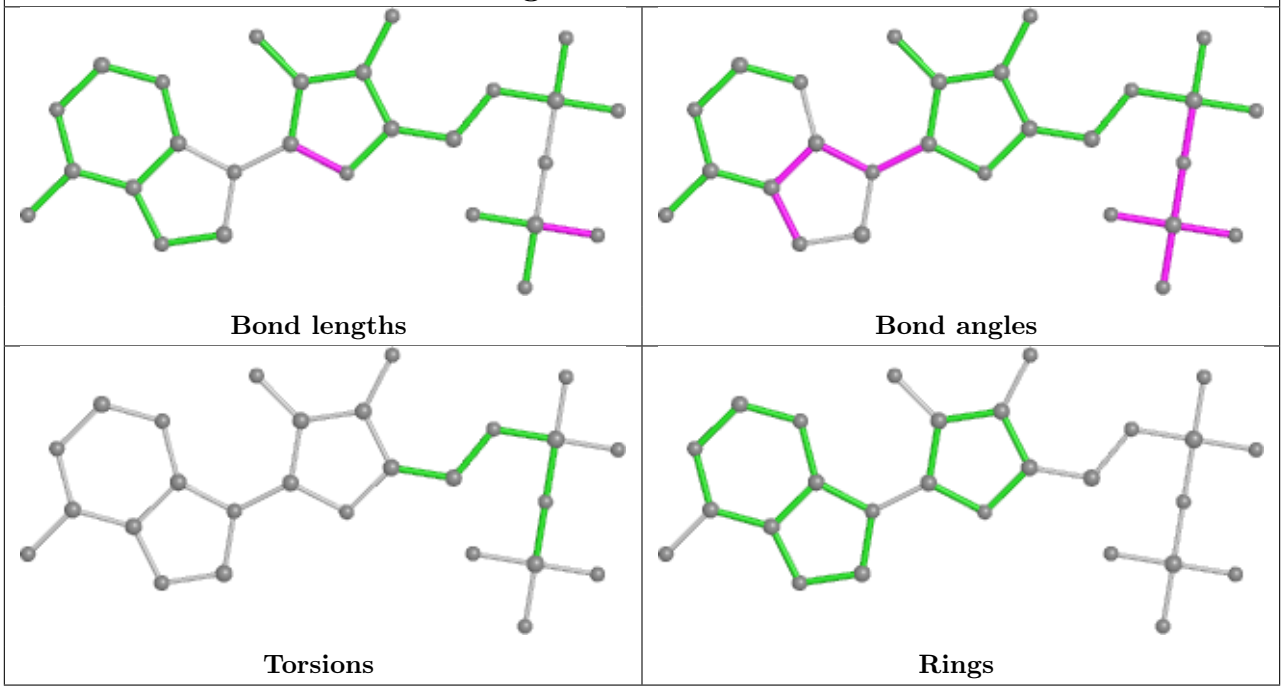
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

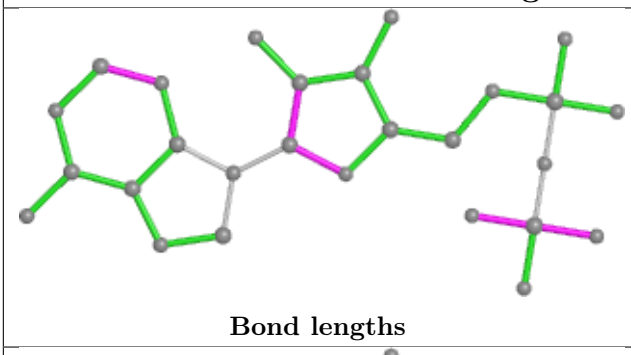
Ligand ADP B 401



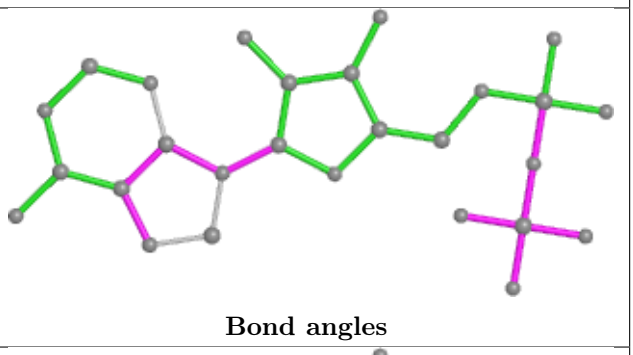
Ligand ADP A 401



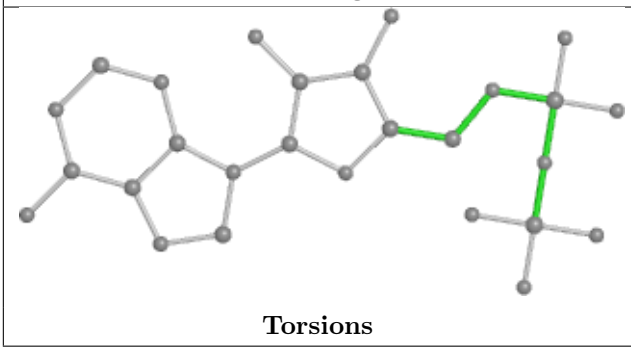
Ligand ADP C 401



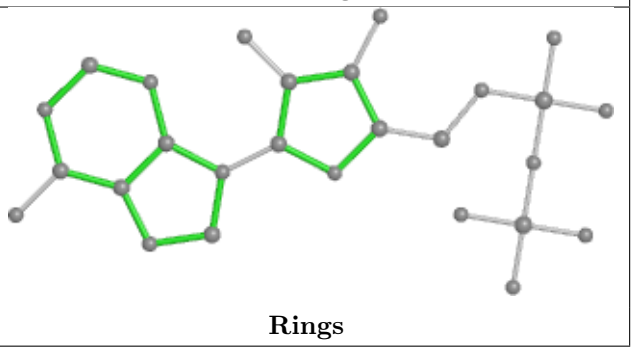
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	287/362 (79%)	0.31	21 (7%) 15 13	171, 343, 482, 756	0
1	B	280/362 (77%)	0.31	19 (6%) 17 14	141, 326, 486, 645	0
1	C	292/362 (80%)	0.41	18 (6%) 20 17	114, 314, 495, 758	0
2	D	30/46 (65%)	0.57	2 (6%) 17 15	303, 376, 577, 705	0
2	E	30/46 (65%)	-0.20	0 100 100	316, 405, 524, 567	0
All	All	919/1178 (78%)	0.33	60 (6%) 18 15	114, 334, 507, 758	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	318	ALA	10.5
1	C	317	CYS	7.0
1	B	4	THR	6.7
1	C	351	GLU	6.1
1	B	25	GLY	5.9
1	C	315	PRO	5.9
1	A	25	GLY	5.2
1	A	351	GLU	5.2
1	B	85	CYS	4.6
1	C	319	GLY	4.4
1	A	352	ASP	4.3
1	B	26	LYS	4.0
1	A	289	GLN	3.9
1	C	160	PHE	3.7
1	B	287	ARG	3.4
1	C	284	ASN	3.4
1	A	26	LYS	3.4
1	B	191	GLY	3.4
1	A	24	GLY	3.4
1	A	29	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	316	LEU	3.2
1	B	315	PRO	3.2
1	B	131	GLY	3.1
1	B	169	PRO	3.1
1	A	273	GLN	3.0
2	D	34	THR	3.0
1	B	190	PHE	3.0
1	A	346	VAL	3.0
1	A	317	CYS	2.9
1	C	83	LEU	2.7
1	C	350	LEU	2.7
1	B	307	GLU	2.7
1	C	162	THR	2.6
1	C	314	MET	2.5
1	B	132	SER	2.4
1	A	318	ALA	2.4
1	B	308	ASP	2.4
1	C	352	ASP	2.4
1	A	328	THR	2.4
1	B	5	VAL	2.3
1	A	237	THR	2.3
1	A	308	ASP	2.3
1	C	217	ASN	2.3
1	A	23	VAL	2.3
1	B	29	VAL	2.3
1	C	213	SER	2.3
1	C	283	HIS	2.3
1	B	272	ASN	2.2
1	A	39	ALA	2.2
1	B	84	SER	2.1
2	D	25	GLY	2.1
1	C	70	PHE	2.1
1	A	315	PRO	2.1
1	C	161	ASP	2.1
1	B	168	ALA	2.1
1	C	52	LEU	2.1
1	B	277	ALA	2.0
1	A	307	GLU	2.0
1	A	52	LEU	2.0
1	A	350	LEU	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)

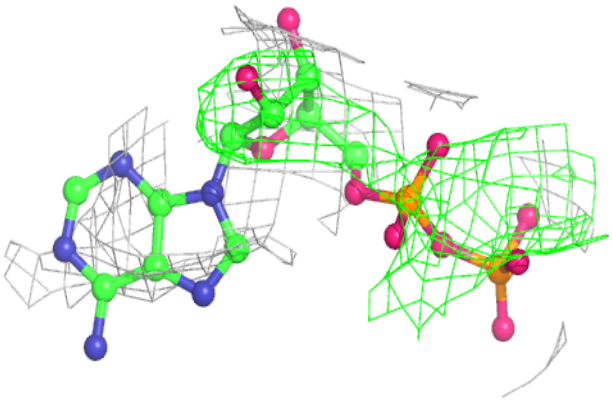
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

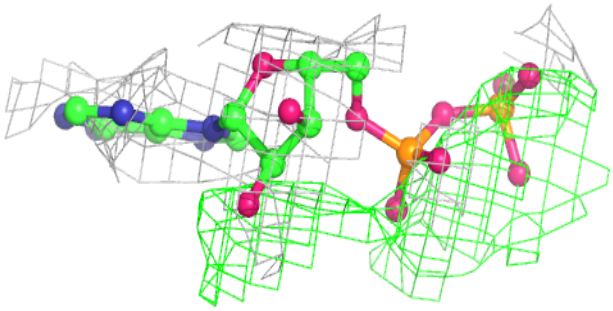
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	C	401	27/27	0.70	0.48	320,325,329,332	0
4	MG	A	402	1/1	0.70	0.28	297,297,297,297	0
3	ADP	A	401	27/27	0.74	0.37	322,328,331,331	0
3	ADP	B	401	27/27	0.82	0.45	333,342,351,356	0
5	ZN	B	363	1/1	0.88	0.14	368,368,368,368	0
4	MG	C	402	1/1	0.92	0.37	282,282,282,282	0
5	ZN	C	363	1/1	0.92	0.08	299,299,299,299	1
4	MG	B	402	1/1	0.93	0.33	246,246,246,246	0

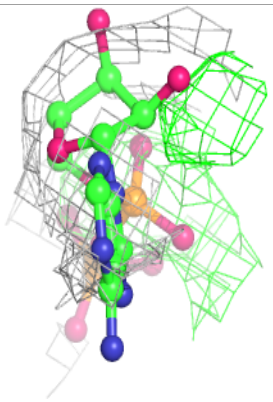
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP C 401:

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

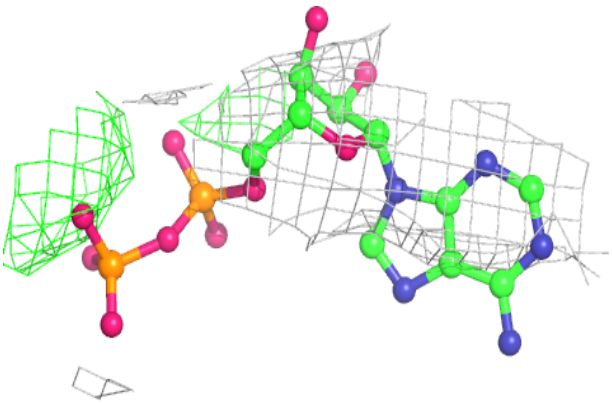


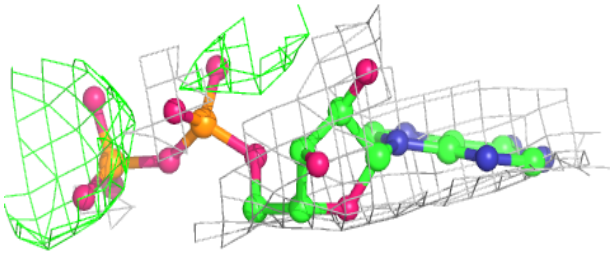


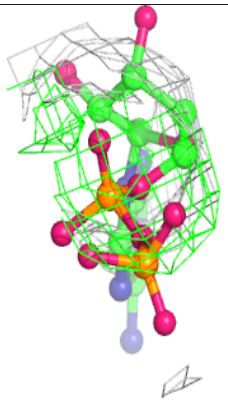


Electron density around ADP A 401:

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

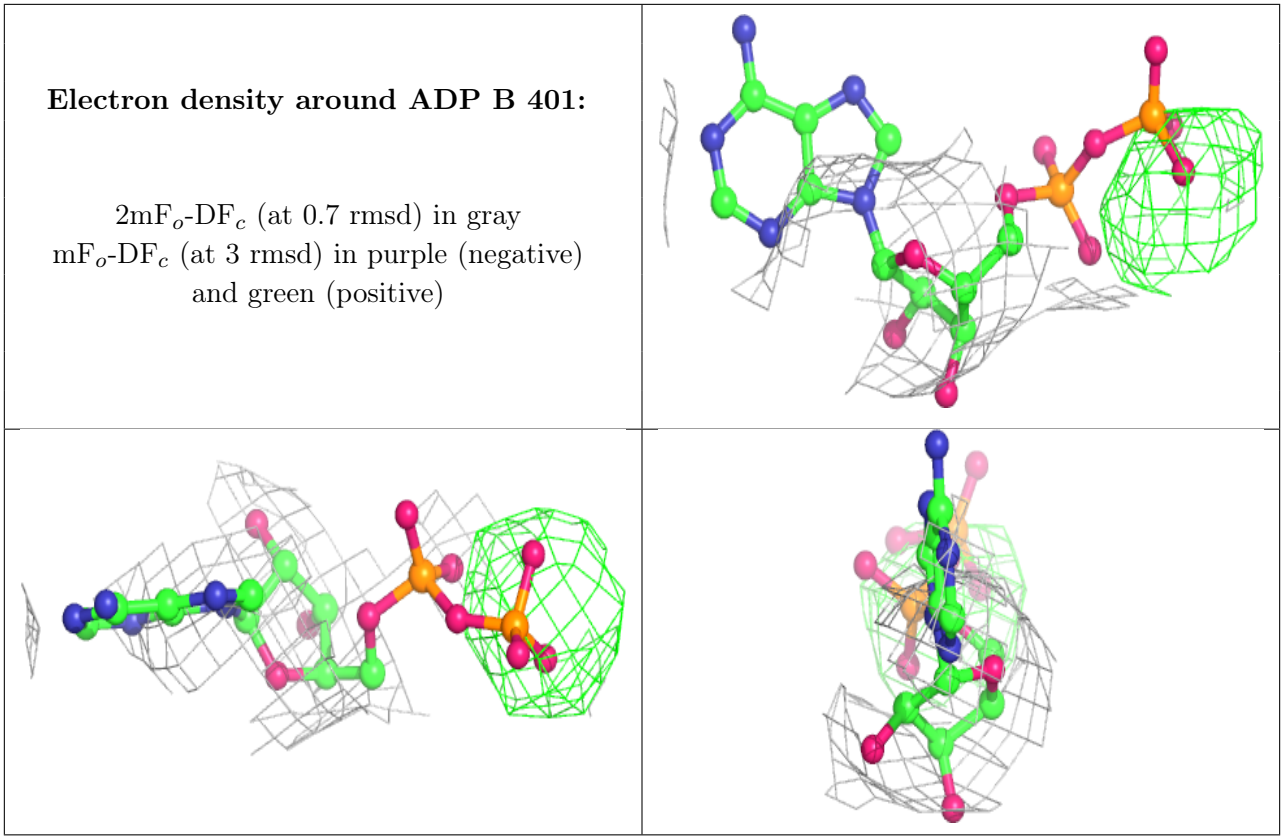






Electron density around ADP B 401:

$2mF_o$-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.