Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:53 am BST

PDB ID	:	1YYF
Title	:	Correction of X-ray Intensities from an HslV-HslU co-crystal containing lattice translocation defects
Authors	:	Wang, J.; Rho, S.H.; Park, H.H.; Eom, S.H.
Deposited on	:	2005-02-24
Resolution	:	4.16 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 following versions of software and data (see references ⓘ) were used in the production of this report:

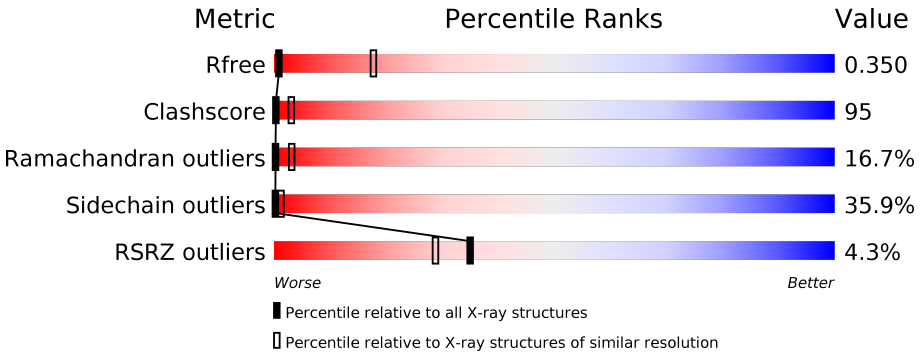
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 4.16 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	1020 (4.54-3.76)
Clashscore	141614	1028 (4.52-3.80)
Ramachandran outliers	138981	1005 (4.54-3.78)
Sidechain outliers	138945	1024 (4.54-3.76)
RSRZ outliers	127900	1055 (4.62-3.70)

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 on 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	443	9% 13% 38% 32% 9% 8%
1	B	443	3% 11% 40% 29% 12% 8%
2	C	181	19% 50% 25% 5%
2	D	181	20% 46% 30%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9215 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.

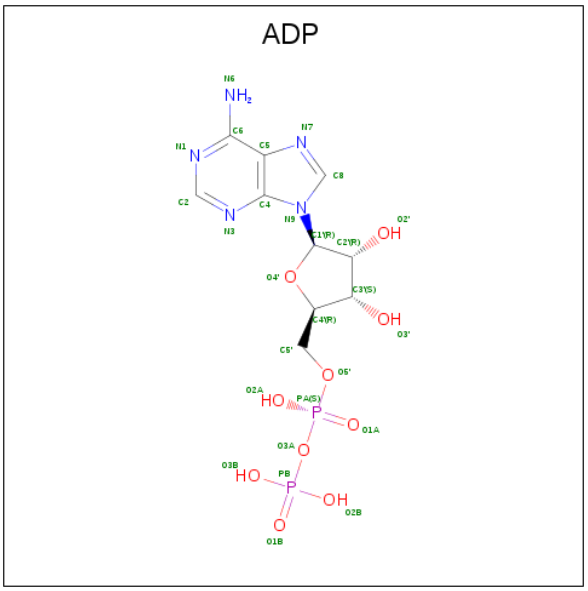
- Molecule 1 is a protein called ATP-dependent hsl protease ATP-binding subunit hslU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3222	2013	575	623	11			
1	B	408	Total	C	N	O	S	0	0	0
			3223	2013	575	624	11			

- Molecule 2 is a protein called ATP-dependent protease hslV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	180	Total	C	N	O	S	0	0	0
			1358	855	237	260	6			
2	C	180	Total	C	N	O	S	0	0	0
			1358	855	237	260	6			

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

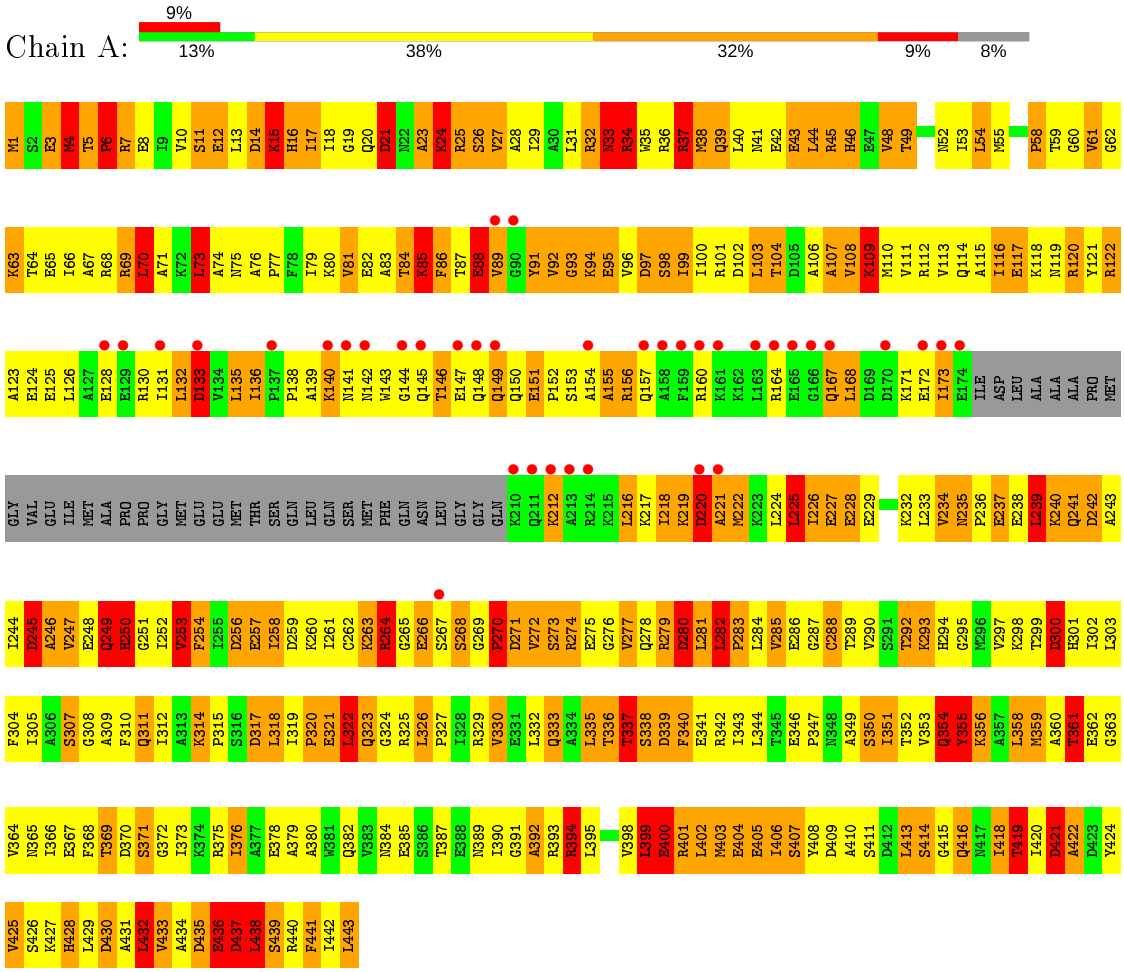


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

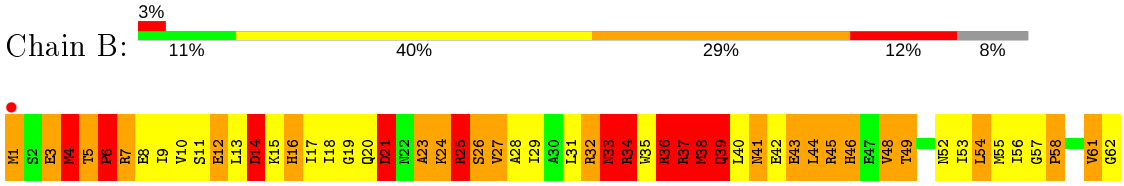
3 Residue-property plots (i)

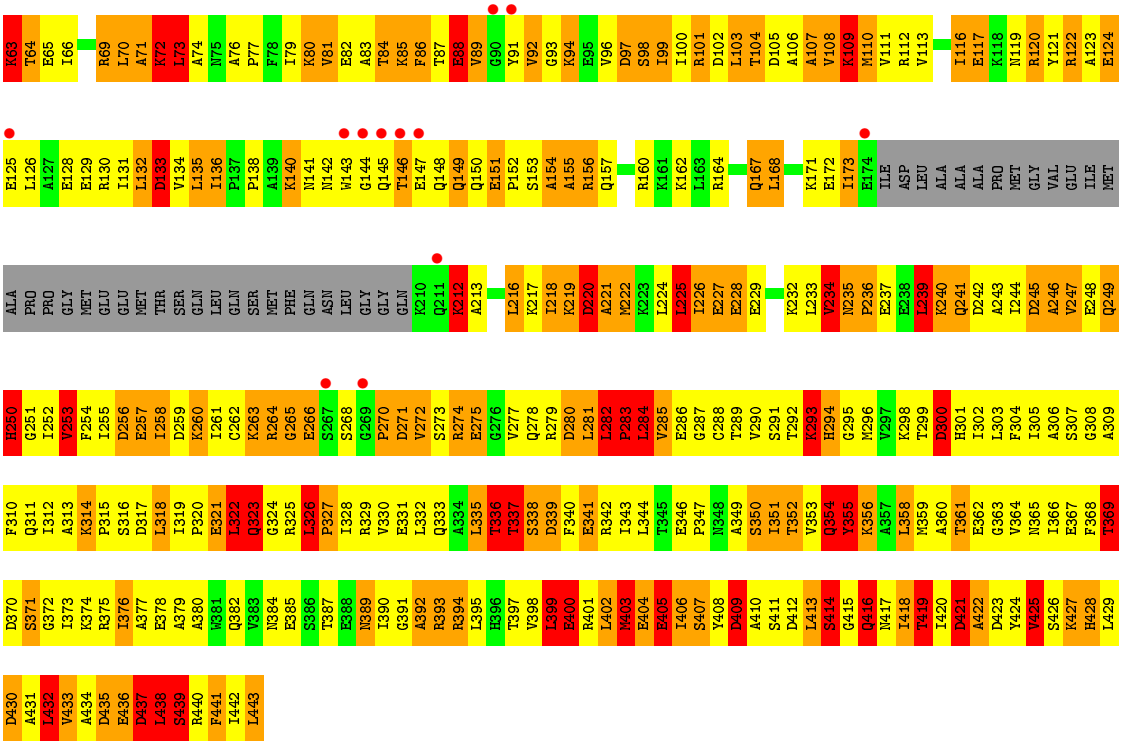
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: ATP-dependent hsl protease ATP-binding subunit hslU



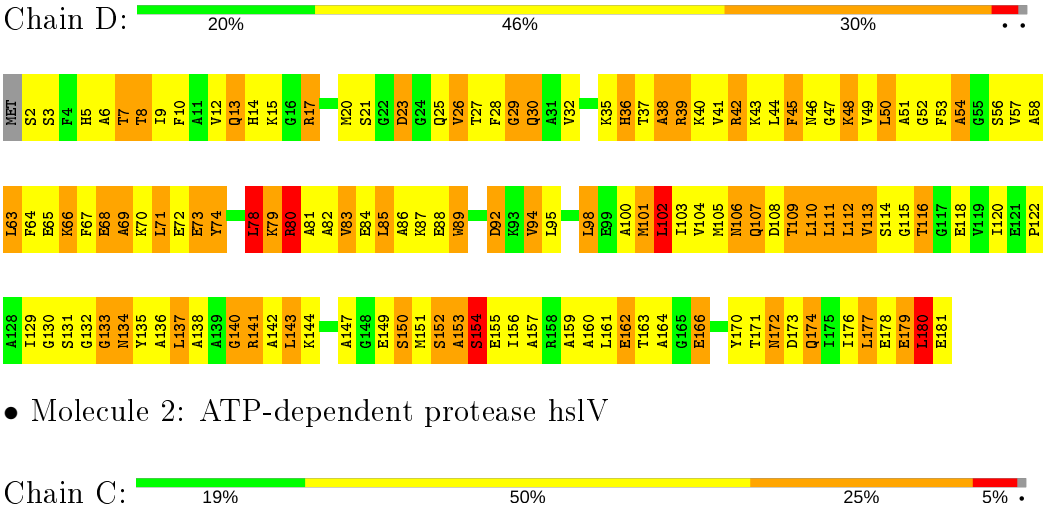
- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU





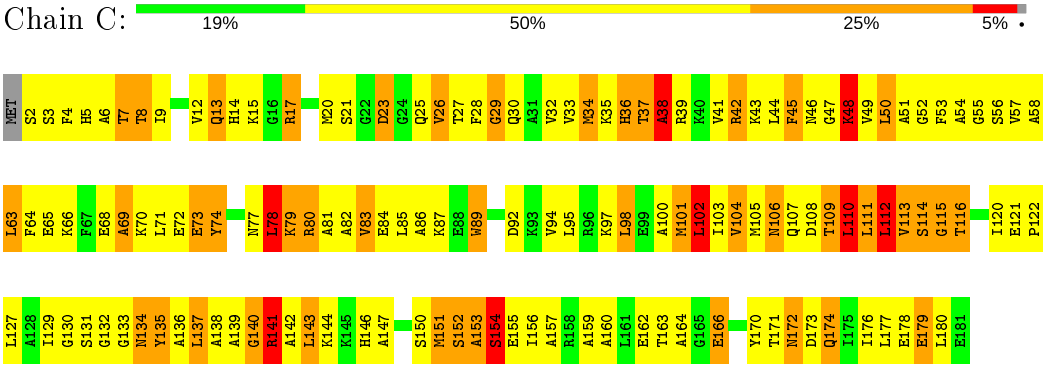
• Molecule 2: ATP-dependent protease hslV

Chain D:



• Molecule 2: ATP-dependent protease hslV

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	181.20Å 181.20Å 529.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.92 – 4.16 34.83 – 4.16	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.92-4.16) 99.5 (34.83-4.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 4.12Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.277 , 0.346 0.294 , 0.350	Depositor DCC
R_{free} test set	1299 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 57.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	9215	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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

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	1.32	18/3261 (0.6%)	1.44	45/4394 (1.0%)
1	B	1.32	18/3262 (0.6%)	1.45	46/4395 (1.0%)
2	C	1.62	17/1375 (1.2%)	1.47	20/1847 (1.1%)
2	D	1.60	16/1375 (1.2%)	1.48	15/1847 (0.8%)
All	All	1.41	69/9273 (0.7%)	1.45	126/12483 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	8
2	D	0	1
All	All	0	17

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321	GLU	CG-CD	8.74	1.65	1.51
1	A	1	MET	CG-SD	8.11	2.02	1.81
2	C	38	ALA	CA-CB	7.97	1.69	1.52
1	B	38	MET	SD-CE	7.72	2.21	1.77
1	B	1	MET	CG-SD	7.56	2.00	1.81
2	D	42	ARG	CG-CD	7.50	1.70	1.51
1	A	441	PHE	CB-CG	-7.35	1.38	1.51
1	A	355	TYR	CD2-CE2	7.27	1.50	1.39
1	B	405	GLU	CG-CD	7.20	1.62	1.51
2	C	42	ARG	CG-CD	7.17	1.69	1.51
2	C	61	PHE	CE1-CZ	7.16	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	355	TYR	CE2-CZ	6.98	1.47	1.38
1	A	38	MET	SD-CE	6.76	2.15	1.77
2	D	166	GLU	CD-OE1	6.76	1.33	1.25
1	B	355	TYR	CD2-CE2	6.67	1.49	1.39
2	D	40	LYS	CD-CE	6.64	1.67	1.51
2	C	34	MET	CG-SD	6.42	1.97	1.81
2	D	38	ALA	CA-CB	6.40	1.65	1.52
1	B	443	LEU	CG-CD1	-6.38	1.28	1.51
2	C	34	MET	SD-CE	6.29	2.13	1.77
2	D	61	PHE	CD1-CE1	6.19	1.51	1.39
2	C	42	ARG	NE-CZ	6.18	1.41	1.33
1	A	314	LYS	CB-CG	6.13	1.69	1.52
1	B	441	PHE	CB-CG	-6.13	1.41	1.51
2	D	61	PHE	CB-CG	6.09	1.61	1.51
1	A	89	VAL	CA-CB	6.06	1.67	1.54
2	D	61	PHE	CD2-CE2	6.04	1.51	1.39
2	C	38	ALA	CA-C	5.99	1.68	1.52
1	A	271	ASP	CB-CG	5.99	1.64	1.51
2	C	48	LYS	CD-CE	5.92	1.66	1.51
1	B	403	MET	SD-CE	5.90	2.10	1.77
1	A	400	GLU	CG-CD	5.90	1.60	1.51
2	C	79	LYS	CD-CE	5.90	1.66	1.51
2	C	166	GLU	CD-OE2	5.87	1.32	1.25
1	A	33	ASN	CB-CG	5.85	1.64	1.51
2	C	61	PHE	CD2-CE2	5.81	1.50	1.39
1	A	95	GLU	CG-CD	5.81	1.60	1.51
2	C	61	PHE	CG-CD2	5.78	1.47	1.38
1	B	33	ASN	CB-CG	5.78	1.64	1.51
1	B	234	VAL	CA-CB	5.77	1.66	1.54
1	B	110	MET	SD-CE	5.76	2.10	1.77
2	D	166	GLU	CD-OE2	5.74	1.31	1.25
1	A	355	TYR	CE2-CZ	5.73	1.46	1.38
1	B	404	GLU	CD-OE1	5.73	1.31	1.25
2	D	89	TRP	CB-CG	-5.65	1.40	1.50
1	B	367	GLU	CG-CD	5.63	1.60	1.51
1	B	309	ALA	CA-CB	-5.61	1.40	1.52
1	B	89	VAL	CA-CB	5.61	1.66	1.54
1	B	400	GLU	CG-CD	5.60	1.60	1.51
2	D	42	ARG	CB-CG	5.55	1.67	1.52
2	D	30	GLN	CB-CG	5.53	1.67	1.52
1	A	254	PHE	CB-CG	-5.53	1.42	1.51
2	C	151	MET	CG-SD	5.53	1.95	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	79	LYS	CD-CE	5.38	1.64	1.51
2	C	61	PHE	CD1-CE1	5.37	1.50	1.39
1	B	71	ALA	CA-CB	-5.35	1.41	1.52
1	A	405	GLU	CG-CD	5.33	1.59	1.51
2	C	42	ARG	CB-CG	5.32	1.67	1.52
2	D	162	GLU	CG-CD	5.29	1.59	1.51
2	D	30	GLN	CG-CD	5.27	1.63	1.51
2	C	89	TRP	CB-CG	-5.25	1.40	1.50
2	D	166	GLU	CG-CD	5.18	1.59	1.51
2	C	113	VAL	CA-CB	-5.13	1.44	1.54
1	A	249	GLN	CB-CG	5.08	1.66	1.52
1	A	367	GLU	CG-CD	5.05	1.59	1.51
2	D	61	PHE	CG-CD1	5.05	1.46	1.38
1	A	321	GLU	CG-CD	5.05	1.59	1.51
1	A	37	ARG	NE-CZ	5.01	1.39	1.33
1	A	419	THR	CA-CB	5.01	1.66	1.53

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	271	ASP	CB-CG-OD2	11.15	128.33	118.30
1	B	271	ASP	CB-CG-OD2	10.42	127.68	118.30
2	D	23	ASP	CB-CG-OD2	9.73	127.06	118.30
2	D	102	LEU	CB-CG-CD1	-9.57	94.73	111.00
2	D	173	ASP	CB-CG-OD2	9.37	126.73	118.30
1	A	438	LEU	CA-CB-CG	-8.92	94.78	115.30
2	C	23	ASP	CB-CG-OD2	8.67	126.10	118.30
1	A	21	ASP	CB-CG-OD2	8.64	126.08	118.30
1	B	256	ASP	CB-CG-OD2	8.46	125.91	118.30
1	B	326	LEU	CA-CB-CG	-8.29	96.24	115.30
1	B	21	ASP	CB-CG-OD2	8.25	125.73	118.30
1	A	330	VAL	CB-CA-C	-8.14	95.93	111.40
1	B	438	LEU	CA-CB-CG	-8.08	96.72	115.30
1	A	326	LEU	CA-CB-CG	-8.04	96.80	115.30
1	A	249	GLN	CB-CA-C	-8.02	94.35	110.40
2	D	59	ASP	CB-CG-OD2	7.68	125.22	118.30
2	C	50	LEU	CA-CB-CG	-7.56	97.92	115.30
1	A	73	LEU	CA-CB-CG	-7.40	98.28	115.30
1	A	437	ASP	CB-CG-OD2	7.36	124.92	118.30
1	A	326	LEU	CB-CG-CD1	-7.33	98.54	111.00
1	B	437	ASP	CB-CG-OD2	7.32	124.89	118.30
1	A	318	LEU	CA-CB-CG	-7.27	98.58	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	102	LEU	CB-CG-CD1	-7.25	98.68	111.00
1	B	409	ASP	CB-CG-OD2	7.19	124.77	118.30
1	A	401	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	B	73	LEU	CA-CB-CG	-7.13	98.89	115.30
1	A	320	PRO	N-CD-CG	-7.04	92.64	103.20
1	A	34	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	322	LEU	CB-CG-CD1	-6.98	99.14	111.00
1	B	443	LEU	CA-CB-CG	6.91	131.19	115.30
1	A	317	ASP	CB-CG-OD2	6.87	124.48	118.30
1	B	133	ASP	CB-CG-OD2	6.86	124.47	118.30
1	A	1	MET	CB-CG-SD	6.79	132.77	112.40
1	B	367	GLU	CA-CB-CG	6.70	128.13	113.40
2	C	173	ASP	CB-CG-OD2	6.66	124.30	118.30
1	B	355	TYR	CB-CG-CD1	-6.57	117.06	121.00
1	B	284	LEU	CA-CB-CG	-6.57	100.19	115.30
1	A	256	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	435	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	239	LEU	CA-CB-CG	6.49	130.23	115.30
1	B	318	LEU	CA-CB-CG	-6.48	100.39	115.30
2	C	143	LEU	CA-CB-CG	-6.42	100.54	115.30
1	A	432	LEU	N-CA-C	-6.42	93.68	111.00
1	A	399	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	B	37	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	C	42	ARG	NE-CZ-NH1	6.37	123.48	120.30
2	C	59	ASP	CB-CG-OD2	6.36	124.02	118.30
1	B	418	ILE	CB-CA-C	-6.35	98.90	111.60
1	B	1	MET	CB-CG-SD	6.33	131.39	112.40
2	D	141	ARG	NE-CZ-NH2	-6.28	117.16	120.30
2	C	114	SER	CB-CA-C	-6.25	98.23	110.10
2	C	66	LYS	CD-CE-NZ	6.23	126.02	111.70
2	C	141	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	339	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	394	ARG	CG-CD-NE	6.19	124.80	111.80
2	C	38	ALA	N-CA-C	6.15	127.59	111.00
1	B	220	ASP	CB-CG-OD2	6.14	123.82	118.30
1	B	327	PRO	N-CD-CG	-6.11	94.03	103.20
1	B	413	LEU	CA-CB-CG	-6.10	101.27	115.30
2	C	113	VAL	CB-CA-C	-6.10	99.81	111.40
1	A	242	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	216	LEU	CA-CB-CG	6.01	129.12	115.30
2	D	50	LEU	CA-CB-CG	-6.00	101.50	115.30
1	B	400	GLU	OE1-CD-OE2	-6.00	116.10	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	37	THR	N-CA-C	5.99	127.18	111.00
1	B	435	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	105	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	419	THR	N-CA-C	-5.91	95.04	111.00
1	B	239	LEU	CA-CB-CG	5.89	128.86	115.30
2	D	38	ALA	N-CA-C	5.87	126.84	111.00
1	B	421	ASP	CB-CG-OD2	5.86	123.58	118.30
2	D	39	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	72	LYS	CD-CE-NZ	5.83	125.10	111.70
2	D	80	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	419	THR	N-CA-C	-5.82	95.28	111.00
2	D	37	THR	N-CA-C	5.82	126.72	111.00
1	A	15	LYS	CB-CG-CD	5.79	126.65	111.60
2	D	40	LYS	CD-CE-NZ	5.77	124.96	111.70
1	B	36	ARG	CG-CD-NE	5.71	123.80	111.80
1	A	81	VAL	CB-CA-C	-5.67	100.62	111.40
2	D	180	LEU	CA-CB-CG	5.66	128.32	115.30
2	D	113	VAL	CB-CA-C	-5.65	100.67	111.40
1	A	34	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	D	85	LEU	CB-CG-CD2	-5.62	101.44	111.00
1	A	400	GLU	OE1-CD-OE2	-5.62	116.56	123.30
1	B	38	MET	CG-SD-CE	5.61	109.17	100.20
1	B	81	VAL	CB-CA-C	-5.57	100.81	111.40
1	B	34	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	245	ASP	CB-CG-OD2	5.46	123.21	118.30
1	B	432	LEU	N-CA-C	-5.45	96.30	111.00
1	B	423	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	133	ASP	CB-CG-OD2	5.39	123.15	118.30
2	C	123	ASP	CB-CG-OD2	5.38	123.15	118.30
2	C	112	LEU	CA-CB-CG	-5.37	102.95	115.30
1	A	70	LEU	CB-CG-CD1	5.34	120.08	111.00
1	A	220	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	216	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	418	ILE	CB-CA-C	-5.33	100.95	111.60
1	B	355	TYR	CA-CB-CG	-5.32	103.30	113.40
1	B	36	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	B	369	THR	CB-CA-C	-5.31	97.27	111.60
1	A	1	MET	CA-CB-CG	5.30	122.32	113.30
2	C	48	LYS	CD-CE-NZ	5.30	123.88	111.70
2	D	66	LYS	CD-CE-NZ	5.26	123.81	111.70
1	B	272	VAL	CB-CA-C	5.26	121.39	111.40
1	B	321	GLU	OE1-CD-OE2	-5.26	116.99	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	143	LEU	CB-CG-CD2	-5.25	102.07	111.00
1	A	97	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	370	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	253	VAL	CB-CA-C	-5.18	101.55	111.40
1	A	421	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	63	LYS	CD-CE-NZ	5.16	123.57	111.70
1	A	370	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	339	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	58	PRO	N-CD-CG	-5.13	95.50	103.20
1	B	322	LEU	CB-CG-CD2	-5.13	102.28	111.00
2	C	135	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	B	34	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	413	LEU	CA-CB-CG	-5.07	103.63	115.30
1	B	405	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	A	409	ASP	CB-CG-OD2	5.04	122.83	118.30
2	C	151	MET	CA-CB-CG	5.04	121.86	113.30
2	C	110	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	B	253	VAL	CB-CA-C	-5.03	101.85	111.40
1	A	340	PHE	CB-CA-C	-5.02	100.36	110.40
1	A	271	ASP	OD1-CG-OD2	-5.01	113.78	123.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ILE	Peptide
1	A	151	GLU	Peptide
1	A	219	LYS	Peptide
1	A	250	HIS	Peptide
1	A	262	CYS	Peptide
1	A	270	PRO	Peptide
1	A	33	ASN	Peptide
1	A	48	VAL	Peptide
1	B	116	ILE	Peptide
1	B	151	GLU	Peptide
1	B	219	LYS	Peptide
1	B	250	HIS	Peptide
1	B	262	CYS	Peptide
1	B	33	ASN	Peptide
1	B	336	THR	Peptide
1	B	48	VAL	Peptide
2	D	54	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3222	0	3296	638	1
1	B	3223	0	3296	687	1
2	C	1358	0	1374	220	0
2	D	1358	0	1374	235	0
3	A	27	0	12	5	0
3	B	27	0	12	8	0
All	All	9215	0	9364	1757	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 95.

All (1757) 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:168:LEU:HD12	1:B:219:LYS:CE	1.16	1.55
1:A:168:LEU:HD12	1:A:219:LYS:CE	1.16	1.53
1:A:100:ILE:CD1	1:A:284:LEU:HD22	1.31	1.52
1:B:258:ILE:CD1	1:B:306:ALA:CB	1.90	1.49
1:B:258:ILE:CD1	1:B:306:ALA:HB1	1.05	1.49
1:A:1:MET:SD	1:A:1:MET:CG	2.02	1.46
1:B:1:MET:CE	1:B:1:MET:SD	2.04	1.46
1:A:100:ILE:HD11	1:A:284:LEU:CD2	1.47	1.45
1:A:282:LEU:HB3	1:A:283:PRO:CD	1.41	1.45
1:A:135:LEU:HD23	1:A:171:LYS:CE	1.46	1.44
1:A:168:LEU:CD1	1:A:219:LYS:CE	1.96	1.43
1:B:258:ILE:HD11	1:B:306:ALA:CB	1.46	1.43
1:B:135:LEU:HD23	1:B:171:LYS:CE	1.49	1.42
1:A:167:GLN:OE1	1:A:219:LYS:CE	1.65	1.41
1:B:110:MET:SD	1:B:110:MET:CE	2.10	1.40
1:B:168:LEU:CD1	1:B:219:LYS:CE	1.99	1.39
1:B:403:MET:SD	1:B:403:MET:CE	2.10	1.38
2:C:34:MET:CE	2:C:34:MET:SD	2.13	1.36
1:A:38:MET:CE	1:A:38:MET:SD	2.15	1.34
1:B:135:LEU:CG	1:B:171:LYS:NZ	1.91	1.30
1:B:38:MET:CE	1:B:38:MET:SD	2.21	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:HD12	1:A:219:LYS:CD	1.62	1.27
1:B:403:MET:CE	1:B:420:ILE:HD13	1.64	1.27
1:A:100:ILE:CD1	1:A:284:LEU:CD2	2.03	1.27
1:A:168:LEU:CD1	1:A:219:LYS:HE3	1.58	1.26
1:A:292:THR:HG23	1:A:295:GLY:O	1.28	1.26
2:D:106:ASN:ND2	2:D:109:THR:H	1.33	1.25
1:B:168:LEU:HD12	1:B:219:LYS:CD	1.68	1.23
2:C:106:ASN:ND2	2:C:109:THR:H	1.36	1.22
2:D:9:ILE:CD1	2:D:53:PHE:O	1.87	1.22
1:B:135:LEU:CG	1:B:171:LYS:HZ2	1.53	1.21
1:A:359:MET:CG	1:A:366:ILE:HD11	1.71	1.20
1:B:168:LEU:CD1	1:B:219:LYS:HE3	1.61	1.19
1:B:83:ALA:HB1	1:B:261:ILE:CD1	1.73	1.17
2:D:20:MET:HE2	2:D:41:VAL:HG13	1.18	1.17
1:A:282:LEU:CB	1:A:283:PRO:HD2	1.70	1.17
1:A:403:MET:CE	1:A:420:ILE:HD13	1.74	1.17
1:A:135:LEU:HD22	1:A:171:LYS:NZ	1.49	1.15
1:B:32:ARG:HG2	1:B:36:ARG:HE	1.05	1.15
1:A:135:LEU:CG	1:A:171:LYS:NZ	2.07	1.15
1:A:282:LEU:CB	1:A:283:PRO:CD	2.21	1.15
2:D:23:ASP:HB2	2:D:172:ASN:ND2	1.62	1.14
1:B:237:GLU:H	1:B:240:LYS:CE	1.60	1.14
1:B:359:MET:HG2	1:B:366:ILE:CD1	1.78	1.13
2:D:20:MET:CE	2:D:41:VAL:HG13	1.77	1.13
1:A:390:ILE:HD12	1:A:394:ARG:HH12	1.07	1.13
2:C:20:MET:CE	2:C:41:VAL:HG13	1.78	1.13
1:B:243:ALA:O	1:B:246:ALA:HB3	1.48	1.12
1:B:122:ARG:NH2	1:B:126:LEU:HD11	1.63	1.12
1:A:168:LEU:CD1	1:A:219:LYS:CD	2.25	1.11
2:C:23:ASP:HB2	2:C:172:ASN:ND2	1.64	1.11
1:A:359:MET:CG	1:A:366:ILE:CD1	2.29	1.11
1:A:83:ALA:HB1	1:A:261:ILE:HD11	1.22	1.10
1:A:335:LEU:CD1	1:A:335:LEU:H	1.57	1.10
1:A:167:GLN:OE1	1:A:219:LYS:HE2	0.91	1.09
1:B:401:ARG:HH21	1:B:442:ILE:CG2	1.66	1.08
2:C:57:VAL:HA	2:C:60:ALA:HB3	1.30	1.08
1:B:256:ASP:O	1:B:257:GLU:HB2	1.47	1.07
1:B:335:LEU:H	1:B:335:LEU:HD12	1.02	1.07
1:A:335:LEU:HD12	1:A:335:LEU:N	1.64	1.07
1:B:135:LEU:HD22	1:B:171:LYS:NZ	1.64	1.07
1:A:122:ARG:NH2	1:A:126:LEU:HD11	1.68	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:GLU:N	1:B:240:LYS:HE3	1.71	1.06
1:A:116:ILE:HG22	1:A:116:ILE:O	1.50	1.06
1:B:288:CYS:SG	1:B:299:THR:HG21	1.95	1.06
1:B:403:MET:HE3	1:B:420:ILE:HD13	1.33	1.06
2:D:17:ARG:HG2	2:D:17:ARG:HH11	0.97	1.06
1:B:100:ILE:HD12	1:B:290:VAL:HG21	1.32	1.06
1:B:442:ILE:O	1:B:442:ILE:HG22	1.56	1.06
1:A:282:LEU:HB3	1:A:283:PRO:HD3	1.35	1.06
1:A:442:ILE:HG22	1:A:442:ILE:O	1.46	1.06
2:C:17:ARG:HH11	2:C:17:ARG:HG2	1.07	1.06
1:B:100:ILE:HD11	1:B:284:LEU:CD2	1.85	1.06
1:A:32:ARG:HG2	1:A:36:ARG:HE	1.21	1.05
1:A:359:MET:HG2	1:A:366:ILE:CD1	1.85	1.05
1:B:168:LEU:CD1	1:B:219:LYS:CD	2.31	1.05
1:B:130:ARG:HD3	1:B:225:LEU:HD11	1.34	1.05
1:B:322:LEU:HD12	1:B:326:LEU:CD1	1.87	1.05
1:B:390:ILE:HD12	1:B:394:ARG:NH1	1.71	1.05
1:A:247:VAL:O	1:A:250:HIS:HA	1.57	1.05
1:B:403:MET:CE	1:B:420:ILE:CD1	2.34	1.05
1:B:390:ILE:HD12	1:B:394:ARG:HH12	0.92	1.04
1:B:239:LEU:HD13	1:B:240:LYS:HD3	1.32	1.04
2:C:80:ARG:HH11	2:C:80:ARG:HG2	1.18	1.04
1:B:83:ALA:HB1	1:B:261:ILE:HD11	1.05	1.04
1:B:258:ILE:HD12	1:B:306:ALA:CB	1.72	1.04
1:B:237:GLU:H	1:B:240:LYS:HE3	0.87	1.04
1:A:438:LEU:HD21	1:A:442:ILE:HD12	1.35	1.04
1:B:282:LEU:HB3	1:B:283:PRO:HD3	1.37	1.03
1:A:168:LEU:CD1	1:A:219:LYS:HD2	1.85	1.03
1:A:5:THR:HG23	1:A:8:GLU:HG3	1.41	1.03
2:C:12:VAL:HG23	2:C:126:ILE:HG12	1.37	1.03
1:B:359:MET:CG	1:B:366:ILE:CD1	2.36	1.02
1:A:168:LEU:HD11	1:A:219:LYS:HD2	1.41	1.02
1:A:282:LEU:HB3	1:A:283:PRO:HD2	1.28	1.02
2:D:20:MET:HE1	2:D:51:ALA:C	1.80	1.02
1:B:258:ILE:HD11	1:B:306:ALA:HB2	1.35	1.01
1:A:361:THR:HG21	1:B:36:ARG:HG3	1.39	1.01
1:A:108:VAL:C	1:A:110:MET:H	1.58	1.01
1:B:282:LEU:HB3	1:B:283:PRO:CD	1.87	1.01
1:B:359:MET:CG	1:B:366:ILE:HD11	1.90	1.01
1:A:392:ALA:O	1:A:395:LEU:HD12	1.61	1.01
1:A:261:ILE:HD13	1:A:277:VAL:CG1	1.91	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ILE:HG22	1:B:135:LEU:HD11	1.43	1.00
2:C:12:VAL:CG2	2:C:126:ILE:HG12	1.90	1.00
1:B:168:LEU:CD1	1:B:219:LYS:HD2	1.90	1.00
1:B:86:PHE:HD2	1:B:96:VAL:HG12	1.23	0.99
1:B:3:GLU:O	1:B:4:MET:HB2	1.63	0.99
1:A:359:MET:HG3	1:A:366:ILE:HD11	1.41	0.99
2:C:20:MET:HE2	2:C:41:VAL:HG13	1.45	0.99
2:D:57:VAL:HA	2:D:60:ALA:HB3	1.44	0.99
1:A:100:ILE:HD12	1:A:284:LEU:CD2	1.90	0.99
1:B:18:ILE:HD12	1:B:343:ILE:CA	1.93	0.99
2:C:172:ASN:H	2:C:172:ASN:HD22	1.12	0.98
1:B:268:SER:CB	1:B:312:ILE:HG21	1.93	0.98
1:A:83:ALA:HB1	1:A:261:ILE:CD1	1.93	0.98
1:A:292:THR:CG2	1:A:295:GLY:O	2.10	0.98
1:A:61:VAL:HB	1:A:335:LEU:HD11	1.45	0.98
1:A:108:VAL:HG12	1:A:109:LYS:H	1.28	0.98
2:D:12:VAL:CG2	2:D:126:ILE:HG12	1.93	0.98
2:D:23:ASP:HB2	2:D:172:ASN:HD21	1.23	0.98
1:A:167:GLN:OE1	1:A:219:LYS:CD	2.11	0.97
1:A:130:ARG:HD3	1:A:225:LEU:HD11	1.43	0.97
2:D:80:ARG:HH11	2:D:80:ARG:HG2	1.26	0.97
1:B:392:ALA:O	1:B:395:LEU:HD12	1.64	0.97
1:A:261:ILE:HG21	1:A:277:VAL:HG12	1.46	0.97
1:A:237:GLU:H	1:A:240:LYS:HE3	1.27	0.97
2:C:78:LEU:HD23	2:C:111:LEU:HD22	1.45	0.97
2:D:106:ASN:HD21	2:D:109:THR:H	1.08	0.97
2:C:106:ASN:HD21	2:C:109:THR:H	1.03	0.96
2:C:103:ILE:HG13	2:C:129:ILE:CD1	1.94	0.96
2:C:103:ILE:HG13	2:C:129:ILE:HD12	1.46	0.96
1:A:261:ILE:HD13	1:A:277:VAL:HG11	1.45	0.96
1:A:168:LEU:CD1	1:A:219:LYS:NZ	2.28	0.96
2:C:9:ILE:CD1	2:C:53:PHE:O	2.14	0.96
1:B:168:LEU:CD1	1:B:219:LYS:NZ	2.28	0.96
2:C:110:LEU:C	2:C:111:LEU:HD13	1.86	0.95
1:A:268:SER:HB3	1:A:312:ILE:HG21	1.44	0.95
1:B:135:LEU:CD2	1:B:171:LYS:NZ	0.80	0.95
1:A:86:PHE:HD2	1:A:96:VAL:HG12	1.30	0.95
2:C:20:MET:HE3	2:C:41:VAL:HG13	1.46	0.95
1:A:135:LEU:CG	1:A:171:LYS:HZ2	1.71	0.95
1:A:18:ILE:CD1	1:A:342:ARG:C	2.35	0.95
1:B:322:LEU:CD1	1:B:326:LEU:CD1	2.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ILE:CD1	1:B:343:ILE:N	2.30	0.94
1:B:32:ARG:HG2	1:B:36:ARG:NE	1.82	0.94
1:B:369:THR:HB	1:B:371:SER:H	1.31	0.94
1:A:335:LEU:HD12	1:A:335:LEU:H	0.78	0.94
1:A:18:ILE:CD1	1:A:343:ILE:N	2.31	0.94
1:B:61:VAL:HB	1:B:335:LEU:HD11	1.47	0.94
1:A:403:MET:HE3	1:A:420:ILE:HD13	1.49	0.94
1:B:76:ALA:HB1	1:B:251:GLY:HA2	1.50	0.94
1:B:27:VAL:HG23	1:B:70:LEU:CD2	1.97	0.94
1:B:314:LYS:O	1:B:317:ASP:HB2	1.66	0.93
1:B:349:ALA:O	1:B:350:SER:O	1.86	0.93
1:A:76:ALA:HB1	1:A:251:GLY:HA2	1.48	0.93
1:B:261:ILE:HG22	1:B:261:ILE:O	1.68	0.93
2:C:23:ASP:HB2	2:C:172:ASN:HD21	1.30	0.93
1:A:18:ILE:HD13	1:A:342:ARG:HB2	1.51	0.93
3:B:906:ADP:H8	3:B:906:ADP:H5'1	1.32	0.93
2:C:78:LEU:HD23	2:C:111:LEU:CD2	1.97	0.93
2:C:101:MET:HB3	2:C:112:LEU:HD21	1.50	0.93
1:B:52:ASN:OD1	1:B:304:PHE:HB2	1.68	0.93
1:A:361:THR:CG2	1:B:36:ARG:HG3	1.99	0.93
2:C:108:ASP:HB3	2:C:109:THR:HG22	1.50	0.93
1:A:256:ASP:O	1:A:257:GLU:HB2	1.67	0.92
1:B:401:ARG:HH21	1:B:442:ILE:HG21	1.34	0.92
2:C:106:ASN:HD21	2:C:109:THR:N	1.68	0.92
1:A:310:PHE:HE1	1:A:315:PRO:HA	1.33	0.92
2:D:17:ARG:CG	2:D:17:ARG:HH11	1.81	0.92
1:A:27:VAL:HG23	1:A:70:LEU:CD2	2.00	0.92
1:A:135:LEU:CD2	1:A:171:LYS:NZ	0.78	0.92
2:D:110:LEU:C	2:D:111:LEU:HD13	1.88	0.92
1:A:431:ALA:HA	1:A:434:ALA:CB	2.00	0.92
1:B:322:LEU:CD1	1:B:326:LEU:HD11	1.99	0.92
2:D:106:ASN:ND2	2:D:109:THR:N	2.17	0.92
1:A:119:ASN:HD22	1:A:122:ARG:HG2	1.36	0.91
1:A:261:ILE:HG22	1:A:261:ILE:O	1.65	0.91
1:B:168:LEU:HD11	1:B:219:LYS:HD2	1.47	0.91
1:B:83:ALA:CB	1:B:261:ILE:HD11	1.96	0.91
1:B:18:ILE:CD1	1:B:343:ILE:HA	2.00	0.91
1:B:401:ARG:NH2	1:B:442:ILE:HG21	1.83	0.91
2:D:9:ILE:HD11	2:D:53:PHE:O	1.67	0.91
1:B:335:LEU:H	1:B:335:LEU:CD1	1.77	0.91
2:C:20:MET:HE1	2:C:51:ALA:C	1.91	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:56:SER:O	2:C:60:ALA:N	2.04	0.91
2:D:50:LEU:HG	2:D:180:LEU:CD2	2.01	0.91
1:A:359:MET:CB	1:A:366:ILE:HD12	2.00	0.90
1:B:235:ASN:N	1:B:236:PRO:HD3	1.85	0.90
1:B:403:MET:HE1	1:B:420:ILE:HD13	1.53	0.90
1:B:100:ILE:HD11	1:B:284:LEU:HD21	1.52	0.90
1:B:235:ASN:O	1:B:239:LEU:CD1	2.20	0.90
1:A:100:ILE:HD13	1:A:299:THR:HG22	1.54	0.90
1:A:131:ILE:HG22	1:A:135:LEU:HD11	1.54	0.90
1:A:325:ARG:O	1:A:327:PRO:HD2	1.71	0.90
1:A:20:GLN:HE22	1:A:332:LEU:HA	1.35	0.90
1:B:261:ILE:HG21	1:B:277:VAL:HG12	1.52	0.90
2:C:61:PHE:O	2:C:64:PHE:HB2	1.72	0.90
1:B:391:GLY:C	1:B:393:ARG:H	1.74	0.90
1:A:390:ILE:HD12	1:A:394:ARG:NH1	1.86	0.89
1:B:282:LEU:CB	1:B:283:PRO:CD	2.48	0.89
1:B:335:LEU:HD12	1:B:335:LEU:N	1.87	0.89
2:C:106:ASN:ND2	2:C:109:THR:N	2.20	0.89
2:D:12:VAL:HG23	2:D:126:ILE:HG12	1.54	0.89
1:B:100:ILE:CD1	1:B:290:VAL:HG21	2.03	0.89
1:A:235:ASN:N	1:A:236:PRO:HD3	1.87	0.89
1:A:86:PHE:CE2	1:A:96:VAL:HA	2.07	0.89
2:C:17:ARG:HH11	2:C:17:ARG:CG	1.86	0.89
1:B:108:VAL:C	1:B:110:MET:H	1.72	0.88
1:B:135:LEU:CD2	1:B:171:LYS:CE	2.25	0.88
2:C:152:SER:O	2:C:156:ILE:HG13	1.73	0.88
2:D:129:ILE:HG22	2:D:130:GLY:N	1.87	0.88
1:A:3:GLU:O	1:A:4:MET:HB2	1.73	0.88
1:A:401:ARG:HH21	1:A:442:ILE:CG2	1.86	0.88
2:D:17:ARG:HG2	2:D:17:ARG:NH1	1.76	0.88
1:A:108:VAL:C	1:A:110:MET:N	2.24	0.88
1:B:73:LEU:HG	1:B:74:ALA:N	1.88	0.88
2:D:26:VAL:HG12	2:D:35:LYS:H	1.38	0.88
1:B:258:ILE:HD11	1:B:306:ALA:HB1	1.08	0.87
1:A:282:LEU:HB2	1:A:283:PRO:HD2	1.54	0.87
1:B:431:ALA:HA	1:B:434:ALA:CB	2.04	0.87
1:A:27:VAL:HG23	1:A:70:LEU:HD23	1.55	0.87
2:D:61:PHE:O	2:D:64:PHE:HB2	1.75	0.87
1:A:268:SER:CB	1:A:312:ILE:HG21	2.02	0.87
1:A:441:PHE:HD1	1:B:56:ILE:HD13	1.35	0.87
1:A:442:ILE:CG2	1:A:442:ILE:O	2.20	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ALA:HA	1:A:434:ALA:HB2	1.57	0.87
3:B:906:ADP:C8	3:B:906:ADP:H5'1	2.10	0.86
1:A:135:LEU:HD22	1:A:171:LYS:HZ1	1.16	0.86
1:B:18:ILE:CD1	1:B:343:ILE:CA	2.53	0.86
2:D:106:ASN:HD21	2:D:109:THR:N	1.71	0.86
1:A:391:GLY:C	1:A:393:ARG:H	1.75	0.86
1:B:18:ILE:CD1	1:B:342:ARG:C	2.43	0.86
1:A:438:LEU:CD2	1:A:442:ILE:HD12	2.05	0.86
1:B:268:SER:HB3	1:B:312:ILE:CG2	2.06	0.86
1:B:442:ILE:O	1:B:442:ILE:CG2	2.24	0.86
1:A:355:TYR:O	1:A:356:LYS:O	1.94	0.86
1:A:100:ILE:HD12	1:A:284:LEU:HD21	1.58	0.86
1:B:135:LEU:HG	1:B:171:LYS:HZ2	1.37	0.86
1:B:5:THR:HG23	1:B:8:GLU:HG3	1.56	0.86
1:A:268:SER:HB3	1:A:312:ILE:CG2	2.04	0.85
1:A:18:ILE:HD11	1:A:342:ARG:O	1.75	0.85
1:B:130:ARG:HD3	1:B:225:LEU:CD1	2.06	0.85
2:C:26:VAL:HG12	2:C:35:LYS:H	1.38	0.85
1:B:20:GLN:HE22	1:B:332:LEU:HA	1.40	0.85
2:D:172:ASN:HD22	2:D:172:ASN:H	1.19	0.85
1:B:86:PHE:CD2	1:B:96:VAL:HG12	2.10	0.85
1:A:355:TYR:O	1:A:356:LYS:C	2.15	0.85
1:A:403:MET:CE	1:A:420:ILE:CD1	2.54	0.85
1:B:336:THR:H	1:B:339:ASP:HB2	1.41	0.85
1:B:359:MET:CB	1:B:366:ILE:HD12	2.06	0.85
1:A:425:VAL:HG12	1:A:426:SER:N	1.90	0.85
1:A:86:PHE:HD1	1:A:86:PHE:N	1.74	0.85
1:A:79:ILE:HD11	1:A:102:ASP:O	1.75	0.85
1:B:135:LEU:CD2	1:B:171:LYS:HZ1	0.80	0.84
1:B:399:LEU:O	1:B:401:ARG:N	2.08	0.84
2:C:25:GLN:OE1	2:C:172:ASN:HB3	1.77	0.84
1:A:108:VAL:O	1:A:110:MET:N	2.10	0.84
1:B:243:ALA:O	1:B:246:ALA:CB	2.24	0.84
1:B:401:ARG:NH2	1:B:442:ILE:CG2	2.40	0.84
1:A:275:GLU:HG3	1:A:319:ILE:HD11	1.57	0.84
2:D:110:LEU:O	2:D:111:LEU:HD13	1.78	0.84
1:A:359:MET:HB3	1:A:366:ILE:HD12	1.58	0.84
1:A:399:LEU:O	1:A:401:ARG:N	2.09	0.84
1:A:100:ILE:HD13	1:A:299:THR:CG2	2.07	0.84
1:A:243:ALA:O	1:A:246:ALA:HB3	1.77	0.84
1:B:6:PRO:HD3	1:B:32:ARG:HD2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:MET:HG2	1:B:366:ILE:HD11	1.52	0.84
1:A:403:MET:HE1	1:A:420:ILE:HD13	1.58	0.83
1:B:13:LEU:O	1:B:15:LYS:N	2.11	0.83
1:B:355:TYR:O	1:B:356:LYS:C	2.16	0.83
2:C:112:LEU:HD23	2:C:113:VAL:H	1.39	0.83
1:B:350:SER:HB3	1:B:353:VAL:HG23	1.60	0.83
1:B:100:ILE:CD1	1:B:284:LEU:HD21	2.08	0.83
1:A:349:ALA:O	1:A:350:SER:O	1.97	0.83
1:A:153:SER:HB3	1:A:157:GLN:HB2	1.61	0.83
1:A:310:PHE:HE1	1:A:315:PRO:CA	1.91	0.83
1:A:18:ILE:HD11	1:A:342:ARG:C	1.99	0.83
1:A:18:ILE:HD12	1:A:343:ILE:N	1.93	0.82
2:C:110:LEU:O	2:C:111:LEU:HD13	1.78	0.82
2:C:17:ARG:NH1	2:C:17:ARG:HG2	1.86	0.82
2:C:72:GLU:O	2:C:74:TYR:N	2.12	0.82
1:A:135:LEU:HD21	1:A:171:LYS:NZ	1.15	0.82
1:A:298:LYS:HG2	1:A:300:ASP:HB2	1.61	0.82
1:B:6:PRO:CD	1:B:32:ARG:HD2	2.10	0.82
1:A:369:THR:HB	1:A:371:SER:H	1.45	0.82
1:B:70:LEU:C	1:B:70:LEU:HD12	2.00	0.82
1:B:153:SER:HB3	1:B:157:GLN:HB2	1.62	0.82
1:A:413:LEU:N	1:A:413:LEU:HD23	1.93	0.81
1:B:220:ASP:N	1:B:220:ASP:OD1	2.09	0.81
2:D:20:MET:HE2	2:D:41:VAL:CG1	2.08	0.81
2:C:25:GLN:HB2	2:C:172:ASN:CG	2.01	0.81
1:A:108:VAL:HG12	1:A:109:LYS:N	1.94	0.81
1:A:253:VAL:HG21	1:A:304:PHE:CE2	2.15	0.81
1:A:167:GLN:CD	1:A:219:LYS:HE2	2.00	0.81
1:A:237:GLU:N	1:A:240:LYS:HE3	1.94	0.81
1:A:26:SER:O	1:A:29:ILE:N	2.13	0.81
1:A:343:ILE:O	1:A:347:PRO:HG3	1.80	0.81
1:B:18:ILE:HD12	1:B:343:ILE:N	1.92	0.81
1:A:5:THR:HG23	1:A:8:GLU:CG	2.09	0.81
1:A:135:LEU:CG	1:A:171:LYS:HZ3	1.83	0.81
1:B:438:LEU:HD21	1:B:442:ILE:HD12	1.63	0.81
1:B:431:ALA:HA	1:B:434:ALA:HB2	1.63	0.80
1:A:13:LEU:O	1:A:15:LYS:N	2.13	0.80
1:A:52:ASN:OD1	1:A:304:PHE:HB2	1.80	0.80
2:D:78:LEU:HD23	2:D:111:LEU:HD22	1.61	0.80
1:A:168:LEU:HD12	1:A:219:LYS:HE3	0.81	0.80
2:C:112:LEU:CD2	2:C:113:VAL:N	2.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:VAL:HG23	1:A:330:VAL:O	1.81	0.80
1:B:292:THR:HG22	1:B:295:GLY:O	1.81	0.80
1:A:401:ARG:NH2	1:A:442:ILE:CG2	2.44	0.80
1:B:359:MET:HG3	1:B:366:ILE:HD11	1.63	0.80
1:B:18:ILE:HD12	1:B:343:ILE:CG1	2.12	0.80
1:A:167:GLN:OE1	1:A:219:LYS:CG	2.30	0.80
2:C:129:ILE:HG22	2:C:130:GLY:N	1.96	0.80
1:B:268:SER:HB3	1:B:312:ILE:HG21	1.64	0.79
1:B:268:SER:CB	1:B:312:ILE:CG2	2.60	0.79
1:B:168:LEU:HD12	1:B:219:LYS:HE3	0.79	0.79
1:B:18:ILE:HD12	1:B:343:ILE:HA	1.58	0.79
1:B:322:LEU:HD11	1:B:326:LEU:HD11	1.63	0.79
1:A:135:LEU:HD21	1:A:171:LYS:HZ1	0.83	0.79
1:A:54:LEU:HB3	1:A:329:ARG:HD3	1.63	0.79
1:A:442:ILE:HG23	1:B:329:ARG:HB2	1.64	0.79
1:A:424:TYR:CE2	1:A:428:HIS:CE1	2.71	0.79
1:B:235:ASN:O	1:B:239:LEU:HD11	1.81	0.79
1:B:391:GLY:O	1:B:393:ARG:N	2.16	0.79
1:B:27:VAL:HG23	1:B:70:LEU:HD23	1.63	0.79
1:B:259:ASP:HB3	1:B:310:PHE:CE2	2.18	0.79
2:C:80:ARG:HG2	2:C:80:ARG:NH1	1.97	0.79
1:B:108:VAL:HG12	1:B:109:LYS:H	1.48	0.79
1:B:413:LEU:O	1:B:416:GLN:N	2.15	0.79
1:A:346:GLU:N	1:A:347:PRO:HD2	1.97	0.78
1:A:86:PHE:N	1:A:86:PHE:CD1	2.47	0.78
1:B:256:ASP:O	1:B:257:GLU:CB	2.31	0.78
2:C:112:LEU:CD2	2:C:113:VAL:H	1.95	0.78
2:C:103:ILE:HD11	2:C:129:ILE:HG13	1.63	0.78
2:D:129:ILE:CG2	2:D:130:GLY:N	2.46	0.78
1:B:336:THR:N	1:B:339:ASP:HB2	1.98	0.78
1:B:391:GLY:C	1:B:393:ARG:N	2.34	0.78
1:A:359:MET:CB	1:A:366:ILE:CD1	2.61	0.78
1:A:372:GLY:O	1:A:376:ILE:HG13	1.83	0.78
1:A:424:TYR:CE2	1:A:428:HIS:NE2	2.51	0.78
1:B:239:LEU:HD13	1:B:240:LYS:CD	2.12	0.78
1:A:18:ILE:HD13	1:A:342:ARG:CB	2.13	0.78
1:A:391:GLY:C	1:A:393:ARG:N	2.36	0.78
1:B:251:GLY:C	1:B:252:ILE:HG13	2.02	0.78
2:C:110:LEU:HD22	2:C:111:LEU:N	1.99	0.78
1:A:86:PHE:CD2	1:A:96:VAL:HG12	2.17	0.78
1:B:100:ILE:HD13	1:B:299:THR:HG22	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLN:OE1	1:A:219:LYS:HG2	1.84	0.78
2:C:172:ASN:N	2:C:172:ASN:HD22	1.82	0.78
2:C:45:PHE:O	2:C:48:LYS:HB2	1.84	0.78
1:B:430:ASP:O	1:B:433:VAL:HG22	1.84	0.78
1:B:106:ALA:O	1:B:108:VAL:N	2.14	0.77
1:B:100:ILE:HD11	1:B:284:LEU:HD23	1.64	0.77
1:A:239:LEU:HD13	1:A:240:LYS:HD3	1.65	0.77
1:A:253:VAL:CG2	1:A:304:PHE:CE2	2.67	0.77
1:A:391:GLY:O	1:A:393:ARG:N	2.17	0.77
1:B:258:ILE:HD12	1:B:306:ALA:HB1	0.79	0.77
2:D:12:VAL:HG22	2:D:13:GLN:N	1.98	0.77
1:A:420:ILE:HG23	1:A:424:TYR:HD1	1.49	0.77
1:B:235:ASN:O	1:B:239:LEU:HD12	1.85	0.77
1:B:399:LEU:C	1:B:401:ARG:H	1.87	0.77
2:C:114:SER:OG	2:C:114:SER:O	2.01	0.77
2:D:106:ASN:HD22	2:D:109:THR:H	1.31	0.77
1:A:438:LEU:HD21	1:A:442:ILE:CD1	2.14	0.77
1:A:245:ASP:O	1:A:249:GLN:N	2.16	0.77
1:B:54:LEU:HD12	1:B:55:MET:N	1.99	0.77
1:A:240:LYS:O	1:A:242:ASP:N	2.17	0.77
1:A:350:SER:HB3	1:A:353:VAL:HG23	1.67	0.77
1:A:432:LEU:H	1:A:434:ALA:H	1.33	0.77
1:B:413:LEU:HD23	1:B:413:LEU:N	2.00	0.77
2:D:50:LEU:HG	2:D:180:LEU:HD21	1.65	0.77
1:A:135:LEU:CD2	1:A:171:LYS:HZ1	0.91	0.76
1:A:430:ASP:O	1:A:433:VAL:HG22	1.86	0.76
1:B:136:ILE:CG2	1:B:136:ILE:O	2.33	0.76
1:A:310:PHE:CE1	1:A:315:PRO:HA	2.20	0.76
1:B:343:ILE:O	1:B:347:PRO:HG3	1.85	0.76
1:A:220:ASP:OD1	1:A:220:ASP:N	2.18	0.76
1:B:27:VAL:CG2	1:B:70:LEU:HD23	2.15	0.76
1:B:288:CYS:SG	1:B:299:THR:CG2	2.72	0.76
2:D:103:ILE:HG13	2:D:129:ILE:HD12	1.67	0.76
2:D:56:SER:O	2:D:60:ALA:N	2.14	0.76
1:A:251:GLY:C	1:A:252:ILE:HG13	2.05	0.76
1:A:438:LEU:O	1:A:441:PHE:N	2.17	0.76
1:B:54:LEU:HB3	1:B:329:ARG:HD3	1.67	0.76
1:A:375:ARG:HB2	1:A:425:VAL:HG11	1.68	0.76
1:A:441:PHE:CD1	1:B:56:ILE:HD13	2.19	0.76
1:A:241:GLN:HA	1:A:244:ILE:HD12	1.67	0.76
2:C:139:ALA:O	2:C:142:ALA:HB3	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:122:PRO:HG3	2:C:127:LEU:HG	1.68	0.76
2:D:89:TRP:CD1	2:D:95:LEU:HB3	2.20	0.76
1:A:128:GLU:O	1:A:132:LEU:HG	1.86	0.75
1:A:135:LEU:CD2	1:A:171:LYS:CE	2.26	0.75
2:D:20:MET:HE1	2:D:52:GLY:N	2.01	0.75
1:A:81:VAL:HG21	1:A:99:ILE:HG23	1.68	0.75
1:B:425:VAL:HG12	1:B:426:SER:N	2.01	0.75
1:A:257:GLU:O	1:A:259:ASP:N	2.19	0.75
1:A:270:PRO:HD2	1:A:274:ARG:CD	2.17	0.75
1:A:86:PHE:HE2	1:A:96:VAL:HA	1.47	0.75
1:B:13:LEU:C	1:B:15:LYS:H	1.88	0.75
1:A:16:HIS:HD2	1:A:69:ARG:HG2	1.50	0.75
1:B:86:PHE:HE2	1:B:96:VAL:HA	1.51	0.75
2:D:12:VAL:HG22	2:D:13:GLN:H	1.49	0.75
1:B:420:ILE:HG23	1:B:424:TYR:HD1	1.49	0.75
2:D:72:GLU:O	2:D:74:TYR:N	2.19	0.75
1:B:359:MET:HB3	1:B:366:ILE:HD12	1.67	0.75
2:D:108:ASP:HB3	2:D:109:THR:HG22	1.69	0.75
2:D:9:ILE:HD13	2:D:53:PHE:O	1.86	0.74
1:A:116:ILE:O	1:A:116:ILE:CG2	2.27	0.74
1:A:235:ASN:O	1:A:239:LEU:CD1	2.36	0.74
1:B:5:THR:H	1:B:8:GLU:HG3	1.52	0.74
2:D:50:LEU:HG	2:D:180:LEU:HD23	1.67	0.74
1:B:135:LEU:CG	1:B:171:LYS:HZ3	1.80	0.74
1:B:375:ARG:HB2	1:B:425:VAL:HG11	1.68	0.74
1:B:86:PHE:HD1	1:B:86:PHE:N	1.84	0.74
1:B:5:THR:HG23	1:B:8:GLU:CG	2.18	0.74
1:A:320:PRO:HG2	1:A:321:GLU:OE2	1.88	0.74
1:A:5:THR:H	1:A:8:GLU:HG3	1.52	0.74
2:C:57:VAL:HA	2:C:60:ALA:CB	2.16	0.74
2:D:13:GLN:HG3	2:D:105:MET:HE1	1.70	0.74
1:A:130:ARG:O	1:A:173:ILE:HG21	1.87	0.74
1:B:237:GLU:HA	1:B:240:LYS:HG2	1.69	0.74
1:B:98:SER:OG	1:B:99:ILE:N	2.21	0.74
2:C:104:VAL:O	2:C:110:LEU:HD23	1.87	0.74
2:C:7:THR:HG22	2:C:23:ASP:OD2	1.88	0.74
1:A:418:ILE:CG2	1:A:419:THR:N	2.51	0.74
1:A:408:TYR:CE1	1:B:6:PRO:HB3	2.23	0.74
1:B:70:LEU:CD1	1:B:70:LEU:C	2.56	0.74
1:A:278:GLN:HE22	1:A:319:ILE:H	1.33	0.73
1:A:4:MET:O	1:A:32:ARG:NH1	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LEU:CD2	1:B:171:LYS:HZ3	0.92	0.73
1:B:424:TYR:O	1:B:425:VAL:C	2.25	0.73
2:D:105:MET:HB3	2:D:110:LEU:CD2	2.18	0.73
1:A:322:LEU:HD12	1:A:322:LEU:C	2.08	0.73
1:B:292:THR:CG2	1:B:295:GLY:O	2.35	0.73
1:B:390:ILE:O	1:B:390:ILE:HG22	1.88	0.73
1:B:418:ILE:CG2	1:B:419:THR:N	2.51	0.73
2:D:67:PHE:HD2	2:D:85:LEU:CD2	2.02	0.73
1:B:119:ASN:HD22	1:B:122:ARG:HG2	1.54	0.73
1:B:136:ILE:HG22	1:B:136:ILE:O	1.88	0.73
1:B:153:SER:C	1:B:155:ALA:H	1.90	0.73
1:B:235:ASN:N	1:B:236:PRO:CD	2.51	0.73
1:B:327:PRO:HG2	1:B:328:ILE:H	1.54	0.73
1:A:168:LEU:HD13	1:A:219:LYS:NZ	2.02	0.73
1:A:373:ILE:HA	1:A:376:ILE:HD12	1.69	0.73
1:B:108:VAL:HG12	1:B:109:LYS:N	2.00	0.73
1:B:438:LEU:O	1:B:441:PHE:N	2.20	0.73
2:C:12:VAL:HG23	2:C:126:ILE:CG1	2.18	0.73
2:D:12:VAL:HG21	2:D:126:ILE:HG12	1.68	0.73
1:A:425:VAL:CG1	1:A:426:SER:N	2.52	0.73
2:C:110:LEU:CD2	2:C:111:LEU:N	2.52	0.73
1:A:13:LEU:HD12	1:A:24:LYS:HB3	1.71	0.73
2:D:101:MET:HB3	2:D:112:LEU:HD21	1.70	0.73
1:A:13:LEU:C	1:A:15:LYS:H	1.89	0.72
2:D:78:LEU:HD23	2:D:111:LEU:CD2	2.19	0.72
2:D:103:ILE:HG13	2:D:129:ILE:CD1	2.19	0.72
2:D:20:MET:HE3	2:D:41:VAL:HG13	1.71	0.72
1:A:418:ILE:HG22	1:A:419:THR:N	2.04	0.72
1:B:18:ILE:HD11	1:B:343:ILE:HA	1.70	0.72
1:A:108:VAL:CG1	1:A:109:LYS:N	2.52	0.72
1:A:235:ASN:N	1:A:236:PRO:CD	2.51	0.72
1:A:69:ARG:O	1:A:70:LEU:C	2.26	0.72
1:A:96:VAL:HG11	1:A:280:ASP:HB3	1.72	0.72
1:B:116:ILE:HG22	1:B:116:ILE:O	1.89	0.72
1:B:350:SER:HB3	1:B:353:VAL:CG2	2.19	0.72
1:A:106:ALA:O	1:A:110:MET:HB2	1.88	0.72
1:A:41:ASN:OD1	1:A:44:LEU:HD12	1.89	0.72
1:B:359:MET:CG	1:B:366:ILE:HD12	2.16	0.72
1:A:235:ASN:O	1:A:239:LEU:HD11	1.90	0.72
1:A:135:LEU:CD2	1:A:171:LYS:HZ3	0.92	0.72
1:B:108:VAL:C	1:B:110:MET:N	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:112:LEU:HD23	2:C:113:VAL:N	2.05	0.72
2:D:110:LEU:HD22	2:D:111:LEU:N	2.05	0.72
1:B:86:PHE:N	1:B:86:PHE:CD1	2.57	0.72
1:A:431:ALA:HA	1:A:434:ALA:HB3	1.71	0.72
1:B:336:THR:H	1:B:339:ASP:CB	2.03	0.71
2:D:152:SER:O	2:D:156:ILE:HG13	1.90	0.71
2:D:43:LYS:NZ	2:D:179:GLU:O	2.21	0.71
1:A:41:ASN:HD21	1:A:43:GLU:HB3	1.56	0.71
1:B:12:GLU:O	1:B:15:LYS:HB2	1.89	0.71
2:C:110:LEU:CD2	2:C:111:LEU:H	2.04	0.71
1:A:425:VAL:HG12	1:A:426:SER:H	1.53	0.71
1:B:18:ILE:HD13	1:B:342:ARG:C	2.08	0.71
1:B:424:TYR:CE2	1:B:428:HIS:CE1	2.79	0.71
1:B:16:HIS:HD2	1:B:69:ARG:HG2	1.54	0.71
2:D:159:ALA:O	2:D:160:ALA:C	2.28	0.71
2:D:9:ILE:HD12	2:D:53:PHE:O	1.86	0.71
1:A:130:ARG:HD3	1:A:225:LEU:CD1	2.19	0.71
1:A:253:VAL:HG23	1:A:304:PHE:CD2	2.26	0.71
1:A:375:ARG:HA	1:A:378:GLU:HB2	1.71	0.71
1:B:346:GLU:N	1:B:347:PRO:HD2	2.05	0.71
2:C:27:THR:HG21	2:C:170:TYR:CD2	2.25	0.71
1:A:237:GLU:H	1:A:240:LYS:CE	2.02	0.71
1:B:226:ILE:O	1:B:229:GLU:HB2	1.91	0.71
1:B:399:LEU:C	1:B:401:ARG:N	2.43	0.71
1:B:375:ARG:O	1:B:376:ILE:C	2.29	0.71
1:A:171:LYS:HD2	1:A:218:ILE:CD1	2.21	0.71
1:A:18:ILE:HD12	1:A:343:ILE:CA	2.21	0.71
1:A:401:ARG:NH2	1:A:442:ILE:HG21	2.05	0.71
1:A:281:LEU:O	1:A:282:LEU:C	2.28	0.70
1:B:79:ILE:HD11	1:B:102:ASP:O	1.91	0.70
1:A:61:VAL:N	3:A:905:ADP:O2B	2.22	0.70
1:B:315:PRO:C	1:B:317:ASP:H	1.93	0.70
1:A:278:GLN:HE22	1:A:319:ILE:N	1.88	0.70
1:A:6:PRO:HD3	1:A:32:ARG:HD2	1.73	0.70
1:B:20:GLN:HE22	1:B:332:LEU:CA	2.04	0.70
1:B:233:LEU:O	1:B:235:ASN:ND2	2.24	0.70
1:B:431:ALA:HA	1:B:434:ALA:HB3	1.72	0.70
1:B:69:ARG:O	1:B:70:LEU:C	2.29	0.70
1:A:279:ARG:O	1:A:282:LEU:HB2	1.90	0.70
1:B:340:PHE:O	1:B:341:GLU:C	2.27	0.70
1:B:18:ILE:HD11	1:B:342:ARG:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:129:ILE:CG2	2:C:130:GLY:N	2.54	0.70
2:C:8:THR:HG21	2:C:132:GLY:H	1.55	0.70
1:B:10:VAL:O	1:B:13:LEU:HB2	1.90	0.70
2:D:45:PHE:O	2:D:48:LYS:HB2	1.90	0.70
1:B:27:VAL:HG23	1:B:70:LEU:HD22	1.72	0.70
1:A:310:PHE:CE1	1:A:315:PRO:CA	2.74	0.70
1:A:34:ARG:O	1:A:35:TRP:C	2.30	0.70
2:D:110:LEU:HD13	2:D:127:LEU:HD12	1.74	0.70
2:D:110:LEU:O	2:D:111:LEU:CD1	2.40	0.70
1:B:278:GLN:HE22	1:B:319:ILE:N	1.90	0.69
1:B:355:TYR:CD2	1:B:403:MET:HG2	2.27	0.69
1:B:86:PHE:CE2	1:B:96:VAL:HA	2.27	0.69
1:A:257:GLU:O	1:A:258:ILE:C	2.31	0.69
1:A:77:PRO:O	1:A:251:GLY:HA3	1.92	0.69
1:B:259:ASP:OD2	1:B:260:LYS:N	2.25	0.69
1:B:261:ILE:CG2	1:B:261:ILE:O	2.40	0.69
1:B:253:VAL:HG21	1:B:304:PHE:CE2	2.28	0.69
2:C:17:ARG:HB3	2:C:153:ALA:CB	2.22	0.69
1:A:261:ILE:O	1:A:261:ILE:CG2	2.38	0.69
1:A:292:THR:HG21	1:A:297:VAL:HG23	1.72	0.69
1:B:240:LYS:O	1:B:242:ASP:N	2.26	0.69
1:B:418:ILE:HG22	1:B:419:THR:N	2.07	0.69
1:A:117:GLU:HA	1:A:120:ARG:HB3	1.73	0.69
1:A:13:LEU:C	1:A:15:LYS:N	2.45	0.69
2:C:12:VAL:HG21	2:C:126:ILE:HG12	1.75	0.69
1:A:149:GLN:O	1:A:152:PRO:HD2	1.92	0.69
1:A:36:ARG:O	1:A:37:ARG:C	2.31	0.69
1:A:358:LEU:HD22	1:B:36:ARG:HB3	1.75	0.69
1:B:270:PRO:HD2	1:B:274:ARG:NE	2.08	0.69
1:B:319:ILE:CG2	1:B:321:GLU:OE2	2.41	0.69
2:C:57:VAL:O	2:C:61:PHE:HB2	1.93	0.69
1:B:281:LEU:O	1:B:282:LEU:C	2.31	0.69
1:B:4:MET:O	1:B:32:ARG:NH1	2.25	0.69
1:B:322:LEU:HD12	1:B:326:LEU:HD13	1.72	0.69
2:D:92:ASP:OD2	2:D:95:LEU:HD12	1.93	0.69
2:C:151:MET:HG3	2:C:156:ILE:HG12	1.75	0.68
2:C:8:THR:CG2	2:C:132:GLY:H	2.06	0.68
2:D:112:LEU:CD2	2:D:113:VAL:H	2.05	0.68
1:A:61:VAL:CG2	1:A:61:VAL:O	2.41	0.68
1:B:93:GLY:O	1:B:94:LYS:HD2	1.92	0.68
2:C:112:LEU:HD22	2:C:113:VAL:N	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:CG2	1:A:70:LEU:HD23	2.22	0.68
1:B:336:THR:O	1:B:340:PHE:N	2.26	0.68
1:B:369:THR:HB	1:B:371:SER:N	2.08	0.68
1:A:390:ILE:HG22	1:A:390:ILE:O	1.93	0.68
1:A:32:ARG:HG2	1:A:36:ARG:NE	2.04	0.68
1:B:292:THR:OG1	1:B:293:LYS:N	2.25	0.68
2:D:134:ASN:O	2:D:135:TYR:C	2.31	0.68
1:A:303:LEU:HG	1:A:304:PHE:N	2.08	0.68
1:A:233:LEU:O	1:A:235:ASN:ND2	2.27	0.68
1:A:240:LYS:O	1:A:243:ALA:N	2.26	0.68
2:D:17:ARG:HB3	2:D:153:ALA:CB	2.23	0.68
1:B:254:PHE:HA	1:B:305:ILE:O	1.94	0.67
1:B:310:PHE:HE1	1:B:315:PRO:HA	1.59	0.67
1:B:61:VAL:HB	1:B:335:LEU:CD1	2.24	0.67
1:B:135:LEU:HD21	1:B:171:LYS:HZ1	0.52	0.67
1:A:399:LEU:C	1:A:401:ARG:N	2.48	0.67
1:B:322:LEU:O	1:B:324:GLY:N	2.28	0.67
1:B:403:MET:HE3	1:B:420:ILE:CD1	2.13	0.67
1:B:428:HIS:C	1:B:429:LEU:HD12	2.15	0.67
2:C:94:VAL:HG12	2:C:95:LEU:HG	1.77	0.67
1:A:73:LEU:HG	1:A:74:ALA:N	1.99	0.67
1:B:13:LEU:C	1:B:15:LYS:N	2.45	0.67
2:D:114:SER:O	2:D:114:SER:OG	2.11	0.67
1:B:54:LEU:HD12	1:B:54:LEU:C	2.16	0.67
2:C:152:SER:O	2:C:156:ILE:CG1	2.42	0.67
1:A:325:ARG:C	1:A:327:PRO:HD2	2.15	0.67
1:A:418:ILE:CG2	1:A:419:THR:H	2.06	0.67
2:C:136:ALA:HB1	2:C:160:ALA:HB1	1.77	0.67
2:C:68:GLU:O	2:C:71:LEU:N	2.28	0.67
2:D:57:VAL:HA	2:D:60:ALA:CB	2.23	0.67
1:B:168:LEU:HD13	1:B:219:LYS:NZ	2.07	0.66
1:B:282:LEU:O	1:B:285:VAL:HG13	1.94	0.66
3:B:906:ADP:H2'	3:B:906:ADP:O5'	1.95	0.66
1:A:18:ILE:HG23	1:A:342:ARG:HH21	1.60	0.66
1:A:88:GLU:O	1:A:91:TYR:HA	1.94	0.66
3:A:905:ADP:H5'1	3:A:905:ADP:H8	1.59	0.66
2:C:83:VAL:HG12	2:C:84:GLU:N	2.08	0.66
2:D:110:LEU:HD22	2:D:127:LEU:HD12	1.77	0.66
1:A:355:TYR:CD2	1:A:403:MET:HG2	2.31	0.66
1:A:402:LEU:HD13	1:A:429:LEU:HD11	1.77	0.66
1:A:314:LYS:O	1:A:317:ASP:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:MET:HB3	1:A:366:ILE:CD1	2.25	0.66
1:A:399:LEU:C	1:A:401:ARG:H	1.99	0.66
1:A:398:VAL:O	1:A:401:ARG:HB3	1.95	0.66
2:D:101:MET:HB3	2:D:112:LEU:CD2	2.26	0.66
1:A:104:THR:HA	1:A:107:ALA:HB3	1.78	0.66
1:B:135:LEU:HD22	1:B:171:LYS:HZ1	1.32	0.66
1:B:237:GLU:N	1:B:240:LYS:CE	2.41	0.66
1:B:320:PRO:O	1:B:323:GLN:HB2	1.96	0.66
1:B:332:LEU:HD12	1:B:332:LEU:N	2.10	0.66
1:A:237:GLU:HA	1:A:240:LYS:HG2	1.78	0.66
1:A:270:PRO:HD2	1:A:274:ARG:HD2	1.76	0.66
1:B:325:ARG:C	1:B:327:PRO:HD2	2.17	0.66
1:A:279:ARG:O	1:A:280:ASP:C	2.34	0.66
1:B:282:LEU:HD11	1:B:321:GLU:HB3	1.78	0.66
2:C:13:GLN:HG3	2:C:105:MET:HE1	1.77	0.66
2:C:95:LEU:HD23	2:C:98:LEU:HD12	1.76	0.66
2:D:110:LEU:CD2	2:D:111:LEU:N	2.59	0.66
1:B:257:GLU:O	1:B:258:ILE:C	2.31	0.65
1:B:34:ARG:O	1:B:35:TRP:C	2.34	0.65
2:D:152:SER:O	2:D:156:ILE:CG1	2.43	0.65
1:A:350:SER:HB3	1:A:353:VAL:CG2	2.26	0.65
1:A:54:LEU:HD12	1:A:55:MET:N	2.11	0.65
1:B:325:ARG:O	1:B:327:PRO:HD2	1.97	0.65
1:B:355:TYR:OH	1:B:400:GLU:OE2	2.08	0.65
2:C:103:ILE:HG13	2:C:129:ILE:HD11	1.76	0.65
2:C:9:ILE:HD12	2:C:53:PHE:O	1.95	0.65
2:D:122:PRO:HG3	2:D:127:LEU:HG	1.77	0.65
1:B:235:ASN:C	1:B:239:LEU:HD12	2.16	0.65
1:A:259:ASP:OD2	1:A:260:LYS:N	2.29	0.65
1:A:392:ALA:O	1:A:395:LEU:CD1	2.43	0.65
2:D:26:VAL:O	2:D:26:VAL:CG1	2.44	0.65
2:D:68:GLU:O	2:D:71:LEU:N	2.28	0.65
1:A:135:LEU:HD22	1:A:171:LYS:HZ3	1.29	0.65
1:A:435:ASP:O	1:A:437:ASP:N	2.30	0.65
1:A:270:PRO:HD2	1:A:274:ARG:NE	2.12	0.65
2:D:44:LEU:CB	2:D:49:VAL:CG2	2.75	0.65
1:A:24:LYS:O	1:A:25:ARG:C	2.35	0.64
2:D:103:ILE:HD11	2:D:129:ILE:HG13	1.78	0.64
1:A:100:ILE:HD12	1:A:290:VAL:HG21	1.78	0.64
1:B:315:PRO:O	1:B:317:ASP:N	2.30	0.64
1:B:34:ARG:HG3	1:B:35:TRP:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:LEU:H	1:B:434:ALA:H	1.46	0.64
1:B:251:GLY:O	1:B:252:ILE:HG13	1.98	0.64
1:B:271:ASP:HB3	1:B:273:SER:H	1.62	0.64
1:B:373:ILE:HA	1:B:376:ILE:HD12	1.78	0.64
1:B:41:ASN:HD21	1:B:43:GLU:HB3	1.61	0.64
1:B:135:LEU:HD21	1:B:171:LYS:NZ	1.14	0.64
2:C:8:THR:HG21	2:C:132:GLY:N	2.12	0.64
2:D:23:ASP:HB2	2:D:172:ASN:HD22	1.58	0.64
1:A:402:LEU:HB3	1:A:403:MET:SD	2.37	0.64
1:B:20:GLN:O	1:B:23:ALA:HB3	1.97	0.64
2:C:60:ALA:O	2:C:61:PHE:C	2.35	0.64
1:B:415:GLY:O	1:B:416:GLN:O	2.16	0.64
2:D:12:VAL:HG23	2:D:126:ILE:CG1	2.26	0.64
1:B:237:GLU:HA	1:B:240:LYS:CG	2.27	0.64
2:D:8:THR:CG2	2:D:132:GLY:H	2.10	0.64
1:A:77:PRO:HD2	1:A:251:GLY:CA	2.27	0.64
1:B:282:LEU:CB	1:B:283:PRO:HD3	2.18	0.64
1:B:77:PRO:O	1:B:251:GLY:HA3	1.98	0.64
1:B:279:ARG:O	1:B:280:ASP:C	2.35	0.64
2:C:138:ALA:O	2:C:142:ALA:HB2	1.96	0.64
2:D:25:GLN:OE1	2:D:172:ASN:HB3	1.96	0.64
1:A:149:GLN:C	1:A:152:PRO:HD2	2.19	0.64
1:A:272:VAL:HB	1:A:275:GLU:HB2	1.79	0.64
1:B:70:LEU:HD12	1:B:70:LEU:O	1.98	0.64
1:A:293:LYS:O	1:A:295:GLY:N	2.30	0.63
1:B:100:ILE:CD1	1:B:299:THR:HG22	2.28	0.63
1:A:249:GLN:HG2	1:A:249:GLN:O	1.98	0.63
1:A:254:PHE:HA	1:A:305:ILE:O	1.99	0.63
1:A:266:GLU:OE1	2:D:66:LYS:NZ	2.31	0.63
1:B:131:ILE:HG22	1:B:135:LEU:CD1	2.26	0.63
1:B:290:VAL:HG12	1:B:291:SER:N	2.13	0.63
2:D:152:SER:O	2:D:156:ILE:HD12	1.97	0.63
1:B:354:GLN:O	1:B:358:LEU:HB2	1.98	0.63
2:C:20:MET:HE1	2:C:52:GLY:N	2.13	0.63
1:B:3:GLU:HG2	1:B:4:MET:H	1.64	0.63
1:A:167:GLN:CD	1:A:219:LYS:HG2	2.18	0.63
1:A:6:PRO:CD	1:A:32:ARG:HD2	2.28	0.63
1:B:130:ARG:CD	1:B:225:LEU:HD11	2.22	0.63
1:A:168:LEU:HD13	1:A:219:LYS:HZ1	1.63	0.63
1:A:403:MET:HB3	1:A:407:SER:HB2	1.80	0.63
1:A:61:VAL:O	1:A:61:VAL:HG23	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:92:ASP:C	2:C:92:ASP:OD1	2.37	0.63
1:A:27:VAL:HG23	1:A:70:LEU:HD22	1.80	0.63
1:B:130:ARG:O	1:B:173:ILE:HG21	1.99	0.63
1:B:278:GLN:NE2	1:B:319:ILE:H	1.97	0.63
1:B:3:GLU:O	1:B:4:MET:CB	2.41	0.63
2:D:25:GLN:HB2	2:D:172:ASN:CG	2.18	0.63
2:C:95:LEU:O	2:C:98:LEU:HB2	1.97	0.63
2:D:152:SER:O	2:D:156:ILE:CD1	2.46	0.63
1:A:12:GLU:O	1:A:15:LYS:HB2	1.99	0.63
1:A:153:SER:C	1:A:155:ALA:H	2.02	0.63
1:A:70:LEU:HD12	1:A:70:LEU:C	2.20	0.63
1:B:3:GLU:CG	1:B:4:MET:H	2.11	0.63
1:B:6:PRO:CD	1:B:32:ARG:CD	2.77	0.63
2:D:112:LEU:HB3	2:D:120:ILE:HB	1.79	0.63
1:A:261:ILE:HG21	1:A:277:VAL:CG1	2.27	0.62
1:B:235:ASN:H	1:B:236:PRO:HD3	1.63	0.62
2:D:83:VAL:O	2:D:86:ALA:N	2.32	0.62
1:A:123:ALA:HA	1:A:126:LEU:HD12	1.81	0.62
1:A:322:LEU:HD12	1:A:322:LEU:O	1.99	0.62
1:A:421:ASP:O	1:A:424:TYR:N	2.32	0.62
1:B:290:VAL:CG1	1:B:291:SER:N	2.63	0.62
1:B:18:ILE:HD12	1:B:343:ILE:HG13	1.82	0.62
1:B:221:ALA:HA	1:B:224:LEU:HB2	1.81	0.62
1:B:236:PRO:HA	1:B:240:LYS:HE2	1.80	0.62
1:B:55:MET:HE1	1:B:63:LYS:HA	1.81	0.62
1:B:221:ALA:H	1:B:224:LEU:HD13	1.64	0.62
1:B:366:ILE:CG2	1:B:420:ILE:HD12	2.29	0.62
1:A:18:ILE:HD12	1:A:343:ILE:CG1	2.30	0.62
1:A:18:ILE:HD13	1:A:342:ARG:C	2.18	0.62
1:B:432:LEU:O	1:B:435:ASP:N	2.33	0.62
1:B:274:ARG:O	1:B:275:GLU:C	2.37	0.62
2:D:172:ASN:O	2:D:172:ASN:ND2	2.32	0.62
2:D:44:LEU:HB2	2:D:49:VAL:CG2	2.30	0.62
2:D:57:VAL:O	2:D:61:PHE:HB2	2.00	0.62
1:A:261:ILE:CD1	1:A:277:VAL:HG11	2.26	0.62
1:B:26:SER:O	1:B:29:ILE:N	2.32	0.62
1:B:401:ARG:HH21	1:B:442:ILE:HG22	1.62	0.62
2:C:54:ALA:HB3	2:C:100:ALA:HB1	1.81	0.62
2:D:12:VAL:HG23	2:D:125:GLY:O	2.00	0.62
2:C:23:ASP:HB2	2:C:172:ASN:HD22	1.59	0.62
1:B:268:SER:OG	1:B:312:ILE:HG21	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD22	1:A:70:LEU:HD11	1.81	0.61
2:C:108:ASP:CB	2:C:109:THR:HG22	2.28	0.61
2:C:110:LEU:O	2:C:111:LEU:CD1	2.48	0.61
2:D:67:PHE:HD2	2:D:85:LEU:HD22	1.63	0.61
1:A:31:LEU:HD22	1:A:70:LEU:CD1	2.30	0.61
1:A:424:TYR:HE2	1:A:428:HIS:CE1	2.19	0.61
1:A:70:LEU:C	1:A:70:LEU:CD1	2.69	0.61
1:B:107:ALA:O	1:B:243:ALA:HB1	2.00	0.61
2:C:112:LEU:HB3	2:C:120:ILE:HB	1.82	0.61
2:D:20:MET:CE	2:D:52:GLY:N	2.62	0.61
1:B:315:PRO:O	1:B:318:LEU:HD12	2.00	0.61
1:A:390:ILE:CD1	1:B:323:GLN:NE2	2.63	0.61
2:C:92:ASP:OD2	2:C:95:LEU:HD12	1.99	0.61
2:D:7:THR:HG22	2:D:23:ASP:OD2	1.99	0.61
1:A:435:ASP:O	1:A:436:GLU:C	2.39	0.61
1:B:435:ASP:O	1:B:437:ASP:N	2.33	0.61
1:B:52:ASN:OD1	1:B:304:PHE:N	2.33	0.61
2:D:8:THR:HG21	2:D:132:GLY:N	2.16	0.61
1:A:79:ILE:CD1	1:A:102:ASP:C	2.69	0.61
1:A:5:THR:O	1:A:6:PRO:C	2.37	0.61
1:B:240:LYS:O	1:B:243:ALA:N	2.32	0.61
1:B:278:GLN:CB	1:B:319:ILE:HD12	2.31	0.61
2:C:23:ASP:CB	2:C:172:ASN:HD21	2.10	0.61
1:A:20:GLN:HE22	1:A:332:LEU:CA	2.12	0.61
1:A:403:MET:CE	1:A:406:ILE:HD12	2.30	0.61
1:B:220:ASP:O	1:B:222:MET:N	2.34	0.61
1:B:278:GLN:HE22	1:B:319:ILE:H	1.48	0.61
1:B:372:GLY:C	1:B:374:LYS:N	2.49	0.61
2:C:104:VAL:O	2:C:110:LEU:CD2	2.48	0.61
2:C:68:GLU:O	2:C:70:LYS:N	2.34	0.61
2:D:44:LEU:HB2	2:D:49:VAL:HG23	1.82	0.61
1:A:220:ASP:O	1:A:222:MET:N	2.33	0.61
2:C:8:THR:HG23	2:C:131:SER:N	2.16	0.61
1:A:278:GLN:NE2	1:A:319:ILE:H	1.97	0.61
1:A:83:ALA:O	1:A:84:THR:C	2.39	0.61
2:D:12:VAL:CG2	2:D:13:GLN:H	2.12	0.61
1:A:325:ARG:C	1:A:327:PRO:CD	2.69	0.61
1:B:398:VAL:O	1:B:401:ARG:HB3	2.01	0.61
2:C:163:THR:O	2:C:166:GLU:HB3	2.01	0.61
2:C:27:THR:HG21	2:C:170:TYR:HD2	1.64	0.61
1:A:263:LYS:HE2	1:A:269:GLY:HA3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ASP:HA	1:B:245:ASP:HB2	1.82	0.61
1:A:420:ILE:HG23	1:A:424:TYR:CD1	2.32	0.60
3:A:905:ADP:H5'1	3:A:905:ADP:C8	2.36	0.60
1:A:408:TYR:CD1	1:B:6:PRO:HB3	2.36	0.60
1:B:108:VAL:CG1	1:B:109:LYS:N	2.64	0.60
1:B:263:LYS:HD2	1:B:272:VAL:HG12	1.81	0.60
1:B:403:MET:HB3	1:B:407:SER:HB2	1.82	0.60
1:A:261:ILE:HD13	1:A:277:VAL:HG12	1.80	0.60
1:A:428:HIS:C	1:A:429:LEU:HD12	2.21	0.60
1:B:425:VAL:CG1	1:B:426:SER:N	2.64	0.60
1:B:122:ARG:CZ	1:B:126:LEU:HD11	2.29	0.60
1:B:338:SER:O	1:B:339:ASP:C	2.40	0.60
1:B:375:ARG:HA	1:B:378:GLU:HB2	1.83	0.60
2:C:110:LEU:HD22	2:C:127:LEU:HD12	1.83	0.60
2:D:79:LYS:O	2:D:82:ALA:HB3	2.01	0.60
1:A:26:SER:O	1:A:28:ALA:N	2.34	0.60
1:A:338:SER:O	1:A:339:ASP:C	2.39	0.60
1:B:252:ILE:HA	1:B:303:LEU:O	2.02	0.60
1:B:278:GLN:HB2	1:B:319:ILE:HD12	1.83	0.60
1:A:274:ARG:O	1:A:275:GLU:C	2.39	0.60
1:A:415:GLY:O	1:A:416:GLN:C	2.38	0.60
1:B:108:VAL:O	1:B:110:MET:N	2.34	0.60
1:B:263:LYS:CD	1:B:272:VAL:HG12	2.31	0.60
1:B:424:TYR:CE2	1:B:428:HIS:NE2	2.70	0.60
2:D:70:LYS:NZ	2:D:84:GLU:HB3	2.16	0.60
2:C:112:LEU:HD13	2:C:120:ILE:HD12	1.83	0.60
2:D:60:ALA:O	2:D:61:PHE:C	2.40	0.60
1:A:131:ILE:HG22	1:A:135:LEU:CD1	2.30	0.60
1:B:307:SER:OG	1:B:308:GLY:N	2.35	0.60
1:B:34:ARG:HE	1:B:250:HIS:CE1	2.19	0.60
1:B:36:ARG:O	1:B:37:ARG:C	2.40	0.60
1:B:415:GLY:O	1:B:416:GLN:C	2.39	0.60
1:B:441:PHE:N	1:B:441:PHE:HD2	1.99	0.60
2:C:132:GLY:O	2:C:133:GLY:C	2.40	0.60
2:D:94:VAL:HG12	2:D:95:LEU:HG	1.83	0.60
1:A:18:ILE:HD12	1:A:343:ILE:HG13	1.82	0.60
1:A:235:ASN:H	1:A:236:PRO:HD3	1.64	0.60
1:A:23:ALA:O	1:A:24:LYS:C	2.39	0.60
2:D:112:LEU:CD2	2:D:113:VAL:N	2.65	0.60
2:D:143:LEU:HD13	2:D:151:MET:SD	2.42	0.60
1:A:354:GLN:O	1:A:358:LEU:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ARG:O	1:A:395:LEU:C	2.38	0.60
1:A:54:LEU:C	1:A:54:LEU:HD12	2.22	0.60
1:B:425:VAL:HG12	1:B:426:SER:H	1.66	0.60
1:B:438:LEU:O	1:B:439:SER:C	2.40	0.60
2:D:112:LEU:HD22	2:D:113:VAL:N	2.17	0.60
1:A:282:LEU:O	1:A:284:LEU:N	2.35	0.59
1:A:406:ILE:HD13	1:A:420:ILE:HD11	1.84	0.59
1:B:18:ILE:N	3:B:906:ADP:N1	2.50	0.59
2:D:104:VAL:O	2:D:110:LEU:HD23	2.02	0.59
1:A:18:ILE:CD1	1:A:343:ILE:CA	2.79	0.59
1:B:247:VAL:O	1:B:250:HIS:HA	2.02	0.59
2:C:106:ASN:HD22	2:C:109:THR:H	1.39	0.59
1:A:403:MET:HE3	1:A:406:ILE:HD12	1.84	0.59
1:A:441:PHE:HA	1:B:315:PRO:HG2	1.83	0.59
1:B:18:ILE:HD13	1:B:342:ARG:HB2	1.84	0.59
1:B:35:TRP:O	1:B:36:ARG:C	2.41	0.59
1:A:408:TYR:HE1	1:B:6:PRO:HB3	1.67	0.59
2:C:21:SER:OG	2:C:157:ALA:HB1	2.02	0.59
1:B:395:LEU:H	1:B:395:LEU:HD12	1.67	0.59
1:B:55:MET:CE	1:B:63:LYS:HA	2.32	0.59
2:C:105:MET:HB3	2:C:110:LEU:CD2	2.32	0.59
2:D:159:ALA:O	2:D:160:ALA:O	2.19	0.59
1:B:31:LEU:HD22	1:B:70:LEU:CD1	2.32	0.59
1:B:355:TYR:O	1:B:356:LYS:O	2.20	0.59
2:C:58:ALA:O	2:C:59:ASP:C	2.41	0.59
1:A:20:GLN:O	1:A:23:ALA:HB3	2.02	0.59
1:A:17:ILE:HD13	1:A:66:ILE:HA	1.84	0.59
1:B:315:PRO:C	1:B:317:ASP:N	2.56	0.59
1:B:20:GLN:HE22	1:B:332:LEU:CB	2.16	0.59
1:B:6:PRO:HD2	1:B:32:ARG:HD2	1.83	0.59
2:C:101:MET:HB3	2:C:112:LEU:CD2	2.28	0.59
2:D:13:GLN:HG3	2:D:105:MET:CE	2.32	0.59
1:A:439:SER:HB3	1:A:443:LEU:HD12	1.84	0.59
1:B:153:SER:O	1:B:155:ALA:N	2.34	0.59
1:A:358:LEU:CD2	1:B:36:ARG:HB3	2.32	0.59
2:D:86:ALA:O	2:D:87:LYS:C	2.41	0.59
1:B:119:ASN:HB3	1:B:233:LEU:HD13	1.85	0.59
2:D:172:ASN:H	2:D:172:ASN:ND2	1.97	0.59
1:B:279:ARG:HG3	1:B:319:ILE:HD13	1.84	0.59
1:A:390:ILE:HD11	1:B:323:GLN:CD	2.23	0.59
1:B:18:ILE:HD11	1:B:347:PRO:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:112:LEU:HD23	2:D:113:VAL:H	1.66	0.59
2:D:12:VAL:CG2	2:D:13:GLN:N	2.66	0.59
1:A:310:PHE:CE1	1:A:315:PRO:N	2.71	0.58
1:B:403:MET:HE2	1:B:420:ILE:CD1	2.29	0.58
2:D:110:LEU:CD2	2:D:111:LEU:H	2.15	0.58
2:D:8:THR:HG21	2:D:132:GLY:H	1.67	0.58
1:A:3:GLU:HG2	1:A:4:MET:H	1.68	0.58
2:D:49:VAL:O	2:D:50:LEU:HD23	2.03	0.58
1:B:253:VAL:CG2	1:B:304:PHE:CE2	2.85	0.58
2:C:101:MET:CB	2:C:112:LEU:HD21	2.30	0.58
2:D:153:ALA:O	2:D:154:SER:C	2.41	0.58
1:A:336:THR:H	1:A:339:ASP:HB2	1.66	0.58
1:A:359:MET:HG2	1:A:366:ILE:HD11	1.52	0.58
1:A:373:ILE:CA	1:A:376:ILE:HD12	2.32	0.58
1:A:402:LEU:HD13	1:A:429:LEU:CD1	2.33	0.58
2:C:103:ILE:CG1	2:C:129:ILE:CD1	2.77	0.58
2:D:23:ASP:CB	2:D:172:ASN:HD21	2.08	0.58
2:D:85:LEU:O	2:D:86:ALA:C	2.42	0.58
2:D:92:ASP:C	2:D:92:ASP:OD1	2.41	0.58
1:B:61:VAL:CB	1:B:335:LEU:HD11	2.29	0.58
1:B:55:MET:HE2	1:B:63:LYS:HB3	1.85	0.58
2:C:43:LYS:NZ	2:C:179:GLU:O	2.26	0.58
2:D:54:ALA:HB3	2:D:100:ALA:HB1	1.86	0.58
2:D:44:LEU:O	2:D:49:VAL:HG22	2.02	0.58
1:A:35:TRP:O	1:A:36:ARG:C	2.42	0.58
1:A:104:THR:HG21	1:A:297:VAL:HG21	1.86	0.58
1:B:103:LEU:HD12	1:B:247:VAL:HG13	1.84	0.58
1:B:135:LEU:CD2	1:B:171:LYS:HZ2	1.23	0.58
1:B:285:VAL:HA	1:B:304:PHE:CE1	2.39	0.58
1:B:424:TYR:O	1:B:425:VAL:O	2.22	0.58
2:D:177:LEU:CD2	2:D:178:GLU:H	2.17	0.58
1:A:19:GLY:O	1:A:20:GLN:HB2	2.03	0.58
1:A:270:PRO:CD	1:A:274:ARG:NE	2.66	0.58
1:A:330:VAL:O	1:A:330:VAL:CG2	2.50	0.58
1:B:18:ILE:CD1	1:B:342:ARG:O	2.51	0.58
2:C:63:LEU:HD11	2:C:89:TRP:CE2	2.38	0.58
1:A:135:LEU:HG	1:A:171:LYS:HZ2	1.66	0.58
2:C:110:LEU:HD23	2:C:111:LEU:H	1.69	0.58
2:C:86:ALA:O	2:C:87:LYS:C	2.42	0.58
1:A:16:HIS:CD2	1:A:69:ARG:HG2	2.35	0.58
1:A:88:GLU:OE2	1:A:91:TYR:C	2.42	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:PHE:CB	1:B:373:ILE:HD11	2.34	0.58
2:D:81:ALA:O	2:D:82:ALA:C	2.43	0.58
1:A:81:VAL:CG2	1:A:99:ILE:HG23	2.33	0.57
1:B:100:ILE:CG1	1:B:284:LEU:HD21	2.33	0.57
1:B:392:ALA:O	1:B:395:LEU:CD1	2.46	0.57
2:D:10:PHE:N	2:D:21:SER:O	2.31	0.57
1:A:227:GLU:C	1:A:229:GLU:H	2.08	0.57
2:C:134:ASN:N	2:C:134:ASN:OD1	2.36	0.57
1:A:276:GLY:O	1:A:279:ARG:N	2.37	0.57
1:B:299:THR:OG1	1:B:300:ASP:N	2.36	0.57
1:B:379:ALA:O	1:B:380:ALA:C	2.43	0.57
1:B:428:HIS:O	1:B:429:LEU:HD12	2.05	0.57
1:A:108:VAL:CG1	1:A:109:LYS:H	2.07	0.57
1:B:224:LEU:O	1:B:225:LEU:C	2.42	0.57
2:C:140:GLY:O	2:C:142:ALA:N	2.37	0.57
2:C:83:VAL:O	2:C:86:ALA:N	2.37	0.57
1:B:249:GLN:O	1:B:250:HIS:HB3	2.02	0.57
2:C:105:MET:HE3	2:C:110:LEU:HG	1.86	0.57
1:B:17:ILE:HD13	1:B:66:ILE:HA	1.86	0.57
1:B:298:LYS:CG	1:B:300:ASP:HB2	2.34	0.57
1:B:56:ILE:HD11	1:B:315:PRO:HG2	1.87	0.57
1:A:253:VAL:HG23	1:A:304:PHE:CE2	2.40	0.57
1:A:390:ILE:HG23	1:B:320:PRO:CB	2.35	0.57
1:B:168:LEU:HD13	1:B:219:LYS:HZ1	1.68	0.57
1:B:336:THR:HG22	1:B:337:THR:OG1	2.05	0.57
1:B:435:ASP:O	1:B:436:GLU:C	2.42	0.57
1:B:438:LEU:O	1:B:440:ARG:N	2.37	0.57
2:C:153:ALA:O	2:C:154:SER:C	2.43	0.57
2:D:105:MET:HB3	2:D:110:LEU:HD21	1.86	0.57
2:D:14:HIS:CE1	2:D:15:LYS:HE2	2.40	0.57
2:C:25:GLN:H	2:C:172:ASN:ND2	2.02	0.57
1:A:340:PHE:O	1:A:341:GLU:C	2.42	0.57
1:B:120:ARG:HG2	1:B:124:GLU:OE2	2.05	0.57
2:D:14:HIS:HB2	2:D:144:LYS:HD2	1.87	0.57
1:B:10:VAL:O	1:B:13:LEU:N	2.38	0.56
2:D:172:ASN:N	2:D:172:ASN:HD22	1.88	0.56
1:A:10:VAL:O	1:A:13:LEU:N	2.35	0.56
1:A:235:ASN:O	1:A:239:LEU:HD12	2.05	0.56
1:A:307:SER:OG	1:A:308:GLY:N	2.38	0.56
1:A:96:VAL:HG11	1:A:280:ASP:CB	2.34	0.56
1:A:408:TYR:HE2	1:B:25:ARG:CZ	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:LYS:O	1:B:295:GLY:N	2.37	0.56
1:B:371:SER:O	1:B:422:ALA:HB2	2.04	0.56
2:C:111:LEU:CD1	2:C:121:GLU:HG3	2.35	0.56
2:C:159:ALA:O	2:C:160:ALA:C	2.42	0.56
1:A:395:LEU:H	1:A:395:LEU:HD12	1.70	0.56
1:A:413:LEU:O	1:A:416:GLN:N	2.38	0.56
1:B:108:VAL:O	1:B:111:VAL:N	2.38	0.56
1:B:261:ILE:HD13	1:B:277:VAL:CG1	2.35	0.56
1:A:354:GLN:OE1	1:B:48:VAL:HG22	2.05	0.56
1:A:41:ASN:ND2	1:A:43:GLU:HB3	2.19	0.56
1:B:322:LEU:HD12	1:B:326:LEU:HD12	1.85	0.56
1:B:70:LEU:CD1	1:B:70:LEU:O	2.53	0.56
2:D:83:VAL:HG12	2:D:84:GLU:N	2.19	0.56
1:A:252:ILE:HA	1:A:303:LEU:O	2.06	0.56
1:A:390:ILE:HD11	1:B:323:GLN:NE2	2.21	0.56
1:B:153:SER:C	1:B:155:ALA:N	2.59	0.56
1:B:399:LEU:O	1:B:402:LEU:N	2.38	0.56
1:B:83:ALA:O	1:B:84:THR:C	2.43	0.56
1:A:366:ILE:CG2	1:A:420:ILE:HD12	2.36	0.56
1:B:322:LEU:O	1:B:326:LEU:HD12	2.06	0.56
1:B:41:ASN:OD1	1:B:44:LEU:HD12	2.04	0.56
1:A:26:SER:O	1:A:27:VAL:C	2.44	0.56
1:A:285:VAL:HA	1:A:304:PHE:CE1	2.41	0.56
1:B:418:ILE:CG2	1:B:419:THR:H	2.15	0.56
2:D:44:LEU:HB3	2:D:49:VAL:CG2	2.36	0.56
1:B:441:PHE:N	1:B:441:PHE:CD2	2.68	0.56
2:C:26:VAL:O	2:C:26:VAL:CG1	2.54	0.56
1:A:106:ALA:O	1:A:108:VAL:N	2.36	0.56
1:B:27:VAL:CG2	1:B:70:LEU:CD2	2.73	0.56
1:B:298:LYS:HG2	1:B:300:ASP:HB2	1.86	0.56
1:B:353:VAL:O	1:B:354:GLN:C	2.43	0.56
2:D:108:ASP:CB	2:D:109:THR:HG22	2.36	0.56
2:D:17:ARG:NH1	2:D:17:ARG:CG	2.52	0.56
1:B:16:HIS:CD2	1:B:69:ARG:HG2	2.40	0.56
1:A:107:ALA:O	1:A:243:ALA:HB1	2.06	0.56
1:A:237:GLU:HA	1:A:240:LYS:CG	2.36	0.56
1:A:3:GLU:O	1:A:4:MET:CB	2.52	0.56
1:A:236:PRO:O	1:A:238:GLU:N	2.38	0.55
1:A:235:ASN:C	1:A:239:LEU:HD12	2.27	0.55
1:A:6:PRO:CD	1:A:32:ARG:CD	2.83	0.55
2:C:17:ARG:HB3	2:C:153:ALA:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:THR:CG2	2:D:132:GLY:N	2.69	0.55
1:A:13:LEU:CD1	1:A:24:LYS:HB3	2.36	0.55
1:B:41:ASN:ND2	1:B:43:GLU:HB3	2.21	0.55
1:B:61:VAL:CG2	1:B:61:VAL:O	2.53	0.55
3:B:906:ADP:C2'	3:B:906:ADP:O5'	2.53	0.55
1:B:98:SER:O	1:B:101:ARG:N	2.40	0.55
1:B:135:LEU:HD22	1:B:171:LYS:HZ3	1.37	0.55
1:B:325:ARG:C	1:B:327:PRO:CD	2.75	0.55
1:B:420:ILE:HG23	1:B:424:TYR:CD1	2.35	0.55
1:A:20:GLN:OE1	1:A:61:VAL:CG2	2.54	0.55
1:A:225:LEU:O	1:A:226:ILE:C	2.45	0.55
1:A:418:ILE:HG23	1:A:419:THR:H	1.72	0.55
1:B:167:GLN:CD	1:B:219:LYS:HG2	2.27	0.55
1:B:240:LYS:HB3	1:B:294:HIS:CD2	2.41	0.55
1:B:52:ASN:CG	1:B:304:PHE:HB2	2.25	0.55
1:B:403:MET:HE1	1:B:420:ILE:CD1	2.23	0.55
2:C:9:ILE:HD11	2:C:53:PHE:O	2.05	0.55
2:D:118:GLU:HG3	2:C:4:PHE:CD1	2.41	0.55
1:A:122:ARG:CZ	1:A:126:LEU:HD11	2.33	0.55
1:B:20:GLN:OE1	1:B:61:VAL:HG21	2.07	0.55
1:B:351:ILE:O	1:B:353:VAL:N	2.39	0.55
2:C:140:GLY:C	2:C:142:ALA:H	2.10	0.55
2:C:35:LYS:HG2	2:C:36:HIS:N	2.21	0.55
2:D:28:PHE:CG	2:D:29:GLY:N	2.75	0.55
1:A:344:LEU:HD11	1:A:376:ILE:HG22	1.88	0.55
1:A:283:PRO:O	1:A:287:GLY:N	2.38	0.55
1:A:18:ILE:CD1	1:A:343:ILE:HA	2.37	0.55
1:A:353:VAL:O	1:A:354:GLN:C	2.45	0.55
1:B:438:LEU:CD2	1:B:442:ILE:HD12	2.37	0.55
2:C:20:MET:HE2	2:C:41:VAL:CG1	2.28	0.55
2:D:136:ALA:HB1	2:D:160:ALA:HB1	1.89	0.55
1:A:119:ASN:HB3	1:A:233:LEU:HD13	1.87	0.55
1:A:100:ILE:CG1	1:A:284:LEU:HD22	2.27	0.55
1:A:384:ASN:OD1	1:A:394:ARG:HD2	2.06	0.55
1:B:257:GLU:O	1:B:259:ASP:N	2.40	0.55
1:B:31:LEU:HD22	1:B:70:LEU:HD11	1.89	0.55
2:D:21:SER:OG	2:D:157:ALA:HB1	2.07	0.55
1:A:86:PHE:CE2	1:A:99:ILE:HD11	2.42	0.55
1:B:149:GLN:C	1:B:152:PRO:HD2	2.26	0.55
1:B:372:GLY:O	1:B:376:ILE:N	2.35	0.55
1:B:86:PHE:CB	1:B:277:VAL:HG21	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:28:PHE:CG	2:C:29:GLY:N	2.75	0.55
2:C:53:PHE:CG	2:C:54:ALA:N	2.75	0.55
2:D:110:LEU:HD22	2:D:110:LEU:C	2.28	0.55
1:A:424:TYR:O	1:A:425:VAL:C	2.46	0.54
1:A:20:GLN:OE1	1:A:61:VAL:HG21	2.07	0.54
1:B:79:ILE:HD11	1:B:102:ASP:C	2.27	0.54
1:B:212:LYS:HZ3	1:B:212:LYS:HB2	1.72	0.54
1:B:299:THR:HA	1:B:302:ILE:HD12	1.89	0.54
1:B:80:LYS:HA	1:B:254:PHE:O	2.07	0.54
2:C:78:LEU:O	2:C:79:LYS:C	2.45	0.54
2:D:95:LEU:HD23	2:D:98:LEU:HD12	1.87	0.54
1:B:390:ILE:HG22	1:B:393:ARG:HD2	1.89	0.54
1:B:390:ILE:CD1	1:B:394:ARG:HH12	1.88	0.54
1:B:61:VAL:O	1:B:61:VAL:HG23	2.07	0.54
1:A:360:ALA:HA	1:A:364:VAL:O	2.07	0.54
1:A:351:ILE:O	1:A:354:GLN:HB2	2.07	0.54
1:B:319:ILE:HG23	1:B:320:PRO:HD2	1.89	0.54
2:C:143:LEU:O	2:C:147:ALA:N	2.32	0.54
2:D:39:ARG:HB2	2:D:39:ARG:CZ	2.37	0.54
1:A:259:ASP:HB3	1:A:310:PHE:CE2	2.42	0.54
1:A:341:GLU:O	1:A:344:LEU:HB2	2.08	0.54
1:A:369:THR:OG1	1:A:421:ASP:HB2	2.08	0.54
1:B:413:LEU:CD2	1:B:413:LEU:N	2.62	0.54
1:A:247:VAL:HG12	1:A:302:ILE:HD11	1.88	0.54
1:B:359:MET:HG2	1:B:366:ILE:HD12	1.79	0.54
1:B:429:LEU:O	1:B:431:ALA:N	2.40	0.54
2:D:132:GLY:O	2:D:133:GLY:C	2.45	0.54
1:B:100:ILE:HD12	1:B:290:VAL:CG2	2.21	0.54
1:B:13:LEU:HD12	1:B:24:LYS:HB3	1.89	0.54
1:B:64:THR:HG23	1:B:254:PHE:CE1	2.42	0.54
2:C:60:ALA:O	2:C:61:PHE:O	2.25	0.54
2:C:89:TRP:CD1	2:C:95:LEU:HB3	2.43	0.54
2:D:129:ILE:CG2	2:D:130:GLY:H	2.20	0.54
2:D:60:ALA:O	2:D:61:PHE:O	2.25	0.54
1:B:70:LEU:HA	1:B:73:LEU:HD21	1.90	0.54
1:B:61:VAL:N	3:B:906:ADP:O2B	2.37	0.54
2:D:112:LEU:HD22	2:D:113:VAL:H	1.71	0.54
1:A:379:ALA:O	1:A:380:ALA:C	2.46	0.53
1:B:282:LEU:CB	1:B:283:PRO:HD2	2.36	0.53
1:B:79:ILE:HG22	1:B:80:LYS:N	2.23	0.53
1:B:96:VAL:HG11	1:B:280:ASP:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:110:LEU:HD22	2:C:111:LEU:H	1.69	0.53
2:D:67:PHE:CD2	2:D:85:LEU:CD2	2.86	0.53
1:A:403:MET:HE3	1:A:420:ILE:CD1	2.31	0.53
1:B:104:THR:HG22	1:B:247:VAL:HG21	1.90	0.53
1:B:100:ILE:CD1	1:B:284:LEU:CD2	2.68	0.53
1:B:253:VAL:HG23	1:B:304:PHE:CD2	2.43	0.53
1:B:365:ASN:HB3	1:B:417:ASN:HB2	1.90	0.53
2:C:80:ARG:HH11	2:C:80:ARG:CG	2.05	0.53
1:A:70:LEU:HD12	1:A:71:ALA:HA	1.89	0.53
1:B:70:LEU:HD12	1:B:71:ALA:HA	1.90	0.53
1:B:69:ARG:O	1:B:73:LEU:HD23	2.09	0.53
2:C:103:ILE:CG1	2:C:129:ILE:HD12	2.30	0.53
2:C:5:HIS:HB2	2:C:27:THR:HB	1.91	0.53
1:A:168:LEU:N	1:A:218:ILE:HG22	2.23	0.53
1:A:362:GLU:OE1	1:B:32:ARG:NE	2.41	0.53
1:B:153:SER:HA	1:B:156:ARG:HB3	1.90	0.53
1:B:6:PRO:HD2	1:B:32:ARG:CD	2.39	0.53
2:D:101:MET:CB	2:D:112:LEU:HD21	2.39	0.53
1:A:399:LEU:O	1:A:402:LEU:N	2.41	0.53
1:B:255:ILE:HD11	1:B:304:PHE:CE2	2.44	0.53
1:A:432:LEU:H	1:A:434:ALA:N	2.05	0.53
1:B:390:ILE:O	1:B:390:ILE:CG2	2.56	0.53
2:C:23:ASP:CB	2:C:172:ASN:ND2	2.55	0.53
1:B:145:GLN:C	1:B:147:GLU:H	2.12	0.53
1:B:368:PHE:HB2	1:B:373:ILE:HD11	1.91	0.53
1:B:79:ILE:CG2	1:B:80:LYS:N	2.72	0.53
1:B:313:ALA:HB1	1:B:317:ASP:OD2	2.08	0.53
2:C:65:GLU:O	2:C:68:GLU:N	2.42	0.53
2:D:110:LEU:CD2	2:D:110:LEU:C	2.73	0.53
1:A:360:ALA:O	1:A:362:GLU:N	2.41	0.53
1:A:88:GLU:HB2	1:A:92:VAL:H	1.73	0.53
1:B:104:THR:HA	1:B:107:ALA:HB3	1.89	0.53
2:C:172:ASN:ND2	2:C:172:ASN:H	1.94	0.53
1:B:394:ARG:O	1:B:395:LEU:C	2.48	0.52
2:C:13:GLN:HG3	2:C:105:MET:CE	2.38	0.52
2:C:79:LYS:O	2:C:82:ALA:HB3	2.09	0.52
2:D:112:LEU:HD13	2:D:120:ILE:HD12	1.90	0.52
1:A:315:PRO:C	1:A:317:ASP:H	2.13	0.52
2:C:25:GLN:HB2	2:C:172:ASN:CB	2.38	0.52
2:D:23:ASP:CB	2:D:172:ASN:ND2	2.54	0.52
1:A:103:LEU:HD12	1:A:247:VAL:HG13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:VAL:HG22	2:C:13:GLN:N	2.24	0.52
2:D:104:VAL:HG22	2:D:111:LEU:HB2	1.91	0.52
2:D:177:LEU:HD22	2:D:178:GLU:N	2.24	0.52
1:A:282:LEU:O	1:A:283:PRO:C	2.47	0.52
1:A:100:ILE:CD1	1:A:299:THR:CG2	2.85	0.52
1:A:432:LEU:O	1:A:435:ASP:N	2.43	0.52
1:A:55:MET:CE	1:A:63:LYS:HA	2.40	0.52
1:B:125:GLU:HA	1:B:128:GLU:CD	2.29	0.52
1:B:338:SER:O	1:B:340:PHE:N	2.42	0.52
1:B:351:ILE:O	1:B:354:GLN:HB2	2.09	0.52
1:B:421:ASP:O	1:B:422:ALA:C	2.48	0.52
1:A:100:ILE:CD1	1:A:290:VAL:HG21	2.40	0.52
1:A:48:VAL:O	1:A:301:HIS:HE1	1.92	0.52
1:A:86:PHE:CZ	1:A:99:ILE:HG13	2.45	0.52
1:B:336:THR:O	1:B:339:ASP:HB2	2.10	0.52
1:B:4:MET:HG2	1:B:8:GLU:HB2	1.91	0.52
1:A:259:ASP:OD1	1:A:309:ALA:N	2.42	0.52
1:B:86:PHE:HB2	1:B:277:VAL:HG21	1.91	0.52
1:B:310:PHE:HE1	1:B:315:PRO:CA	2.23	0.52
1:B:369:THR:OG1	1:B:421:ASP:HB2	2.09	0.52
2:C:152:SER:HB3	2:C:155:GLU:CD	2.30	0.52
2:C:68:GLU:O	2:C:69:ALA:C	2.47	0.52
1:A:6:PRO:HD3	1:A:32:ARG:CD	2.37	0.52
1:B:149:GLN:O	1:B:152:PRO:HD2	2.10	0.52
1:B:337:THR:O	1:B:340:PHE:HB2	2.09	0.52
2:C:178:GLU:OE2	2:C:178:GLU:HA	2.09	0.52
2:C:27:THR:HG21	2:C:170:TYR:CE2	2.45	0.52
2:C:82:ALA:O	2:C:83:VAL:C	2.44	0.52
1:A:394:ARG:HG2	1:A:398:VAL:HG23	1.92	0.52
1:A:61:VAL:HB	1:A:335:LEU:CD1	2.28	0.52
1:B:168:LEU:N	1:B:218:ILE:HG22	2.25	0.52
1:B:360:ALA:HA	1:B:364:VAL:O	2.09	0.52
1:B:413:LEU:O	1:B:416:GLN:HB2	2.10	0.52
2:C:163:THR:O	2:C:164:ALA:C	2.47	0.52
1:A:148:GLN:HA	1:A:151:GLU:HB2	1.91	0.52
1:A:268:SER:OG	1:A:312:ILE:HD13	2.10	0.52
1:A:342:ARG:O	1:A:347:PRO:HD2	2.10	0.52
1:B:322:LEU:C	1:B:324:GLY:H	2.13	0.52
1:B:32:ARG:NH2	1:B:35:TRP:CZ3	2.77	0.52
1:B:3:GLU:HG2	1:B:4:MET:N	2.24	0.52
1:A:31:LEU:HD22	1:A:70:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:MET:HG2	1:A:366:ILE:HD13	1.85	0.52
1:A:67:ALA:O	1:A:68:ARG:C	2.48	0.52
3:A:905:ADP:C5'	3:A:905:ADP:C8	2.93	0.52
1:B:134:VAL:HG13	1:B:171:LYS:HD3	1.92	0.52
2:C:8:THR:CG2	2:C:132:GLY:N	2.71	0.52
1:A:25:ARG:O	1:A:26:SER:C	2.47	0.51
1:A:322:LEU:O	1:A:325:ARG:N	2.33	0.51
1:A:336:THR:N	1:A:339:ASP:HB2	2.25	0.51
1:A:3:GLU:CG	1:A:4:MET:H	2.24	0.51
1:B:336:THR:H	1:B:339:ASP:CG	2.13	0.51
1:B:98:SER:O	1:B:99:ILE:C	2.49	0.51
2:C:110:LEU:HD22	2:C:110:LEU:C	2.31	0.51
2:D:80:ARG:NH1	2:D:80:ARG:HG2	2.05	0.51
1:A:251:GLY:O	1:A:252:ILE:HG13	2.09	0.51
1:A:82:GLU:OE1	1:A:256:ASP:HB3	2.11	0.51
1:B:131:ILE:CG2	1:B:135:LEU:HD11	2.29	0.51
1:B:217:LYS:HB2	1:B:220:ASP:OD2	2.11	0.51
1:B:225:LEU:O	1:B:226:ILE:C	2.49	0.51
1:B:20:GLN:NE2	1:B:332:LEU:CB	2.73	0.51
1:B:52:ASN:OD1	1:B:304:PHE:CB	2.52	0.51
2:C:104:VAL:HG22	2:C:111:LEU:HB2	1.93	0.51
2:D:147:ALA:HB1	2:D:150:SER:HB3	1.92	0.51
1:A:237:GLU:N	1:A:240:LYS:CE	2.66	0.51
1:B:283:PRO:O	1:B:284:LEU:C	2.48	0.51
1:B:322:LEU:C	1:B:324:GLY:N	2.61	0.51
1:B:432:LEU:C	1:B:434:ALA:N	2.64	0.51
2:D:20:MET:HE1	2:D:51:ALA:O	2.08	0.51
1:B:171:LYS:HD2	1:B:218:ILE:CD1	2.41	0.51
1:B:80:LYS:HG3	1:B:254:PHE:HD1	1.75	0.51
2:C:114:SER:O	2:C:116:THR:N	2.44	0.51
1:B:13:LEU:O	1:B:16:HIS:N	2.42	0.51
1:B:344:LEU:HD11	1:B:376:ILE:HG22	1.91	0.51
1:B:429:LEU:O	1:B:430:ASP:C	2.49	0.51
1:A:252:ILE:HG12	1:A:303:LEU:HB3	1.92	0.51
2:D:27:THR:HG21	2:D:170:TYR:CD2	2.46	0.51
1:A:253:VAL:CG2	1:A:304:PHE:CD2	2.92	0.51
1:A:29:ILE:O	1:A:29:ILE:HG22	2.10	0.51
1:A:360:ALA:O	1:A:363:GLY:N	2.25	0.51
1:A:338:SER:O	1:A:340:PHE:N	2.43	0.51
1:B:349:ALA:O	1:B:350:SER:C	2.49	0.51
1:B:418:ILE:HG23	1:B:419:THR:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:172:ASN:N	2:C:172:ASN:ND2	2.53	0.51
2:D:140:GLY:O	2:D:142:ALA:N	2.44	0.51
1:A:318:LEU:HB2	1:A:323:GLN:HG2	1.93	0.51
1:B:303:LEU:HG	1:B:304:PHE:N	2.25	0.51
1:B:421:ASP:O	1:B:424:TYR:N	2.44	0.51
1:B:375:ARG:CB	1:B:425:VAL:HG11	2.41	0.51
1:B:81:VAL:HG21	1:B:99:ILE:HG12	1.93	0.51
1:A:246:ALA:O	1:A:247:VAL:O	2.29	0.50
1:A:5:THR:CG2	1:A:8:GLU:HG3	2.28	0.50
1:B:12:GLU:HA	1:B:15:LYS:HD3	1.93	0.50
1:A:268:SER:CB	1:A:312:ILE:CG2	2.75	0.50
1:A:254:PHE:CZ	1:A:307:SER:HB2	2.46	0.50
1:B:135:LEU:CB	1:B:171:LYS:HZ3	2.22	0.50
1:B:251:GLY:C	1:B:252:ILE:CG1	2.76	0.50
2:D:177:LEU:CD2	2:D:178:GLU:N	2.74	0.50
2:D:39:ARG:HA	2:D:176:ILE:CD1	2.41	0.50
2:D:105:MET:HE3	2:D:110:LEU:HG	1.93	0.50
2:D:177:LEU:HD23	2:D:178:GLU:H	1.76	0.50
2:D:68:GLU:O	2:D:70:LYS:N	2.44	0.50
1:B:399:LEU:O	1:B:400:GLU:C	2.49	0.50
2:D:5:HIS:HB2	2:D:27:THR:HB	1.93	0.50
1:A:149:GLN:C	1:A:151:GLU:H	2.13	0.50
1:A:31:LEU:CD2	1:A:70:LEU:CD1	2.89	0.50
1:A:4:MET:HG2	1:A:8:GLU:HB2	1.92	0.50
2:D:95:LEU:O	2:D:98:LEU:HB2	2.12	0.50
1:A:322:LEU:O	1:A:324:GLY:N	2.44	0.50
1:A:79:ILE:HD11	1:A:102:ASP:C	2.29	0.50
1:B:19:GLY:O	1:B:24:LYS:HE2	2.11	0.50
1:B:37:ARG:HG2	1:B:37:ARG:HH11	1.75	0.50
1:B:83:ALA:O	1:B:84:THR:O	2.29	0.50
1:B:84:THR:O	1:B:86:PHE:N	2.45	0.50
2:C:151:MET:HG3	2:C:156:ILE:CG1	2.40	0.50
1:A:108:VAL:O	1:A:111:VAL:N	2.45	0.50
1:A:25:ARG:O	1:A:26:SER:O	2.30	0.50
1:A:98:SER:OG	1:A:99:ILE:N	2.43	0.50
1:B:79:ILE:CD1	1:B:102:ASP:C	2.79	0.50
1:B:299:THR:HA	1:B:302:ILE:CD1	2.42	0.50
1:B:20:GLN:NE2	1:B:332:LEU:HB3	2.27	0.50
1:B:87:THR:HG23	1:B:88:GLU:N	2.27	0.50
1:A:436:GLU:O	1:A:439:SER:OG	2.28	0.50
1:A:441:PHE:HA	1:B:315:PRO:CG	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:O	1:A:98:SER:HB3	2.11	0.50
1:B:57:GLY:O	1:B:58:PRO:O	2.30	0.50
2:C:153:ALA:O	2:C:155:GLU:N	2.44	0.50
1:A:16:HIS:C	1:A:17:ILE:HG13	2.32	0.50
1:A:311:GLN:HE22	2:D:73:GLU:HA	1.77	0.50
1:B:27:VAL:HA	1:B:53:ILE:CD1	2.42	0.50
2:C:132:GLY:O	2:C:135:TYR:N	2.45	0.50
1:A:135:LEU:CD2	1:A:171:LYS:HZ2	1.06	0.49
1:A:247:VAL:O	1:A:248:GLU:C	2.49	0.49
1:A:277:VAL:O	1:A:278:GLN:C	2.49	0.49
1:A:371:SER:O	1:A:422:ALA:HB2	2.12	0.49
1:B:21:ASP:HA	1:B:24:LYS:HG3	1.94	0.49
1:B:319:ILE:HG23	1:B:321:GLU:OE2	2.12	0.49
1:B:326:LEU:N	1:B:327:PRO:CD	2.74	0.49
1:B:330:VAL:CG2	1:B:330:VAL:O	2.58	0.49
1:B:340:PHE:C	1:B:342:ARG:N	2.65	0.49
3:B:906:ADP:C5'	3:B:906:ADP:C8	2.91	0.49
1:B:88:GLU:O	1:B:91:TYR:HA	2.12	0.49
1:A:364:VAL:HG12	1:A:365:ASN:O	2.12	0.49
1:B:375:ARG:O	1:B:376:ILE:O	2.30	0.49
1:B:439:SER:O	1:B:440:ARG:C	2.46	0.49
1:A:390:ILE:CG2	1:A:390:ILE:O	2.60	0.49
1:A:87:THR:HG23	1:A:88:GLU:N	2.28	0.49
1:B:148:GLN:HA	1:B:151:GLU:HB2	1.93	0.49
1:B:20:GLN:OE1	1:B:61:VAL:CG2	2.60	0.49
1:B:70:LEU:O	1:B:73:LEU:CD2	2.60	0.49
1:A:219:LYS:C	1:A:220:ASP:O	2.49	0.49
1:A:221:ALA:HA	1:A:224:LEU:HB2	1.94	0.49
1:B:43:GLU:HG2	1:B:44:LEU:HG	1.94	0.49
2:C:44:LEU:HB2	2:C:49:VAL:CG2	2.43	0.49
2:C:72:GLU:C	2:C:74:TYR:N	2.66	0.49
1:A:246:ALA:O	1:A:247:VAL:C	2.49	0.49
1:B:21:ASP:O	1:B:24:LYS:HG3	2.12	0.49
2:C:135:TYR:CD2	2:C:135:TYR:N	2.76	0.49
2:C:78:LEU:O	2:C:81:ALA:N	2.45	0.49
1:A:123:ALA:CA	1:A:126:LEU:HD12	2.42	0.49
1:A:351:ILE:O	1:A:353:VAL:N	2.46	0.49
1:A:55:MET:HE2	1:A:63:LYS:HB3	1.95	0.49
1:A:83:ALA:O	1:A:84:THR:O	2.31	0.49
2:C:20:MET:CE	2:C:52:GLY:N	2.75	0.49
1:B:282:LEU:O	1:B:283:PRO:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:PHE:HB3	1:B:373:ILE:HD11	1.94	0.49
1:A:241:GLN:O	1:A:244:ILE:HB	2.13	0.49
1:B:149:GLN:C	1:B:151:GLU:H	2.16	0.49
1:B:17:ILE:CD1	1:B:66:ILE:HA	2.43	0.49
2:C:110:LEU:CD2	2:C:110:LEU:C	2.72	0.49
2:D:172:ASN:N	2:D:172:ASN:ND2	2.55	0.49
1:A:310:PHE:HD1	1:A:314:LYS:CA	2.26	0.49
1:A:69:ARG:O	1:A:73:LEU:HD23	2.13	0.49
1:A:336:THR:H	1:A:339:ASP:CB	2.26	0.48
1:B:250:HIS:CD2	1:B:251:GLY:O	2.65	0.48
1:B:368:PHE:HB3	1:B:373:ILE:CG1	2.41	0.48
1:A:34:ARG:HG3	1:A:35:TRP:N	2.29	0.48
1:A:390:ILE:HG23	1:B:320:PRO:HB3	1.95	0.48
1:A:406:ILE:CD1	1:A:420:ILE:HD11	2.42	0.48
1:B:106:ALA:O	1:B:110:MET:HB2	2.12	0.48
2:C:81:ALA:O	2:C:82:ALA:C	2.51	0.48
2:D:161:LEU:O	2:D:164:ALA:HB3	2.11	0.48
1:B:372:GLY:O	1:B:375:ARG:N	2.46	0.48
1:B:7:ARG:O	1:B:8:GLU:C	2.51	0.48
2:C:62:THR:HG22	2:C:63:LEU:N	2.28	0.48
2:D:41:VAL:HG12	2:D:178:GLU:HG3	1.95	0.48
1:A:375:ARG:CB	1:A:425:VAL:HG11	2.41	0.48
2:C:49:VAL:O	2:C:50:LEU:HD23	2.14	0.48
1:B:408:TYR:C	1:B:410:ALA:H	2.17	0.48
2:C:110:LEU:HD23	2:C:111:LEU:N	2.25	0.48
1:A:421:ASP:O	1:A:422:ALA:C	2.51	0.48
1:A:84:THR:O	1:A:85:LYS:C	2.51	0.48
1:B:62:GLY:O	1:B:66:ILE:HG13	2.14	0.48
2:D:63:LEU:HD11	2:D:89:TRP:CE2	2.48	0.48
1:A:102:ASP:C	1:A:104:THR:H	2.16	0.48
1:B:286:GLU:HA	1:B:325:ARG:NH1	2.28	0.48
1:B:48:VAL:O	1:B:301:HIS:HE1	1.97	0.48
2:D:112:LEU:CB	2:D:120:ILE:HB	2.44	0.48
1:A:70:LEU:O	1:A:73:LEU:HD23	2.13	0.48
1:A:86:PHE:CZ	1:A:99:ILE:CG1	2.97	0.48
1:B:219:LYS:C	1:B:220:ASP:O	2.51	0.48
1:B:310:PHE:CE1	1:B:315:PRO:HA	2.45	0.48
2:C:35:LYS:NZ	2:C:38:ALA:HB2	2.29	0.48
2:D:78:LEU:O	2:D:79:LYS:C	2.51	0.48
1:A:288:CYS:O	1:A:299:THR:HG23	2.14	0.48
1:B:278:GLN:HB3	1:B:319:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ARG:O	1:B:38:MET:C	2.51	0.48
2:C:143:LEU:HD23	2:C:143:LEU:HA	1.38	0.48
2:D:104:VAL:O	2:D:110:LEU:CD2	2.62	0.48
2:D:110:LEU:HA	2:D:110:LEU:HD23	1.36	0.48
1:A:132:LEU:HD21	1:A:160:ARG:HG3	1.95	0.48
1:A:403:MET:N	1:A:403:MET:SD	2.86	0.48
1:A:48:VAL:HG12	1:A:49:THR:H	1.79	0.48
1:A:79:ILE:HD12	1:A:103:LEU:N	2.28	0.48
1:B:322:LEU:O	1:B:323:GLN:C	2.52	0.48
1:A:135:LEU:HD21	1:A:171:LYS:HZ2	1.10	0.47
1:A:320:PRO:O	1:A:321:GLU:C	2.53	0.47
2:C:44:LEU:CB	2:C:49:VAL:HG22	2.44	0.47
2:D:26:VAL:O	2:D:26:VAL:HG12	2.13	0.47
1:A:70:LEU:O	1:A:73:LEU:CD2	2.62	0.47
1:B:261:ILE:CG2	1:B:277:VAL:HG12	2.35	0.47
1:B:377:ALA:O	1:B:380:ALA:N	2.48	0.47
1:B:54:LEU:CD1	1:B:54:LEU:C	2.82	0.47
1:A:282:LEU:O	1:A:285:VAL:HG13	2.14	0.47
1:A:415:GLY:O	1:A:416:GLN:O	2.32	0.47
1:B:244:ILE:O	1:B:245:ASP:C	2.51	0.47
1:B:77:PRO:HD2	1:B:251:GLY:CA	2.45	0.47
1:B:282:LEU:O	1:B:284:LEU:N	2.48	0.47
1:A:246:ALA:O	1:A:250:HIS:N	2.47	0.47
1:A:125:GLU:HA	1:A:128:GLU:CD	2.34	0.47
1:A:135:LEU:CB	1:A:171:LYS:HZ3	2.28	0.47
2:D:174:GLN:HG2	2:D:174:GLN:H	1.52	0.47
2:D:17:ARG:HB3	2:D:153:ALA:HB3	1.97	0.47
1:A:224:LEU:O	1:A:227:GLU:N	2.47	0.47
1:B:128:GLU:C	1:B:130:ARG:H	2.17	0.47
1:B:18:ILE:HG23	1:B:342:ARG:HH21	1.79	0.47
1:B:340:PHE:O	1:B:342:ARG:N	2.47	0.47
1:B:406:ILE:CD1	1:B:420:ILE:HD11	2.45	0.47
1:B:61:VAL:HA	1:B:335:LEU:HD21	1.95	0.47
1:B:82:GLU:OE1	1:B:256:ASP:HB3	2.14	0.47
1:B:86:PHE:HD1	1:B:86:PHE:H	1.62	0.47
2:D:8:THR:HG23	2:D:131:SER:N	2.29	0.47
1:A:276:GLY:O	1:A:277:VAL:C	2.52	0.47
1:B:413:LEU:O	1:B:414:SER:C	2.52	0.47
2:C:12:VAL:HG22	2:C:13:GLN:H	1.79	0.47
1:A:302:ILE:HG22	1:A:303:LEU:N	2.29	0.47
1:A:45:ARG:HH21	1:A:46:HIS:CD2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:GLN:O	1:B:23:ALA:CB	2.62	0.47
1:B:29:ILE:O	1:B:29:ILE:HG22	2.14	0.47
1:B:37:ARG:HB3	1:B:38:MET:H	1.51	0.47
1:A:408:TYR:HE1	1:B:6:PRO:CB	2.28	0.47
2:D:134:ASN:O	2:D:137:LEU:N	2.48	0.47
1:A:322:LEU:C	1:A:324:GLY:N	2.68	0.47
1:A:322:LEU:C	1:A:324:GLY:H	2.17	0.47
1:A:399:LEU:O	1:A:400:GLU:C	2.52	0.47
1:A:355:TYR:CE2	1:A:403:MET:HG2	2.49	0.47
1:B:132:LEU:HD21	1:B:160:ARG:HG3	1.96	0.47
1:B:251:GLY:O	1:B:252:ILE:CG1	2.62	0.47
1:B:278:GLN:HB2	1:B:319:ILE:CD1	2.43	0.47
1:B:18:ILE:HD13	1:B:342:ARG:CB	2.44	0.47
1:B:340:PHE:O	1:B:343:ILE:N	2.47	0.47
1:B:342:ARG:O	1:B:347:PRO:HD2	2.14	0.47
1:B:409:ASP:O	1:B:412:ASP:HB2	2.15	0.47
1:B:425:VAL:O	1:B:427:LYS:N	2.48	0.47
2:C:152:SER:O	2:C:156:ILE:CD1	2.63	0.47
2:D:89:TRP:HD1	2:D:95:LEU:HB3	1.77	0.47
1:A:224:LEU:O	1:A:225:LEU:C	2.53	0.47
1:A:292:THR:O	1:A:293:LYS:O	2.33	0.47
1:A:310:PHE:HE1	1:A:315:PRO:N	2.11	0.47
1:A:315:PRO:O	1:A:318:LEU:HD12	2.15	0.47
1:A:346:GLU:N	1:A:347:PRO:CD	2.74	0.47
1:B:288:CYS:O	1:B:299:THR:HG23	2.14	0.47
2:C:164:ALA:C	2:C:166:GLU:H	2.16	0.47
2:C:25:GLN:HB2	2:C:172:ASN:HB3	1.97	0.47
2:D:163:THR:O	2:D:164:ALA:C	2.52	0.47
1:A:115:ALA:HB2	1:A:118:LYS:NZ	2.30	0.47
1:A:62:GLY:O	1:A:63:LYS:C	2.53	0.47
1:B:100:ILE:HG13	1:B:284:LEU:HD21	1.95	0.47
2:C:110:LEU:HD13	2:C:127:LEU:HD12	1.96	0.47
1:A:10:VAL:HG12	1:A:11:SER:N	2.29	0.46
1:A:168:LEU:HD13	1:A:219:LYS:CE	2.21	0.46
1:A:349:ALA:O	1:A:350:SER:C	2.50	0.46
1:B:20:GLN:OE1	1:B:332:LEU:HB3	2.15	0.46
1:B:271:ASP:HB3	1:B:273:SER:HB3	1.97	0.46
1:B:389:ASN:ND2	1:B:389:ASN:C	2.67	0.46
1:A:150:GLN:O	1:A:153:SER:HB2	2.15	0.46
1:A:31:LEU:CD2	1:A:70:LEU:HD13	2.46	0.46
1:B:100:ILE:CD1	1:B:290:VAL:CG2	2.85	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:THR:OG1	1:B:421:ASP:HA	2.15	0.46
2:D:120:ILE:HD11	2:C:4:PHE:CZ	2.50	0.46
2:D:82:ALA:O	2:D:83:VAL:C	2.50	0.46
1:A:282:LEU:HA	1:A:282:LEU:HD22	1.58	0.46
1:A:315:PRO:C	1:A:317:ASP:N	2.68	0.46
1:A:439:SER:O	1:A:440:ARG:C	2.54	0.46
1:B:278:GLN:NE2	1:B:319:ILE:N	2.58	0.46
2:C:110:LEU:HD23	2:C:110:LEU:HA	1.50	0.46
2:D:53:PHE:CG	2:D:54:ALA:N	2.83	0.46
1:A:243:ALA:O	1:A:246:ALA:CB	2.58	0.46
1:A:286:GLU:HA	1:A:325:ARG:NH1	2.31	0.46
1:A:6:PRO:HD2	1:A:32:ARG:CD	2.45	0.46
1:A:424:TYR:CZ	1:A:428:HIS:NE2	2.75	0.46
1:A:98:SER:O	1:A:101:ARG:HB3	2.15	0.46
1:B:45:ARG:HH21	1:B:46:HIS:CD2	2.33	0.46
1:B:6:PRO:HD3	1:B:32:ARG:CD	2.35	0.46
1:B:4:MET:CG	1:B:8:GLU:HB2	2.45	0.46
1:A:283:PRO:O	1:A:284:LEU:C	2.51	0.46
1:A:100:ILE:HD11	1:A:284:LEU:HD22	0.54	0.46
1:A:319:ILE:HA	1:A:320:PRO:HD2	1.71	0.46
1:B:36:ARG:O	1:B:37:ARG:O	2.34	0.46
1:B:37:ARG:O	1:B:39:GLN:N	2.48	0.46
2:D:25:GLN:N	2:D:172:ASN:OD1	2.49	0.46
1:A:100:ILE:CD1	1:A:299:THR:HG21	2.45	0.46
1:A:441:PHE:HA	1:B:315:PRO:HD2	1.96	0.46
1:A:79:ILE:HD12	1:A:103:LEU:CA	2.46	0.46
1:A:86:PHE:HE2	1:A:96:VAL:CA	2.24	0.46
1:B:150:GLN:O	1:B:153:SER:HB2	2.14	0.46
2:C:105:MET:HB3	2:C:110:LEU:HD21	1.97	0.46
2:D:45:PHE:O	2:D:46:ASN:C	2.54	0.46
1:A:83:ALA:CB	1:A:261:ILE:HD11	2.16	0.46
1:A:20:GLN:OE1	1:A:332:LEU:HB3	2.16	0.46
1:A:408:TYR:C	1:A:410:ALA:H	2.19	0.46
1:B:284:LEU:HA	1:B:284:LEU:HD23	1.66	0.46
1:B:350:SER:HG	1:B:352:THR:HG1	1.64	0.46
2:C:14:HIS:CE1	2:C:15:LYS:HE2	2.51	0.46
2:C:25:GLN:H	2:C:172:ASN:HD21	1.64	0.46
2:D:143:LEU:HD12	2:D:156:ILE:HG23	1.97	0.46
2:C:103:ILE:HD11	2:C:129:ILE:CG1	2.41	0.46
2:C:140:GLY:C	2:C:142:ALA:N	2.68	0.46
2:C:35:LYS:CD	2:C:38:ALA:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:95:LEU:HD23	2:C:98:LEU:CD1	2.45	0.46
2:D:110:LEU:C	2:D:111:LEU:CD1	2.73	0.46
1:A:275:GLU:O	1:A:278:GLN:HB2	2.16	0.46
1:A:292:THR:OG1	1:A:293:LYS:N	2.48	0.46
1:A:66:ILE:HD12	1:A:332:LEU:HD21	1.97	0.46
1:B:116:ILE:O	1:B:117:GLU:HG3	2.16	0.46
2:C:25:GLN:HB2	2:C:172:ASN:ND2	2.31	0.46
2:C:45:PHE:O	2:C:46:ASN:C	2.55	0.46
2:C:51:ALA:HA	2:C:103:ILE:O	2.16	0.46
2:D:110:LEU:HD23	2:D:111:LEU:H	1.81	0.46
1:B:221:ALA:N	1:B:224:LEU:HD13	2.31	0.46
1:B:330:VAL:O	1:B:330:VAL:HG23	2.16	0.46
2:D:106:ASN:O	2:D:107:GLN:C	2.54	0.46
2:D:105:MET:HB3	2:D:110:LEU:HG	1.98	0.46
1:A:81:VAL:HG21	1:A:99:ILE:HG12	1.98	0.45
1:A:251:GLY:C	1:A:252:ILE:CG1	2.78	0.45
1:A:315:PRO:O	1:A:317:ASP:N	2.49	0.45
2:C:33:VAL:O	2:C:33:VAL:HG12	2.16	0.45
2:D:152:SER:HB3	2:D:155:GLU:OE2	2.17	0.45
1:A:100:ILE:CD1	1:A:284:LEU:HD21	2.11	0.45
1:A:226:ILE:O	1:A:229:GLU:HB2	2.17	0.45
1:B:252:ILE:HG12	1:B:303:LEU:HB3	1.98	0.45
2:C:44:LEU:CB	2:C:49:VAL:CG2	2.94	0.45
1:A:21:ASP:HA	1:A:24:LYS:HG3	1.98	0.45
1:B:432:LEU:HB3	1:B:433:VAL:H	1.43	0.45
1:B:54:LEU:CD1	1:B:55:MET:N	2.73	0.45
2:C:89:TRP:CD2	2:C:115:GLY:HA2	2.52	0.45
2:C:89:TRP:HZ3	2:C:113:VAL:O	2.00	0.45
1:B:25:ARG:O	1:B:26:SER:C	2.54	0.45
1:B:117:GLU:HA	1:B:120:ARG:HB3	1.98	0.45
1:B:151:GLU:H	1:B:152:PRO:HD2	1.80	0.45
1:B:390:ILE:HD12	1:B:394:ARG:CZ	2.44	0.45
1:B:40:LEU:HA	1:B:40:LEU:HD23	1.55	0.45
2:C:137:LEU:O	2:C:141:ARG:HG3	2.16	0.45
2:C:39:ARG:CZ	2:C:39:ARG:HB2	2.47	0.45
2:D:67:PHE:HD2	2:D:85:LEU:HD23	1.81	0.45
2:D:89:TRP:NE1	2:D:95:LEU:HB3	2.31	0.45
1:A:123:ALA:CB	1:A:126:LEU:HD12	2.46	0.45
1:A:227:GLU:O	1:A:229:GLU:N	2.41	0.45
1:A:332:LEU:HA	1:A:333:GLN:OE1	2.17	0.45
1:A:31:LEU:HD22	1:A:70:LEU:CD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:THR:O	1:B:6:PRO:C	2.55	0.45
2:C:23:ASP:OD1	2:C:171:THR:HA	2.16	0.45
1:A:119:ASN:HB3	1:A:233:LEU:CD1	2.47	0.45
1:A:168:LEU:H	1:A:218:ILE:HG22	1.81	0.45
1:A:240:LYS:O	1:A:241:GLN:C	2.55	0.45
1:A:273:SER:OG	1:A:273:SER:O	2.33	0.45
1:A:438:LEU:O	1:A:439:SER:C	2.55	0.45
1:B:70:LEU:HA	1:B:73:LEU:CD2	2.47	0.45
1:B:106:ALA:C	1:B:108:VAL:N	2.68	0.45
2:D:26:VAL:O	2:D:26:VAL:HG13	2.17	0.45
2:D:39:ARG:NH1	2:D:39:ARG:HB2	2.32	0.45
2:D:58:ALA:O	2:D:59:ASP:C	2.53	0.45
2:D:89:TRP:CD1	2:D:95:LEU:CB	2.97	0.45
1:A:145:GLN:C	1:A:147:GLU:H	2.20	0.45
1:A:87:THR:CG2	1:A:88:GLU:N	2.80	0.45
1:B:66:ILE:HD12	1:B:332:LEU:HD21	1.98	0.45
2:C:78:LEU:HD23	2:C:111:LEU:HD23	1.93	0.45
1:A:104:THR:HG23	1:A:247:VAL:HG21	1.98	0.44
1:B:135:LEU:HD23	1:B:171:LYS:NZ	0.52	0.44
1:B:320:PRO:HG2	1:B:321:GLU:OE2	2.17	0.44
1:B:83:ALA:HB1	1:B:261:ILE:HD12	1.83	0.44
2:C:35:LYS:HD2	2:C:38:ALA:H	1.81	0.44
1:A:278:GLN:NE2	1:A:318:LEU:HB3	2.32	0.44
1:A:429:LEU:O	1:A:430:ASP:C	2.55	0.44
1:A:60:GLY:N	3:A:905:ADP:O2B	2.50	0.44
1:B:18:ILE:HD12	1:B:343:ILE:CB	2.45	0.44
1:B:104:THR:CG2	1:B:247:VAL:HG21	2.48	0.44
1:B:281:LEU:HD22	1:B:281:LEU:HA	1.25	0.44
1:B:34:ARG:O	1:B:35:TRP:O	2.35	0.44
2:D:10:PHE:CZ	2:D:126:ILE:HG23	2.52	0.44
2:D:26:VAL:HG12	2:D:35:LYS:N	2.20	0.44
1:A:7:ARG:O	1:A:10:VAL:HB	2.17	0.44
1:B:365:ASN:HD22	1:B:417:ASN:HD22	1.65	0.44
2:D:36:HIS:CD2	2:D:36:HIS:N	2.85	0.44
1:A:153:SER:HA	1:A:156:ARG:HB3	1.99	0.44
1:A:256:ASP:O	1:A:257:GLU:CB	2.49	0.44
1:A:290:VAL:HG23	1:A:299:THR:CG2	2.48	0.44
1:A:52:ASN:O	1:A:327:PRO:HG2	2.17	0.44
1:A:98:SER:HA	1:A:101:ARG:NH1	2.32	0.44
1:B:237:GLU:CA	1:B:240:LYS:HG2	2.44	0.44
2:D:65:GLU:O	2:D:68:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:HA	1:A:53:ILE:CD1	2.48	0.44
1:A:325:ARG:O	1:A:327:PRO:CD	2.55	0.44
1:B:23:ALA:O	1:B:24:LYS:C	2.56	0.44
1:B:279:ARG:O	1:B:282:LEU:HB2	2.17	0.44
1:B:441:PHE:HB2	1:B:442:ILE:HG13	1.99	0.44
2:C:83:VAL:O	2:C:85:LEU:N	2.51	0.44
1:A:10:VAL:O	1:A:13:LEU:HB2	2.18	0.44
1:A:171:LYS:HD2	1:A:218:ILE:HD11	1.99	0.44
1:B:353:VAL:C	1:B:355:TYR:N	2.68	0.44
2:D:114:SER:C	2:D:116:THR:H	2.20	0.44
2:D:160:ALA:O	2:D:163:THR:N	2.47	0.44
2:D:27:THR:HG21	2:D:170:TYR:CE2	2.52	0.44
2:D:82:ALA:O	2:D:85:LEU:HB3	2.17	0.44
1:A:171:LYS:HD2	1:A:218:ILE:HD12	1.96	0.44
1:A:403:MET:O	1:A:404:GLU:C	2.56	0.44
1:A:73:LEU:H	1:A:73:LEU:HD23	1.81	0.44
1:B:17:ILE:HG21	1:B:66:ILE:HG12	2.00	0.44
1:B:80:LYS:HG3	1:B:254:PHE:CD1	2.52	0.44
1:B:278:GLN:NE2	1:B:318:LEU:HB3	2.33	0.44
1:B:18:ILE:HD11	1:B:343:ILE:CA	2.38	0.44
1:B:62:GLY:HA2	3:B:906:ADP:O1A	2.18	0.44
2:C:110:LEU:C	2:C:111:LEU:CD1	2.74	0.44
1:A:272:VAL:HB	1:A:275:GLU:CB	2.46	0.44
1:B:268:SER:HB3	1:B:312:ILE:HG23	1.95	0.44
1:B:283:PRO:O	1:B:287:GLY:N	2.36	0.44
2:D:56:SER:O	2:D:59:ASP:N	2.51	0.44
1:A:119:ASN:ND2	1:A:122:ARG:HG2	2.18	0.44
1:B:359:MET:HG2	1:B:366:ILE:HD13	1.86	0.44
1:B:88:GLU:OE2	1:B:91:TYR:C	2.56	0.44
2:C:124:ASP:OD2	2:C:141:ARG:HD2	2.17	0.44
2:C:129:ILE:CG2	2:C:130:GLY:H	2.29	0.44
2:C:72:GLU:O	2:C:73:GLU:C	2.56	0.44
2:D:132:GLY:O	2:D:135:TYR:N	2.51	0.44
2:D:135:TYR:O	2:D:138:ALA:HB3	2.18	0.44
1:A:322:LEU:HD12	1:A:326:LEU:HD11	2.00	0.43
1:A:93:GLY:O	1:A:94:LYS:HD2	2.18	0.43
2:D:110:LEU:HD22	2:D:127:LEU:CD1	2.46	0.43
2:D:17:ARG:HB3	2:D:153:ALA:HB2	1.97	0.43
2:D:83:VAL:O	2:D:86:ALA:HB3	2.17	0.43
1:A:236:PRO:C	1:A:238:GLU:N	2.72	0.43
1:A:88:GLU:OE2	1:A:92:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:GLN:HE22	1:B:318:LEU:HB3	1.82	0.43
1:B:368:PHE:HB3	1:B:373:ILE:HG13	2.00	0.43
2:C:159:ALA:O	2:C:162:GLU:HB2	2.17	0.43
2:D:105:MET:HB3	2:D:110:LEU:CG	2.48	0.43
2:D:89:TRP:HD1	2:D:95:LEU:CB	2.31	0.43
1:A:110:MET:O	1:A:114:GLN:HB2	2.18	0.43
1:A:151:GLU:H	1:A:152:PRO:HD2	1.82	0.43
1:A:79:ILE:HB	1:A:103:LEU:HD23	1.99	0.43
1:B:13:LEU:CD1	1:B:24:LYS:HB3	2.47	0.43
1:B:24:LYS:O	1:B:25:ARG:C	2.56	0.43
1:B:331:GLU:C	1:B:332:LEU:HD12	2.38	0.43
1:B:356:LYS:O	1:B:360:ALA:N	2.50	0.43
2:C:77:ASN:O	2:C:78:LEU:C	2.56	0.43
2:D:10:PHE:O	2:D:21:SER:N	2.51	0.43
1:B:128:GLU:O	1:B:132:LEU:HG	2.19	0.43
1:B:224:LEU:O	1:B:226:ILE:N	2.51	0.43
1:B:298:LYS:HG3	1:B:300:ASP:HB2	2.00	0.43
1:B:310:PHE:N	1:B:310:PHE:CD2	2.85	0.43
1:B:20:GLN:CD	1:B:332:LEU:HB3	2.38	0.43
1:A:73:LEU:C	1:A:75:ASN:H	2.15	0.43
1:B:227:GLU:C	1:B:229:GLU:H	2.21	0.43
1:B:240:LYS:HB3	1:B:294:HIS:NE2	2.33	0.43
2:D:44:LEU:CB	2:D:49:VAL:HG22	2.47	0.43
1:A:336:THR:H	1:A:339:ASP:CG	2.21	0.43
1:B:363:GLY:O	1:B:415:GLY:N	2.51	0.43
1:B:397:THR:O	1:B:398:VAL:C	2.57	0.43
1:B:48:VAL:HG12	1:B:49:THR:H	1.83	0.43
2:C:174:GLN:H	2:C:174:GLN:HG2	1.56	0.43
2:C:17:ARG:NH1	2:C:17:ARG:CG	2.57	0.43
2:C:70:LYS:O	2:C:74:TYR:HD1	2.01	0.43
2:D:68:GLU:O	2:D:69:ALA:C	2.56	0.43
1:A:168:LEU:CD1	1:A:219:LYS:HZ2	2.26	0.43
1:A:254:PHE:CD2	1:A:305:ILE:O	2.72	0.43
1:A:335:LEU:HD23	1:A:343:ILE:HD11	1.99	0.43
1:A:441:PHE:HA	1:B:315:PRO:CD	2.49	0.43
1:B:261:ILE:HD13	1:B:277:VAL:HG12	1.99	0.43
1:B:310:PHE:CE1	1:B:315:PRO:CA	3.01	0.43
2:D:44:LEU:HB3	2:D:49:VAL:HG22	1.99	0.43
1:A:55:MET:HE1	1:A:63:LYS:HA	2.01	0.43
1:B:224:LEU:O	1:B:227:GLU:N	2.51	0.43
1:B:3:GLU:CG	1:B:4:MET:N	2.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:SER:O	1:A:99:ILE:C	2.57	0.43
2:C:137:LEU:HD21	2:C:141:ARG:NH1	2.33	0.43
2:D:62:THR:HG22	2:D:63:LEU:N	2.33	0.43
1:A:153:SER:C	1:A:155:ALA:N	2.71	0.43
1:A:24:LYS:O	1:A:27:VAL:HG13	2.18	0.43
1:A:85:LYS:HB3	1:A:86:PHE:CD1	2.54	0.43
1:B:111:VAL:HG21	1:B:243:ALA:HA	2.00	0.43
1:B:377:ALA:O	1:B:378:GLU:C	2.56	0.43
1:B:57:GLY:HA2	1:B:58:PRO:HD2	1.77	0.43
1:B:73:LEU:HG	1:B:74:ALA:H	1.77	0.43
2:C:141:ARG:H	2:C:141:ARG:HG2	1.74	0.43
1:A:390:ILE:HG22	1:A:393:ARG:HB2	2.01	0.42
1:B:241:GLN:HA	1:B:244:ILE:HD12	2.01	0.42
2:C:53:PHE:CD1	2:C:101:MET:O	2.72	0.42
1:A:136:ILE:O	1:A:136:ILE:CG2	2.67	0.42
1:B:167:GLN:HB2	1:B:168:LEU:H	1.58	0.42
1:B:31:LEU:CD2	1:B:70:LEU:HD13	2.49	0.42
2:D:25:GLN:HB2	2:D:172:ASN:CB	2.49	0.42
2:D:35:LYS:HG2	2:D:36:HIS:N	2.34	0.42
1:A:140:LYS:HE3	1:A:140:LYS:O	2.19	0.42
1:A:310:PHE:N	1:A:310:PHE:CD2	2.87	0.42
1:A:96:VAL:HG21	1:A:280:ASP:HB3	2.01	0.42
1:A:18:ILE:HG23	1:A:342:ARG:NH2	2.30	0.42
1:A:351:ILE:O	1:A:354:GLN:N	2.52	0.42
1:B:14:ASP:OD2	1:B:14:ASP:N	2.52	0.42
1:B:20:GLN:HB3	1:B:20:GLN:HE21	1.52	0.42
1:A:390:ILE:CD1	1:B:323:GLN:CD	2.86	0.42
1:B:391:GLY:O	1:B:392:ALA:C	2.56	0.42
1:B:403:MET:CE	1:B:406:ILE:HD12	2.48	0.42
1:B:97:ASP:OD2	1:B:97:ASP:C	2.57	0.42
1:A:54:LEU:HB2	1:A:326:LEU:HB3	2.01	0.42
2:D:54:ALA:HB3	2:D:100:ALA:CB	2.49	0.42
2:D:67:PHE:CD2	2:D:85:LEU:HD23	2.53	0.42
1:A:337:THR:O	1:A:340:PHE:HB2	2.19	0.42
1:A:372:GLY:C	1:A:376:ILE:HG13	2.39	0.42
1:B:271:ASP:O	1:B:274:ARG:HG2	2.20	0.42
2:C:21:SER:HA	2:C:176:ILE:O	2.19	0.42
2:D:110:LEU:HD23	2:D:111:LEU:N	2.33	0.42
1:A:285:VAL:HA	1:A:304:PHE:HE1	1.83	0.42
1:B:265:GLY:O	1:B:266:GLU:HB2	2.20	0.42
1:B:327:PRO:CG	1:B:328:ILE:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:PHE:O	2:D:29:GLY:O	2.38	0.42
1:A:246:ALA:O	1:A:250:HIS:CA	2.68	0.42
1:A:54:LEU:HB3	1:A:329:ARG:CD	2.43	0.42
1:A:86:PHE:CE2	1:A:99:ILE:CD1	3.03	0.42
1:B:154:ALA:O	1:B:155:ALA:HB2	2.20	0.42
1:B:168:LEU:CD1	1:B:219:LYS:HZ2	2.23	0.42
1:B:218:ILE:O	1:B:220:ASP:O	2.38	0.42
1:B:247:VAL:O	1:B:248:GLU:C	2.57	0.42
1:B:438:LEU:C	1:B:440:ARG:N	2.71	0.42
2:C:9:ILE:HD13	2:C:53:PHE:O	2.09	0.42
2:D:161:LEU:O	2:D:162:GLU:C	2.58	0.42
1:A:107:ALA:O	1:A:108:VAL:HG23	2.20	0.42
1:A:408:TYR:CE2	1:B:25:ARG:HG2	2.55	0.42
1:B:123:ALA:HA	1:B:126:LEU:HD12	2.02	0.42
2:C:164:ALA:O	2:C:166:GLU:N	2.53	0.42
2:D:78:LEU:HD21	2:D:104:VAL:HG23	2.02	0.42
1:B:168:LEU:HD11	1:B:219:LYS:CD	2.18	0.42
1:B:52:ASN:HB2	1:B:325:ARG:O	2.20	0.42
2:C:44:LEU:O	2:C:49:VAL:HG22	2.20	0.42
1:A:302:ILE:CG2	1:A:303:LEU:N	2.83	0.41
1:A:268:SER:CB	1:A:312:ILE:HD13	2.50	0.41
1:A:344:LEU:HA	1:A:344:LEU:HD23	1.89	0.41
1:A:375:ARG:O	1:A:376:ILE:C	2.59	0.41
1:B:359:MET:CB	1:B:366:ILE:CD1	2.79	0.41
2:C:56:SER:OG	2:C:59:ASP:OD1	2.38	0.41
1:A:263:LYS:O	1:A:264:ARG:C	2.58	0.41
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.66	0.41
1:A:32:ARG:O	1:A:36:ARG:HG3	2.19	0.41
1:A:27:VAL:CG2	1:A:70:LEU:CD2	2.84	0.41
1:A:85:LYS:HB3	1:A:86:PHE:HD1	1.85	0.41
1:A:96:VAL:HG23	1:A:97:ASP:N	2.35	0.41
2:C:114:SER:C	2:C:116:THR:H	2.23	0.41
2:D:10:PHE:CE1	2:D:126:ILE:HG23	2.55	0.41
2:D:163:THR:O	2:D:166:GLU:HB3	2.19	0.41
2:D:23:ASP:OD1	2:D:171:THR:HA	2.20	0.41
2:D:68:GLU:HG3	2:D:72:GLU:OE1	2.20	0.41
1:A:253:VAL:HG21	1:A:304:PHE:HE2	1.80	0.41
1:A:310:PHE:CD1	1:A:315:PRO:N	2.87	0.41
1:A:403:MET:O	1:A:407:SER:N	2.52	0.41
1:A:432:LEU:HA	1:A:432:LEU:HD13	1.92	0.41
1:B:116:ILE:CG2	1:B:116:ILE:O	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ASN:HB3	1:B:233:LEU:CD1	2.49	0.41
1:B:336:THR:O	1:B:339:ASP:N	2.53	0.41
2:C:121:GLU:HA	2:C:122:PRO:HD3	1.92	0.41
1:A:160:ARG:HH11	1:A:160:ARG:HG2	1.86	0.41
1:A:368:PHE:HB3	1:A:373:ILE:HD11	2.02	0.41
1:B:24:LYS:H	1:B:24:LYS:HG2	1.50	0.41
1:B:355:TYR:HD2	1:B:403:MET:HG2	1.81	0.41
2:C:63:LEU:HD11	2:C:89:TRP:CZ2	2.55	0.41
2:C:8:THR:HG23	2:C:130:GLY:C	2.41	0.41
2:D:159:ALA:HA	2:D:162:GLU:HB2	2.02	0.41
1:A:131:ILE:CG2	1:A:135:LEU:HD11	2.38	0.41
1:A:281:LEU:O	1:A:282:LEU:O	2.38	0.41
1:A:320:PRO:O	1:A:323:GLN:HB2	2.19	0.41
2:C:17:ARG:HB3	2:C:153:ALA:HB2	1.98	0.41
2:C:35:LYS:HG2	2:C:37:THR:H	1.86	0.41
2:D:51:ALA:HA	2:D:103:ILE:O	2.21	0.41
2:D:72:GLU:C	2:D:74:TYR:N	2.74	0.41
1:A:136:ILE:O	1:A:136:ILE:HG22	2.20	0.41
1:A:338:SER:C	1:A:340:PHE:N	2.73	0.41
1:A:40:LEU:HA	1:A:40:LEU:HD23	1.53	0.41
1:A:428:HIS:O	1:A:429:LEU:HD12	2.20	0.41
1:A:79:ILE:HD12	1:A:103:LEU:HA	2.01	0.41
1:B:102:ASP:C	1:B:104:THR:H	2.23	0.41
1:B:272:VAL:HB	1:B:275:GLU:HB2	2.02	0.41
1:B:274:ARG:O	1:B:277:VAL:N	2.49	0.41
1:B:384:ASN:HB3	1:B:389:ASN:OD1	2.20	0.41
1:B:70:LEU:HD12	1:B:71:ALA:CA	2.51	0.41
1:B:87:THR:CG2	1:B:88:GLU:N	2.83	0.41
2:C:78:LEU:HD21	2:C:104:VAL:HG23	2.02	0.41
1:A:128:GLU:C	1:A:130:ARG:H	2.23	0.41
1:A:168:LEU:HD12	1:A:219:LYS:CG	2.42	0.41
1:A:103:LEU:O	1:A:247:VAL:HG22	2.20	0.41
1:B:374:LYS:O	1:B:378:GLU:HG3	2.21	0.41
1:B:5:THR:O	1:B:8:GLU:N	2.54	0.41
2:C:14:HIS:HB2	2:C:144:LYS:HD2	2.02	0.41
2:C:39:ARG:HB2	2:C:39:ARG:NH1	2.34	0.41
2:D:140:GLY:C	2:D:142:ALA:N	2.74	0.41
1:A:217:LYS:HB2	1:A:220:ASP:OD2	2.21	0.41
1:A:271:ASP:C	1:A:273:SER:H	2.24	0.41
1:A:3:GLU:HG2	1:A:4:MET:N	2.34	0.41
1:A:53:ILE:HB	1:A:305:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:LEU:CD1	1:B:332:LEU:N	2.81	0.41
1:B:31:LEU:O	1:B:34:ARG:HB3	2.19	0.41
1:B:88:GLU:HB3	1:B:92:VAL:HG23	2.02	0.41
2:D:68:GLU:O	2:D:71:LEU:HB2	2.21	0.41
1:B:31:LEU:CD2	1:B:70:LEU:CD1	2.97	0.41
1:A:21:ASP:O	1:A:24:LYS:HG3	2.20	0.41
1:A:34:ARG:HE	1:A:250:HIS:CD2	2.38	0.41
1:B:153:SER:HA	1:B:157:GLN:H	1.86	0.41
1:B:18:ILE:HD12	1:B:343:ILE:HG12	1.96	0.41
1:B:9:ILE:CG2	1:B:28:ALA:HB2	2.51	0.41
1:B:351:ILE:O	1:B:354:GLN:N	2.53	0.41
1:B:408:TYR:O	1:B:410:ALA:N	2.53	0.41
2:D:114:SER:C	2:D:116:THR:N	2.74	0.41
2:D:89:TRP:CD2	2:D:115:GLY:HA2	2.56	0.41
1:A:122:ARG:HH21	1:A:126:LEU:HD11	1.72	0.41
1:A:167:GLN:HB2	1:A:168:LEU:H	1.60	0.41
1:A:375:ARG:O	1:A:376:ILE:O	2.39	0.41
1:A:432:LEU:C	1:A:434:ALA:N	2.75	0.41
1:A:6:PRO:CD	1:A:32:ARG:HD3	2.50	0.41
2:C:102:LEU:HD23	2:C:102:LEU:HA	1.79	0.41
2:D:25:GLN:HB2	2:D:172:ASN:HB3	2.03	0.41
1:A:319:ILE:HG23	1:A:320:PRO:HD2	2.03	0.40
1:B:103:LEU:CD1	1:B:247:VAL:HG13	2.48	0.40
1:B:86:PHE:HB3	1:B:277:VAL:HG21	2.03	0.40
1:B:320:PRO:O	1:B:321:GLU:C	2.60	0.40
1:B:424:TYR:HB3	1:B:425:VAL:H	1.70	0.40
1:A:37:ARG:HG2	1:A:37:ARG:HH11	1.87	0.40
1:B:79:ILE:HD12	1:B:103:LEU:N	2.36	0.40
1:B:10:VAL:O	1:B:13:LEU:CB	2.64	0.40
1:B:401:ARG:HD3	1:B:401:ARG:O	2.21	0.40
2:C:53:PHE:CE2	2:C:55:GLY:HA3	2.56	0.40
2:D:140:GLY:C	2:D:142:ALA:H	2.24	0.40
2:D:177:LEU:HA	2:D:177:LEU:HD23	1.77	0.40
1:A:259:ASP:HB3	1:A:310:PHE:CD2	2.56	0.40
1:A:17:ILE:HG21	1:A:66:ILE:HG12	2.03	0.40
1:A:86:PHE:CE2	1:A:99:ILE:HG13	2.56	0.40
1:B:323:GLN:O	1:B:329:ARG:NH2	2.54	0.40
1:B:402:LEU:HD13	1:B:429:LEU:CD1	2.51	0.40
2:C:143:LEU:O	2:C:146:HIS:N	2.52	0.40
1:A:391:GLY:O	1:A:392:ALA:C	2.59	0.40
1:A:408:TYR:HB2	1:B:29:ILE:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ILE:HD11	1:B:315:PRO:CG	2.50	0.40
2:D:102:LEU:O	2:D:112:LEU:HD23	2.21	0.40
1:A:221:ALA:H	1:A:224:LEU:HD13	1.86	0.40
1:A:275:GLU:CG	1:A:319:ILE:HD11	2.41	0.40
1:A:390:ILE:HG22	1:A:393:ARG:CB	2.51	0.40
1:B:79:ILE:CG1	1:B:103:LEU:HD23	2.52	0.40
1:B:128:GLU:C	1:B:130:ARG:N	2.75	0.40
1:B:263:LYS:HD2	1:B:272:VAL:CG1	2.48	0.40
1:B:338:SER:C	1:B:340:PHE:N	2.73	0.40
1:B:406:ILE:HD13	1:B:420:ILE:HD11	2.02	0.40
1:B:72:LYS:O	1:B:72:LYS:HG2	2.21	0.40
2:C:25:GLN:N	2:C:172:ASN:OD1	2.54	0.40
1:A:266:GLU:HB3	2:D:66:LYS:HE3	2.03	0.40
2:D:66:LYS:HZ2	2:D:88:GLU:HG2	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:NE	1:B:362:GLU:OE1[3_665]	2.06	0.14

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	404/443 (91%)	240 (59%)	83 (20%)	81 (20%)	0 2
1	B	404/443 (91%)	229 (57%)	88 (22%)	87 (22%)	0 1
2	C	178/181 (98%)	141 (79%)	24 (14%)	13 (7%)	1 16
2	D	178/181 (98%)	145 (82%)	20 (11%)	13 (7%)	1 16
All	All	1164/1248 (93%)	755 (65%)	215 (18%)	194 (17%)	0 3

All (194) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	PRO
1	A	14	ASP
1	A	27	VAL
1	A	37	ARG
1	A	58	PRO
1	A	84	THR
1	A	85	LYS
1	A	92	VAL
1	A	107	ALA
1	A	108	VAL
1	A	112	ARG
1	A	133	ASP
1	A	141	ASN
1	A	155	ALA
1	A	234	VAL
1	A	237	GLU
1	A	241	GLN
1	A	246	ALA
1	A	247	VAL
1	A	250	HIS
1	A	258	ILE
1	A	282	LEU
1	A	293	LYS
1	A	300	ASP
1	A	350	SER
1	A	351	ILE
1	A	352	THR
1	A	392	ALA
1	A	405	GLU
1	A	425	VAL
1	A	430	ASP
1	A	432	LEU
1	A	436	GLU
1	B	4	MET
1	B	6	PRO
1	B	14	ASP
1	B	34	ARG
1	B	37	ARG
1	B	58	PRO
1	B	84	THR
1	B	85	LYS
1	B	92	VAL

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Mol	Chain	Res	Type
1	B	107	ALA
1	B	108	VAL
1	B	141	ASN
1	B	144	GLY
1	B	146	THR
1	B	154	ALA
1	B	155	ALA
1	B	241	GLN
1	B	246	ALA
1	B	250	HIS
1	B	282	LEU
1	B	293	LYS
1	B	300	ASP
1	B	337	THR
1	B	350	SER
1	B	352	THR
1	B	392	ALA
1	B	405	GLU
1	B	425	VAL
1	B	430	ASP
1	B	432	LEU
1	B	433	VAL
2	D	6	ALA
2	D	69	ALA
2	D	73	GLU
2	D	141	ARG
2	D	153	ALA
2	C	69	ALA
2	C	73	GLU
2	C	141	ARG
2	C	153	ALA
2	C	154	SER
1	A	4	MET
1	A	26	SER
1	A	34	ARG
1	A	88	GLU
1	A	109	LYS
1	A	144	GLY
1	A	146	THR
1	A	154	ALA
1	A	220	ASP
1	A	221	ALA

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Mol	Chain	Res	Type
1	A	226	ILE
1	A	228	GLU
1	A	264	ARG
1	A	265	GLY
1	A	270	PRO
1	A	280	ASP
1	A	337	THR
1	A	356	LYS
1	A	400	GLU
1	A	414	SER
1	A	433	VAL
1	B	27	VAL
1	B	39	GLN
1	B	88	GLU
1	B	99	ILE
1	B	112	ARG
1	B	133	ASP
1	B	212	LYS
1	B	226	ILE
1	B	234	VAL
1	B	247	VAL
1	B	258	ILE
1	B	264	ARG
1	B	265	GLY
1	B	266	GLU
1	B	270	PRO
1	B	280	ASP
1	B	316	SER
1	B	323	GLN
1	B	351	ILE
1	B	361	THR
1	B	376	ILE
1	B	400	GLU
1	B	414	SER
1	B	416	GLN
1	B	436	GLU
2	D	29	GLY
2	D	133	GLY
2	D	140	GLY
2	D	154	SER
2	C	6	ALA
2	C	140	GLY

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Mol	Chain	Res	Type
1	A	23	ALA
1	A	25	ARG
1	A	39	GLN
1	A	91	TYR
1	A	138	PRO
1	A	212	LYS
1	A	225	LEU
1	A	279	ARG
1	A	283	PRO
1	A	361	THR
1	A	376	ILE
1	A	399	LEU
1	A	416	GLN
1	B	25	ARG
1	B	26	SER
1	B	36	ARG
1	B	109	LYS
1	B	129	GLU
1	B	140	LYS
1	B	213	ALA
1	B	220	ASP
1	B	341	GLU
1	B	356	LYS
1	B	422	ALA
1	B	439	SER
2	D	38	ALA
2	D	47	GLY
2	C	29	GLY
2	C	38	ALA
2	C	47	GLY
2	C	78	LEU
2	C	115	GLY
1	A	24	LYS
1	A	43	GLU
1	A	99	ILE
1	A	257	GLU
1	A	266	GLU
1	A	354	GLN
1	A	422	ALA
1	B	23	ALA
1	B	38	MET
1	B	101	ARG

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Mol	Chain	Res	Type
1	B	138	PRO
1	B	221	ALA
1	B	228	GLU
1	B	257	GLU
1	B	284	LEU
1	B	354	GLN
1	B	387	THR
1	B	399	LEU
1	B	409	ASP
2	D	68	GLU
2	D	78	LEU
2	C	60	ALA
1	A	17	ILE
1	A	139	ALA
1	A	355	TYR
1	A	387	THR
1	A	406	ILE
1	B	43	GLU
1	B	225	LEU
1	B	41	ASN
1	B	355	TYR
1	B	406	ILE
1	B	236	PRO
1	A	272	VAL
1	B	283	PRO
1	A	93	GLY

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	350/377 (93%)	222 (63%)	128 (37%)	0 1
1	B	350/377 (93%)	216 (62%)	134 (38%)	0 0
2	C	138/139 (99%)	95 (69%)	43 (31%)	0 2
2	D	138/139 (99%)	93 (67%)	45 (33%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	976/1032 (95%)	626 (64%)	350 (36%)	0 1

All (350) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	4	MET
1	A	5	THR
1	A	6	PRO
1	A	7	ARG
1	A	11	SER
1	A	12	GLU
1	A	14	ASP
1	A	15	LYS
1	A	16	HIS
1	A	21	ASP
1	A	24	LYS
1	A	32	ARG
1	A	33	ASN
1	A	39	GLN
1	A	42	GLU
1	A	44	LEU
1	A	45	ARG
1	A	46	HIS
1	A	49	THR
1	A	54	LEU
1	A	59	THR
1	A	61	VAL
1	A	63	LYS
1	A	64	THR
1	A	65	GLU
1	A	69	ARG
1	A	70	LEU
1	A	73	LEU
1	A	80	LYS
1	A	85	LYS
1	A	86	PHE
1	A	88	GLU
1	A	89	VAL
1	A	94	LYS
1	A	98	SER
1	A	103	LEU

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Mol	Chain	Res	Type
1	A	104	THR
1	A	109	LYS
1	A	113	VAL
1	A	117	GLU
1	A	120	ARG
1	A	121	TYR
1	A	122	ARG
1	A	124	GLU
1	A	132	LEU
1	A	133	ASP
1	A	135	LEU
1	A	136	ILE
1	A	140	LYS
1	A	142	ASN
1	A	143	TRP
1	A	146	THR
1	A	149	GLN
1	A	156	ARG
1	A	164	ARG
1	A	167	GLN
1	A	168	LEU
1	A	172	GLU
1	A	173	ILE
1	A	212	LYS
1	A	216	LEU
1	A	218	ILE
1	A	220	ASP
1	A	222	MET
1	A	225	LEU
1	A	227	GLU
1	A	228	GLU
1	A	232	LYS
1	A	234	VAL
1	A	235	ASN
1	A	239	LEU
1	A	240	LYS
1	A	245	ASP
1	A	249	GLN
1	A	250	HIS
1	A	253	VAL
1	A	263	LYS
1	A	264	ARG

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Mol	Chain	Res	Type
1	A	267	SER
1	A	268	SER
1	A	273	SER
1	A	274	ARG
1	A	277	VAL
1	A	280	ASP
1	A	281	LEU
1	A	282	LEU
1	A	285	VAL
1	A	288	CYS
1	A	289	THR
1	A	292	THR
1	A	294	HIS
1	A	300	ASP
1	A	307	SER
1	A	311	GLN
1	A	322	LEU
1	A	323	GLN
1	A	333	GLN
1	A	335	LEU
1	A	336	THR
1	A	337	THR
1	A	338	SER
1	A	354	GLN
1	A	358	LEU
1	A	359	MET
1	A	361	THR
1	A	369	THR
1	A	371	SER
1	A	382	GLN
1	A	385	GLU
1	A	389	ASN
1	A	394	ARG
1	A	402	LEU
1	A	403	MET
1	A	404	GLU
1	A	407	SER
1	A	411	SER
1	A	414	SER
1	A	419	THR
1	A	421	ASP
1	A	427	LYS

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Mol	Chain	Res	Type
1	A	428	HIS
1	A	432	LEU
1	A	436	GLU
1	A	437	ASP
1	A	438	LEU
1	A	439	SER
1	A	443	LEU
1	B	3	GLU
1	B	4	MET
1	B	5	THR
1	B	6	PRO
1	B	7	ARG
1	B	11	SER
1	B	12	GLU
1	B	14	ASP
1	B	16	HIS
1	B	21	ASP
1	B	24	LYS
1	B	25	ARG
1	B	32	ARG
1	B	33	ASN
1	B	36	ARG
1	B	38	MET
1	B	39	GLN
1	B	42	GLU
1	B	44	LEU
1	B	45	ARG
1	B	46	HIS
1	B	49	THR
1	B	54	LEU
1	B	61	VAL
1	B	63	LYS
1	B	64	THR
1	B	65	GLU
1	B	69	ARG
1	B	70	LEU
1	B	72	LYS
1	B	73	LEU
1	B	80	LYS
1	B	85	LYS
1	B	86	PHE
1	B	88	GLU

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Mol	Chain	Res	Type
1	B	89	VAL
1	B	94	LYS
1	B	97	ASP
1	B	98	SER
1	B	103	LEU
1	B	104	THR
1	B	109	LYS
1	B	113	VAL
1	B	117	GLU
1	B	120	ARG
1	B	121	TYR
1	B	122	ARG
1	B	124	GLU
1	B	132	LEU
1	B	133	ASP
1	B	135	LEU
1	B	136	ILE
1	B	140	LYS
1	B	142	ASN
1	B	143	TRP
1	B	146	THR
1	B	149	GLN
1	B	156	ARG
1	B	162	LYS
1	B	164	ARG
1	B	167	GLN
1	B	168	LEU
1	B	172	GLU
1	B	173	ILE
1	B	212	LYS
1	B	216	LEU
1	B	218	ILE
1	B	220	ASP
1	B	222	MET
1	B	225	LEU
1	B	227	GLU
1	B	228	GLU
1	B	232	LYS
1	B	234	VAL
1	B	235	ASN
1	B	239	LEU
1	B	240	LYS

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Mol	Chain	Res	Type
1	B	245	ASP
1	B	249	GLN
1	B	250	HIS
1	B	253	VAL
1	B	260	LYS
1	B	263	LYS
1	B	264	ARG
1	B	274	ARG
1	B	275	GLU
1	B	281	LEU
1	B	282	LEU
1	B	283	PRO
1	B	285	VAL
1	B	289	THR
1	B	293	LYS
1	B	294	HIS
1	B	296	MET
1	B	300	ASP
1	B	311	GLN
1	B	314	LYS
1	B	322	LEU
1	B	323	GLN
1	B	326	LEU
1	B	333	GLN
1	B	335	LEU
1	B	336	THR
1	B	337	THR
1	B	338	SER
1	B	354	GLN
1	B	358	LEU
1	B	361	THR
1	B	369	THR
1	B	371	SER
1	B	382	GLN
1	B	385	GLU
1	B	389	ASN
1	B	393	ARG
1	B	394	ARG
1	B	399	LEU
1	B	402	LEU
1	B	403	MET
1	B	404	GLU

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Mol	Chain	Res	Type
1	B	405	GLU
1	B	407	SER
1	B	411	SER
1	B	414	SER
1	B	416	GLN
1	B	419	THR
1	B	421	ASP
1	B	425	VAL
1	B	427	LYS
1	B	428	HIS
1	B	432	LEU
1	B	437	ASP
1	B	438	LEU
1	B	439	SER
1	B	443	LEU
2	D	2	SER
2	D	3	SER
2	D	7	THR
2	D	8	THR
2	D	13	GLN
2	D	17	ARG
2	D	26	VAL
2	D	30	GLN
2	D	32	VAL
2	D	36	HIS
2	D	42	ARG
2	D	45	PHE
2	D	48	LYS
2	D	61	PHE
2	D	63	LEU
2	D	71	LEU
2	D	74	TYR
2	D	78	LEU
2	D	80	ARG
2	D	83	VAL
2	D	92	ASP
2	D	94	VAL
2	D	98	LEU
2	D	101	MET
2	D	102	LEU
2	D	106	ASN
2	D	107	GLN

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Mol	Chain	Res	Type
2	D	109	THR
2	D	110	LEU
2	D	111	LEU
2	D	112	LEU
2	D	116	THR
2	D	134	ASN
2	D	137	LEU
2	D	143	LEU
2	D	149	GLU
2	D	150	SER
2	D	152	SER
2	D	154	SER
2	D	172	ASN
2	D	174	GLN
2	D	177	LEU
2	D	179	GLU
2	D	180	LEU
2	D	181	GLU
2	C	2	SER
2	C	3	SER
2	C	7	THR
2	C	8	THR
2	C	13	GLN
2	C	17	ARG
2	C	26	VAL
2	C	30	GLN
2	C	32	VAL
2	C	36	HIS
2	C	42	ARG
2	C	45	PHE
2	C	48	LYS
2	C	61	PHE
2	C	62	THR
2	C	63	LEU
2	C	74	TYR
2	C	78	LEU
2	C	80	ARG
2	C	83	VAL
2	C	97	LYS
2	C	98	LEU
2	C	101	MET
2	C	102	LEU

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Mol	Chain	Res	Type
2	C	104	VAL
2	C	106	ASN
2	C	107	GLN
2	C	109	THR
2	C	110	LEU
2	C	111	LEU
2	C	112	LEU
2	C	116	THR
2	C	134	ASN
2	C	137	LEU
2	C	141	ARG
2	C	150	SER
2	C	152	SER
2	C	154	SER
2	C	172	ASN
2	C	174	GLN
2	C	177	LEU
2	C	179	GLU
2	C	180	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	33	ASN
1	A	119	ASN
1	A	278	GLN
1	A	417	ASN
1	B	20	GLN
1	B	33	ASN
1	B	39	GLN
1	B	119	ASN
1	B	250	HIS
1	B	278	GLN
1	B	323	GLN
1	B	365	ASN
2	D	36	HIS
2	D	106	ASN
2	D	172	ASN
2	D	174	GLN
2	C	14	HIS
2	C	36	HIS

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Mol	Chain	Res	Type
2	C	106	ASN
2	C	172	ASN
2	C	174	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ADP	B	906	-	24,29,29	1.25	2 (8%)	29,45,45	1.63	9 (31%)
3	ADP	A	905	-	24,29,29	1.34	4 (16%)	29,45,45	1.72	7 (24%)

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	906	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	905	-	-	2/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	905	ADP	C2-N3	4.36	1.39	1.32
3	B	906	ADP	C2-N3	3.77	1.38	1.32
3	B	906	ADP	C2-N1	2.79	1.39	1.33
3	A	905	ADP	O4'-C4'	-2.46	1.39	1.45
3	A	905	ADP	C2-N1	2.18	1.38	1.33
3	A	905	ADP	C2'-C1'	-2.05	1.50	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	905	ADP	N3-C2-N1	-5.08	120.73	128.68
3	B	906	ADP	N3-C2-N1	-3.36	123.42	128.68
3	A	905	ADP	O3B-PB-O2B	3.26	120.08	107.64
3	B	906	ADP	C2'-C3'-C4'	-3.13	96.56	102.64
3	A	905	ADP	O4'-C1'-C2'	2.87	111.12	106.93
3	A	905	ADP	C5-C6-N6	-2.84	116.04	120.35
3	B	906	ADP	O4'-C1'-C2'	-2.55	103.20	106.93
3	B	906	ADP	O3B-PB-O3A	2.50	113.03	104.64
3	B	906	ADP	O3B-PB-O2B	2.30	116.41	107.64
3	A	905	ADP	C2'-C3'-C4'	2.29	107.09	102.64
3	B	906	ADP	O2'-C2'-C1'	2.26	119.19	110.85
3	A	905	ADP	C4-C5-N7	-2.25	107.06	109.40
3	B	906	ADP	O5'-PA-O1A	-2.24	100.32	109.07
3	B	906	ADP	C3'-C2'-C1'	2.15	104.21	100.98
3	A	905	ADP	O2'-C2'-C3'	2.00	118.30	111.82
3	B	906	ADP	O2A-PA-O5'	2.00	117.03	107.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	906	ADP	O4'-C4'-C5'-O5'
3	B	906	ADP	C3'-C4'-C5'-O5'
3	A	905	ADP	O4'-C4'-C5'-O5'
3	A	905	ADP	C3'-C4'-C5'-O5'
3	B	906	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	B	906	ADP	PA-O3A-PB-O2B

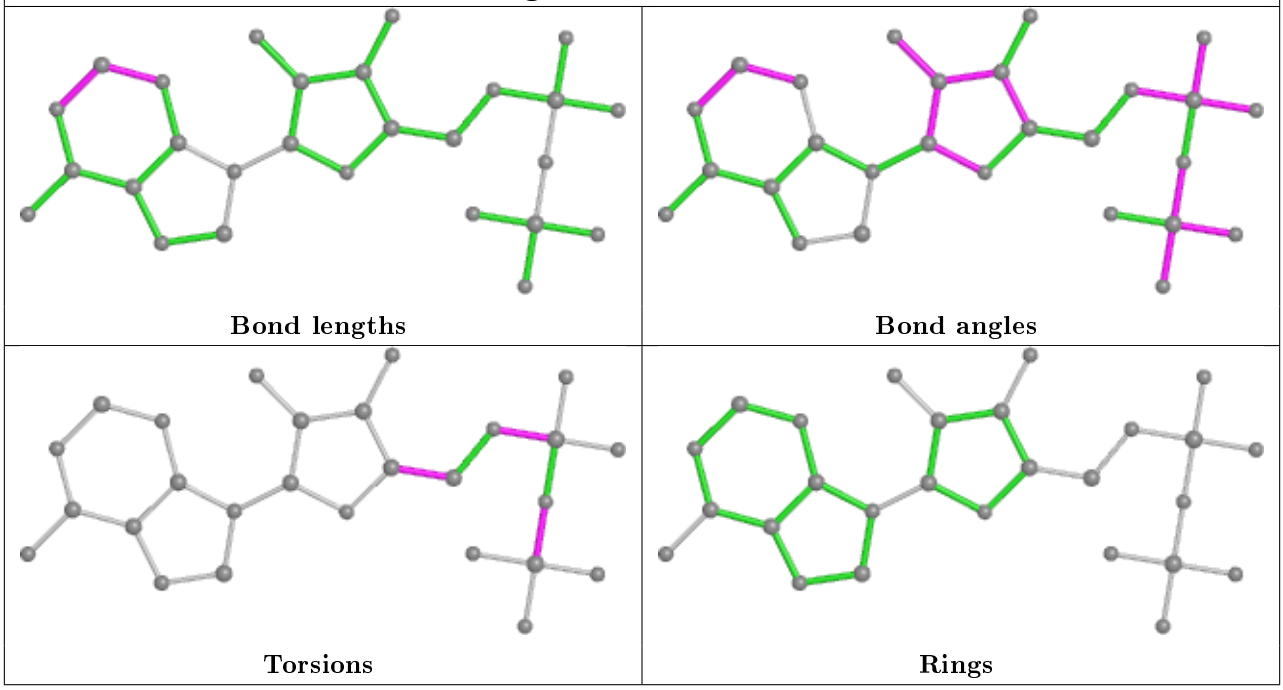
There are no ring outliers.

2 monomers are involved in 13 short contacts:

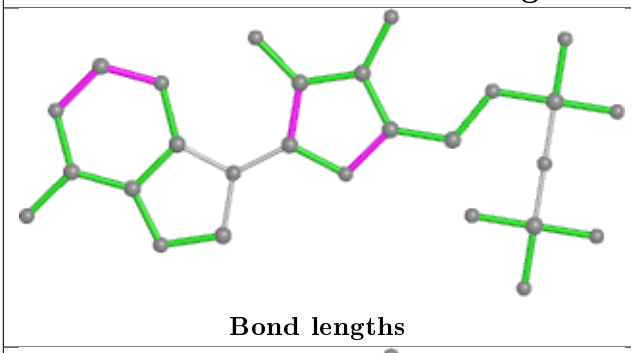
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	906	ADP	8	0
3	A	905	ADP	5	0

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

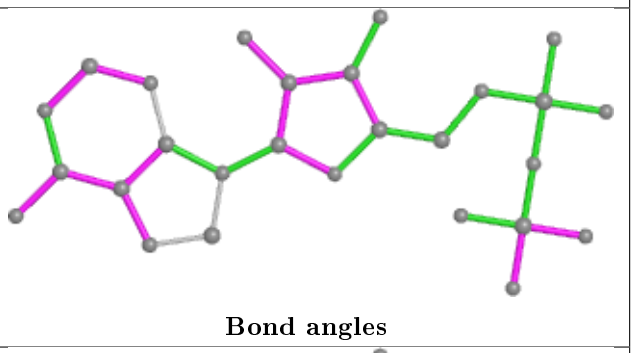
Ligand ADP B 906



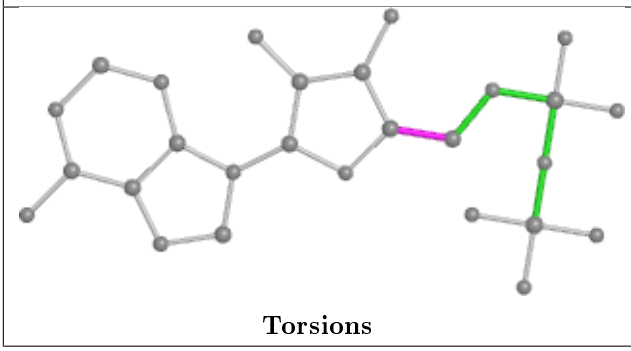
Ligand ADP A 905



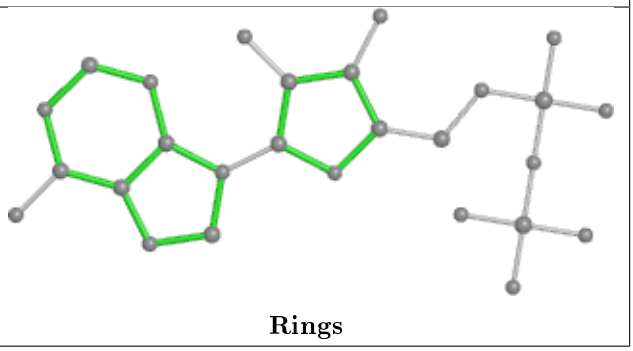
Bond lengths



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	408/443 (92%)	0.01	38 (9%) 8 8	16, 55, 94, 96	0
1	B	408/443 (92%)	-0.24	13 (3%) 47 37	16, 55, 93, 95	0
2	C	180/181 (99%)	-0.75	0 100 100	3, 23, 45, 55	0
2	D	180/181 (99%)	-0.73	0 100 100	3, 23, 45, 55	0
All	All	1176/1248 (94%)	-0.30	51 (4%) 35 29	3, 45, 93, 96	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	213	ALA	4.6
1	A	147	GLU	4.6
1	A	221	ALA	4.4
1	B	145	GLN	3.9
1	A	166	GLY	3.8
1	A	140	LYS	3.7
1	A	142	ASN	3.6
1	A	170	ASP	3.6
1	B	146	THR	3.6
1	A	220	ASP	3.6
1	A	212	LYS	3.5
1	A	90	GLY	3.5
1	A	159	PHE	3.4
1	A	211	GLN	3.3
1	B	267	SER	3.2
1	A	133	ASP	3.2
1	B	147	GLU	3.2
1	A	164	ARG	3.1
1	A	158	ALA	3.0
1	A	167	GLN	3.0
1	A	129	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	144	GLY	2.9
1	A	214	ARG	2.9
1	A	161	LYS	2.9
1	A	210	LYS	2.9
1	A	174	GLU	2.9
1	A	141	ASN	2.8
1	A	154	ALA	2.7
1	A	172	GLU	2.7
1	B	90	GLY	2.6
1	A	160	ARG	2.6
1	A	165	GLU	2.5
1	A	131	ILE	2.5
1	A	267	SER	2.5
1	A	137	PRO	2.4
1	A	149	GLN	2.4
1	B	269	GLY	2.4
1	A	157	GLN	2.3
1	A	148	GLN	2.3
1	A	173	ILE	2.3
1	A	89	VAL	2.3
1	A	145	GLN	2.3
1	B	125	GLU	2.2
1	B	91	TYR	2.2
1	B	1	MET	2.2
1	A	144	GLY	2.2
1	A	128	GLU	2.1
1	A	163	LEU	2.1
1	B	143	TRP	2.1
1	B	211	GLN	2.1
1	B	174	GLU	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 carbohydrates in this entry.

6.4 Ligands

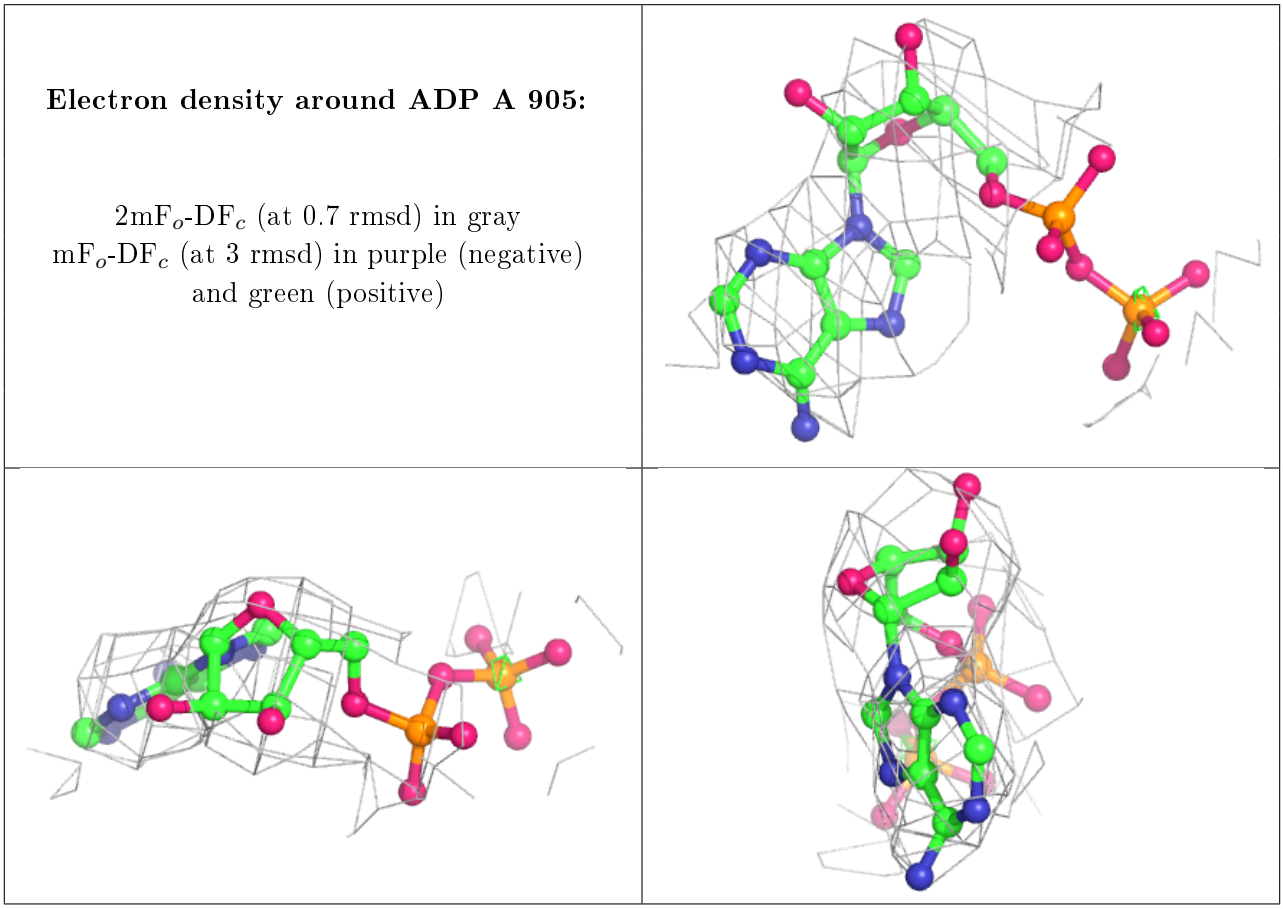
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	A	905	27/27	0.87	0.32	85,101,106,106	0
3	ADP	B	906	27/27	0.90	0.27	79,89,97,98	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.

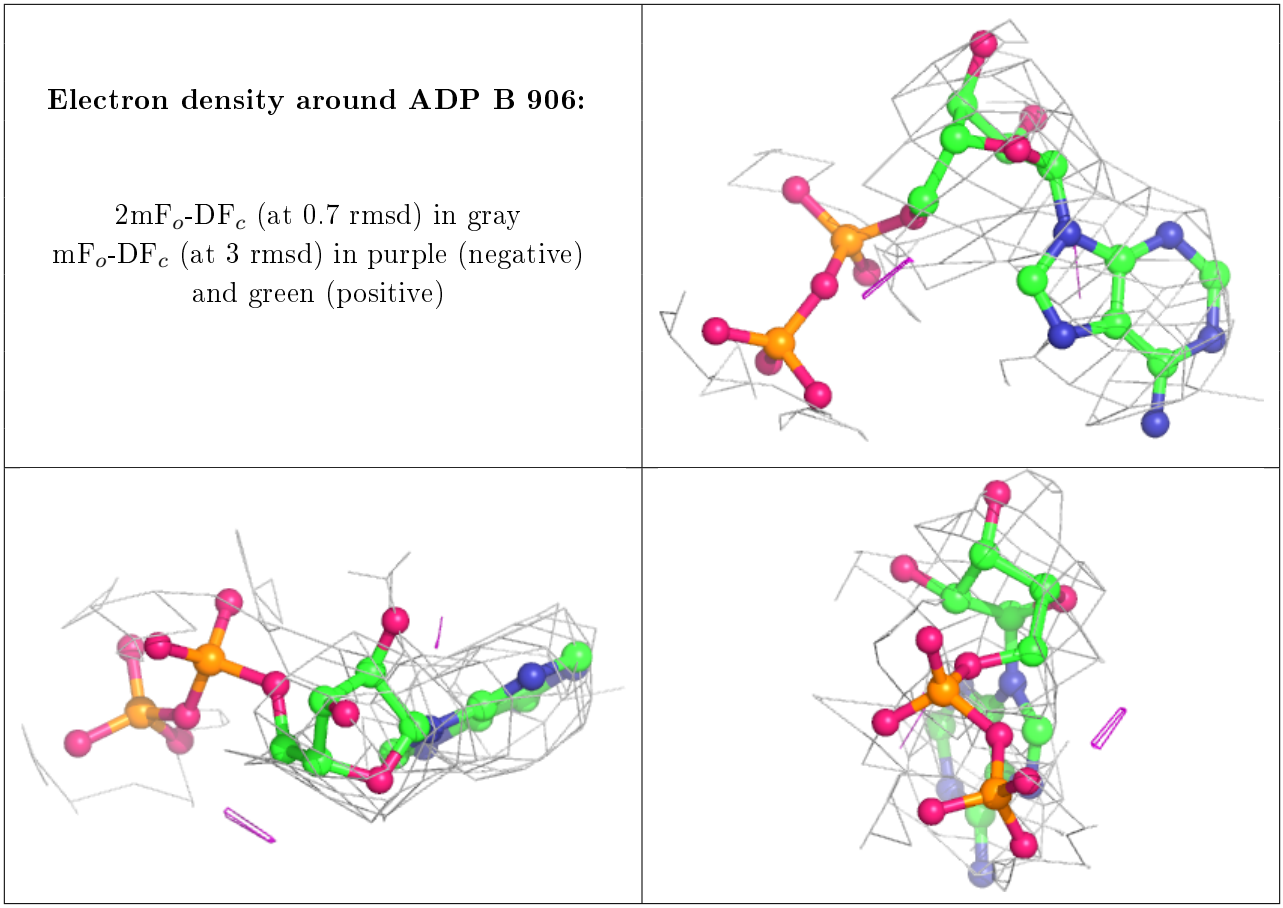
Electron density around ADP A 905:

$2mF_o$-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 906:

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



6.5 Other polymers

There are no such residues in this entry.