



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:55 PM UTC

PDB ID : 1YYF / pdb_00001yyf
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 types of validation reports are described at

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

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

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

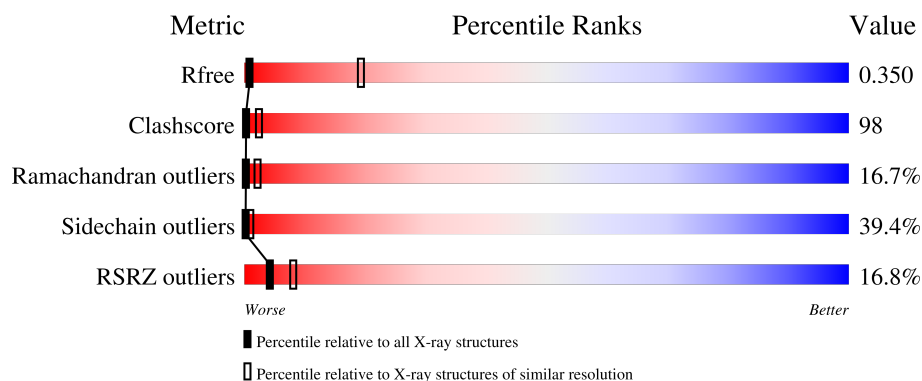
1 Overall quality at a glance

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}	180053	1077 (4.50-3.82)
Clashscore	190562	1019 (4.48-3.84)
Ramachandran outliers	187476	1035 (4.50-3.82)
Sidechain outliers	187428	1022 (4.50-3.82)
RSRZ outliers	180081	1074 (4.50-3.82)

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

Mol	Chain	Length	Quality of chain
1	A	443	25% 10% 36% 31% 15% 8%
1	B	443	19% 9% 36% 33% 14% 8%
2	C	181	% 16% 43% 33% 8% .
2	D	181	% 14% 47% 33% 6% .

2 Entry composition [i](#)

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.

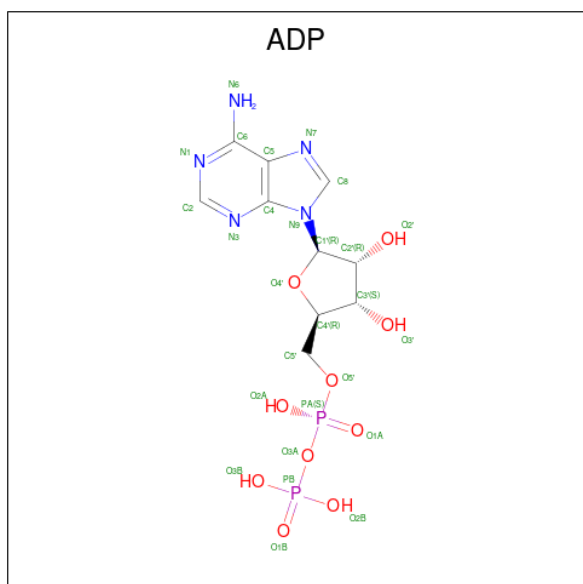
- Molecule 1 is a protein called ATP-dependent hsl protease ATP-binding subunit hslU.

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 (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

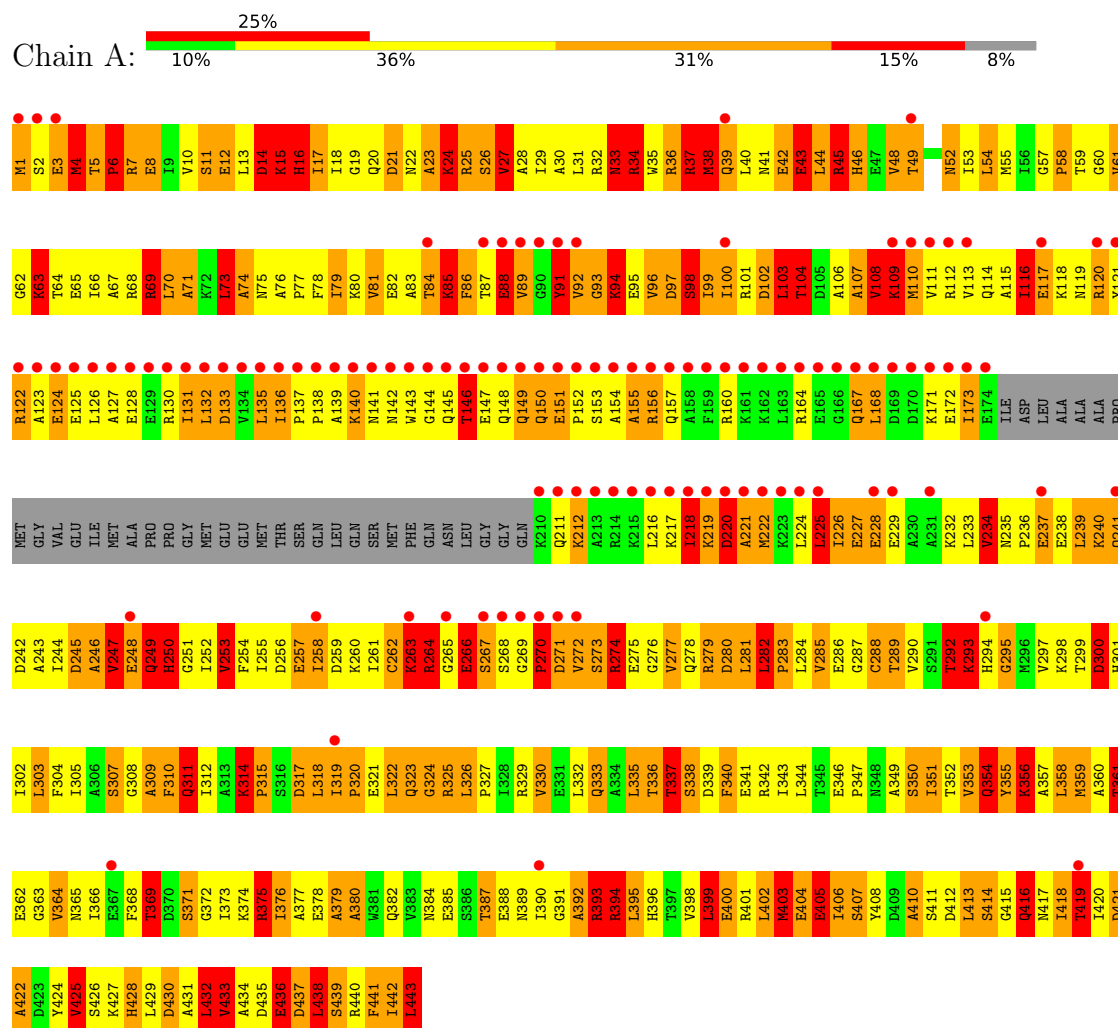


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

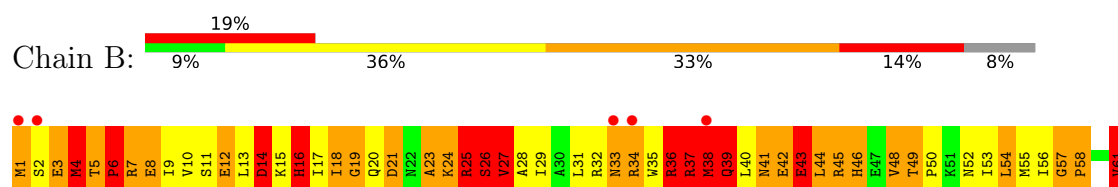
3 Residue-property plots

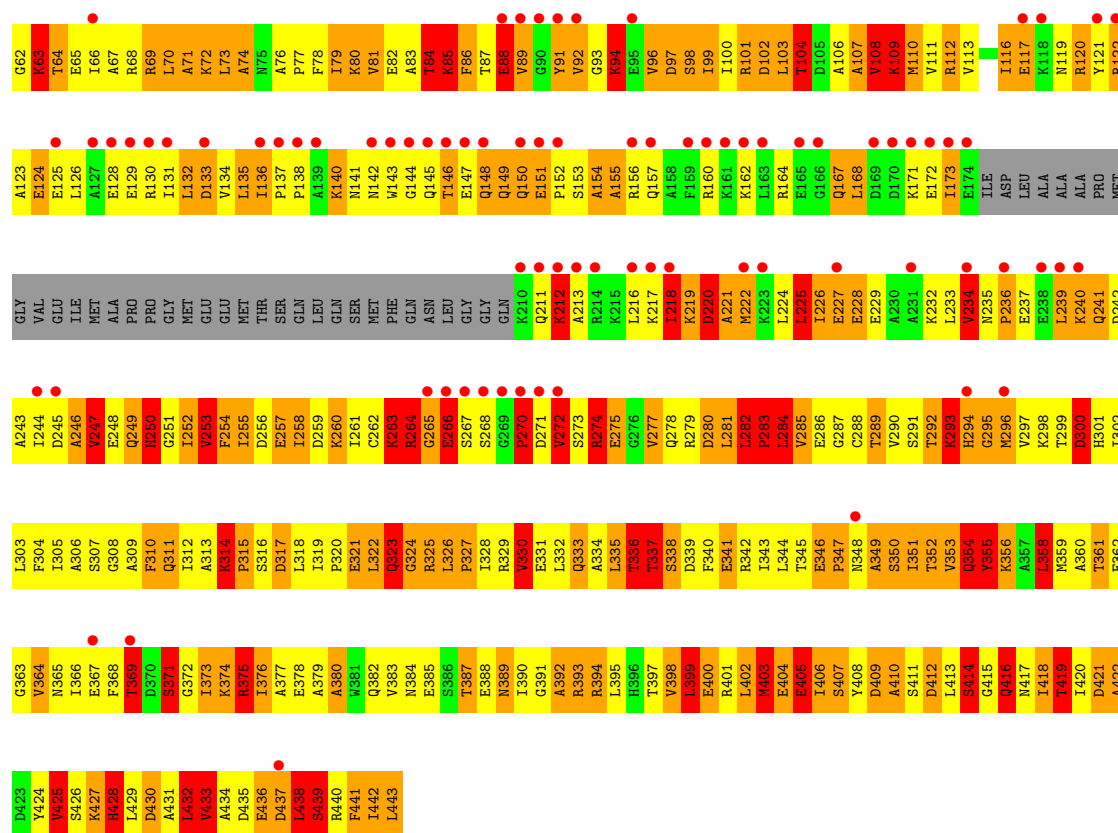
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

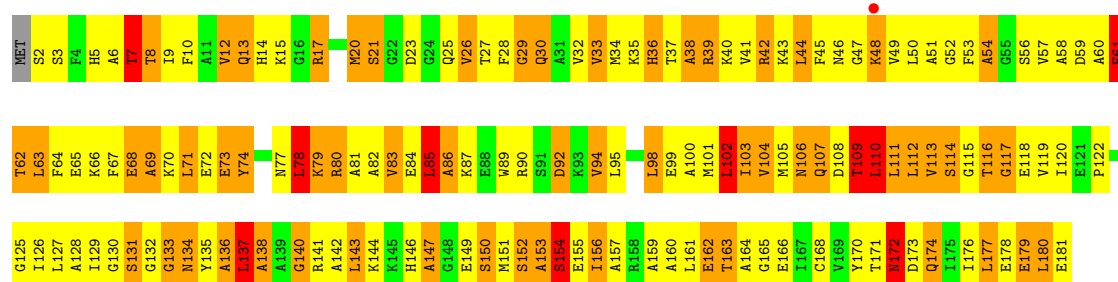
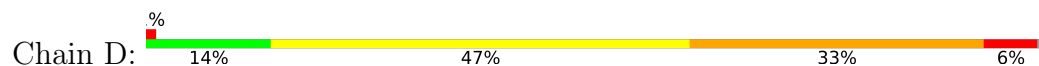


- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU

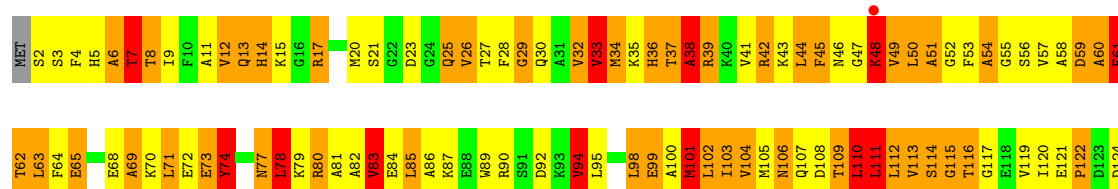
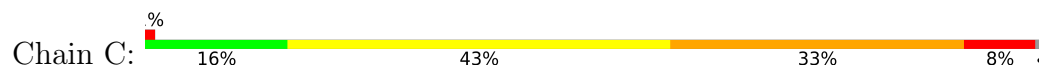




• Molecule 2: ATP-dependent protease hslV



• Molecule 2: ATP-dependent protease hslV



G125	I126	L127	A128	I129	G130	S131	G132	G133	N134	Y135	A136	L137	A138	A139	G140	R141	A142	L143	K144	K145	H146	A147		S150	M151	S152	A153	S154	E155	I156	A157	R158	A159	A160	L161	E162	T163	A164	G165	E166	I167	G168	W169	Y170	T171	N172	D173	Q174	L175	L176	L177	E178	E179	L180	E181
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4 Data and refinement statistics

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 34.92 – 4.16	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.92-4.16) 99.3 (34.92-4.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 4.12Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.277 , 0.346 0.295 , 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 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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	1.68	45/3261 (1.4%)	1.76	87/4394 (2.0%)
1	B	1.70	41/3262 (1.3%)	1.75	78/4395 (1.8%)
2	C	1.98	32/1375 (2.3%)	1.80	30/1847 (1.6%)
2	D	1.92	26/1375 (1.9%)	1.81	31/1847 (1.7%)
All	All	1.77	144/9273 (1.6%)	1.77	226/12483 (1.8%)

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 (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	MET	SD-CE	16.62	2.21	1.79
1	A	38	MET	SD-CE	14.47	2.15	1.79
2	C	34	MET	SD-CE	13.42	2.13	1.79
1	B	403	MET	SD-CE	12.55	2.10	1.79
1	B	110	MET	SD-CE	12.21	2.10	1.79
2	C	38	ALA	CA-C	11.76	1.68	1.52
1	B	89	VAL	CA-CB	10.48	1.66	1.54
1	A	89	VAL	CA-CB	9.99	1.67	1.54
1	B	1	MET	SD-CE	9.98	2.04	1.79
1	A	419	THR	CA-CB	9.47	1.66	1.53
2	D	38	ALA	CA-C	9.44	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	LYS	CA-C	9.36	1.63	1.52
1	B	405	GLU	CA-C	9.35	1.65	1.52
2	C	38	ALA	CA-CB	9.30	1.69	1.53
1	B	234	VAL	CA-CB	9.12	1.66	1.54
1	B	419	THR	CA-CB	9.10	1.65	1.53
1	B	309	ALA	CA-CB	-9.08	1.40	1.53
1	A	1	MET	CG-SD	8.60	2.02	1.80
1	A	249	GLN	CA-C	-8.07	1.42	1.52
2	D	103	ILE	CA-C	-8.06	1.42	1.52
1	B	1	MET	CG-SD	8.02	2.00	1.80
1	A	403	MET	SD-CE	7.91	1.99	1.79
1	B	94	LYS	CA-C	7.85	1.61	1.52
2	C	51	ALA	CA-C	-7.78	1.43	1.52
1	A	89	VAL	CA-C	7.78	1.62	1.52
1	A	1	MET	SD-CE	7.73	1.98	1.79
2	C	113	VAL	CA-CB	-7.71	1.44	1.54
1	B	71	ALA	CA-CB	-7.68	1.41	1.53
2	D	7	THR	CA-CB	-7.62	1.41	1.53
1	A	110	MET	SD-CE	7.53	1.98	1.79
2	C	33	VAL	CA-CB	-7.48	1.45	1.54
1	A	137	PRO	CA-C	7.44	1.59	1.52
2	D	34	MET	SD-CE	7.40	1.98	1.79
1	B	443	LEU	CG-CD1	-7.37	1.28	1.52
2	D	38	ALA	CA-CB	7.36	1.65	1.53
2	C	42	ARG	NE-CZ	7.30	1.41	1.33
2	D	136	ALA	CA-C	7.20	1.62	1.52
1	A	247	VAL	CA-CB	-7.00	1.45	1.54
2	C	34	MET	CG-SD	6.84	1.97	1.80
1	B	61	VAL	CA-C	-6.69	1.44	1.52
1	A	405	GLU	CA-C	6.68	1.61	1.52
2	C	119	VAL	CA-CB	-6.66	1.45	1.54
1	B	96	VAL	C-O	-6.64	1.17	1.24
2	D	33	VAL	CA-CB	-6.60	1.46	1.54
2	C	122	PRO	CA-C	-6.58	1.45	1.52
1	B	2	SER	CA-C	6.53	1.61	1.52
1	A	309	ALA	CA-CB	-6.53	1.44	1.53
2	C	54	ALA	CA-CB	-6.49	1.45	1.54
1	B	270	PRO	CA-C	6.45	1.61	1.52
2	C	113	VAL	CA-C	-6.41	1.44	1.52
1	B	18	ILE	CA-C	-6.38	1.44	1.52
1	A	441	PHE	CA-C	-6.29	1.44	1.52
1	A	69	ARG	CA-C	-6.27	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	38	ALA	N-CA	6.26	1.54	1.46
1	A	104	THR	CA-C	-6.24	1.44	1.52
1	A	71	ALA	CA-CB	-6.20	1.43	1.53
1	B	89	VAL	CA-C	6.19	1.59	1.52
2	C	162	GLU	CA-C	6.15	1.60	1.52
1	A	340	PHE	CA-C	-6.13	1.45	1.52
2	C	7	THR	CA-C	-6.13	1.44	1.52
1	A	63	LYS	CA-C	6.12	1.60	1.52
1	B	383	VAL	CA-CB	-6.08	1.47	1.54
2	D	42	ARG	CG-CD	6.08	1.70	1.52
2	C	101	MET	SD-CE	6.07	1.94	1.79
2	C	114	SER	CA-C	-6.05	1.45	1.52
2	D	40	LYS	CA-C	6.03	1.60	1.52
1	B	84	THR	CA-CB	6.02	1.63	1.53
2	D	162	GLU	CA-C	6.00	1.61	1.52
1	B	266	GLU	CA-C	5.96	1.60	1.52
2	C	11	ALA	CA-CB	-5.96	1.43	1.53
1	B	94	LYS	C-O	5.94	1.31	1.24
1	A	387	THR	CA-CB	-5.93	1.43	1.53
1	A	37	ARG	NE-CZ	5.92	1.39	1.33
2	C	151	MET	CG-SD	5.91	1.95	1.80
1	B	63	LYS	CA-C	5.88	1.60	1.52
1	B	91	TYR	N-CA	5.87	1.53	1.46
1	A	379	ALA	CA-CB	-5.81	1.44	1.53
2	C	6	ALA	CA-C	5.81	1.60	1.52
2	C	42	ARG	CG-CD	5.81	1.69	1.52
1	A	270	PRO	CA-C	5.80	1.60	1.52
1	B	398	VAL	CA-CB	-5.76	1.48	1.54
2	C	165	GLY	C-O	5.71	1.31	1.23
2	D	109	THR	CA-C	5.67	1.59	1.52
2	D	114	SER	CA-C	-5.67	1.45	1.52
2	C	142	ALA	CA-CB	-5.66	1.44	1.53
2	D	7	THR	CA-C	-5.65	1.45	1.52
1	A	380	ALA	CA-CB	-5.61	1.44	1.53
1	B	317	ASP	CA-C	-5.60	1.45	1.52
1	B	345	THR	CA-C	5.59	1.58	1.52
1	B	254	PHE	N-CA	-5.57	1.39	1.46
1	B	387	THR	CA-CB	-5.56	1.44	1.53
1	A	314	LYS	CB-CG	5.55	1.69	1.52
2	D	119	VAL	CA-CB	-5.53	1.47	1.54
2	D	138	ALA	CA-CB	-5.52	1.44	1.53
1	B	104	THR	CA-CB	-5.51	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	109	THR	CA-CB	5.45	1.62	1.53
1	A	375	ARG	NE-CZ	5.43	1.39	1.33
2	D	79	LYS	CG-CD	5.43	1.68	1.52
1	B	37	ARG	NE-CZ	5.42	1.39	1.33
1	A	248	GLU	CA-C	5.41	1.60	1.52
1	A	247	VAL	CA-C	-5.41	1.45	1.52
1	B	284	LEU	CA-C	-5.40	1.45	1.52
1	A	100	ILE	N-CA	5.39	1.52	1.46
1	A	317	ASP	CA-C	-5.36	1.45	1.52
1	B	252	ILE	N-CA	-5.34	1.39	1.46
2	D	147	ALA	CA-CB	-5.33	1.44	1.53
1	A	271	ASP	CA-C	5.32	1.59	1.52
1	B	371	SER	CA-C	-5.32	1.44	1.52
1	B	296	MET	SD-CE	5.32	1.92	1.79
1	A	36	ARG	CA-C	-5.29	1.45	1.52
2	C	83	VAL	CA-CB	-5.29	1.48	1.54
2	D	34	MET	CG-SD	5.27	1.94	1.80
2	C	94	VAL	CA-CB	5.26	1.60	1.54
2	C	137	LEU	CA-C	-5.23	1.45	1.52
1	B	321	GLU	CG-CD	5.21	1.65	1.52
2	D	168	CYS	N-CA	5.20	1.52	1.46
2	C	39	ARG	C-O	5.20	1.30	1.23
2	C	103	ILE	CA-C	-5.19	1.46	1.52
2	C	42	ARG	CD-NE	5.19	1.53	1.46
1	A	2	SER	N-CA	5.18	1.52	1.46
1	A	34	ARG	CA-C	5.18	1.59	1.52
1	B	353	VAL	CA-C	-5.17	1.46	1.52
1	A	266	GLU	CA-C	5.16	1.59	1.52
1	B	102	ASP	CA-C	-5.16	1.46	1.52
2	C	48	LYS	CG-CD	5.16	1.68	1.52
2	C	74	TYR	CA-CB	5.14	1.58	1.53
1	A	89	VAL	N-CA	5.14	1.52	1.46
2	D	40	LYS	CD-CE	5.14	1.67	1.52
1	A	441	PHE	CB-CG	-5.13	1.38	1.50
1	A	96	VAL	CA-C	-5.13	1.45	1.52
1	A	317	ASP	C-O	-5.10	1.17	1.24
2	D	110	LEU	CA-C	5.10	1.58	1.52
1	A	267	SER	CA-C	5.08	1.59	1.52
2	D	113	VAL	CA-CB	-5.07	1.47	1.54
2	C	45	PHE	CA-C	-5.05	1.46	1.52
1	A	98	SER	C-O	-5.04	1.18	1.24
1	A	1	MET	CA-C	5.04	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	LEU	CG-CD1	-5.04	1.35	1.52
2	D	12	VAL	CA-CB	-5.04	1.47	1.55
1	B	334	ALA	CA-C	-5.04	1.46	1.52
2	D	42	ARG	CB-CG	5.03	1.67	1.52
1	A	91	TYR	N-CA	5.01	1.52	1.46
2	D	30	GLN	CB-CG	5.01	1.67	1.52
1	B	375	ARG	NE-CZ	5.01	1.38	1.33

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	37	THR	N-CA-C	10.59	127.18	114.04
1	A	104	THR	N-CA-C	-10.49	99.23	113.18
1	B	74	ALA	N-CA-C	-10.32	99.84	111.71
1	A	249	GLN	CB-CA-C	-10.29	94.35	110.81
1	B	211	GLN	OE1-CD-NE2	-9.83	112.77	122.60
1	A	150	GLN	OE1-CD-NE2	-9.80	112.80	122.60
1	B	150	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	A	211	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	A	74	ALA	N-CA-C	-9.71	101.36	113.01
1	A	311	GLN	N-CA-C	-9.58	101.59	113.38
2	C	110	LEU	N-CA-C	9.39	123.72	108.32
1	B	311	GLN	N-CA-C	-8.97	101.77	112.89
1	B	274	ARG	N-CA-C	-8.73	102.43	113.43
1	B	418	ILE	N-CA-C	8.69	123.03	108.86
2	D	156	ILE	N-CA-C	-8.69	102.08	110.42
1	A	330	VAL	CB-CA-C	-8.47	95.93	111.18
2	D	110	LEU	N-CA-C	8.45	122.66	108.13
2	D	86	ALA	N-CA-C	-8.20	101.01	111.02
1	A	432	LEU	N-CA-C	-8.04	93.68	110.80
2	C	38	ALA	N-CA-C	7.88	127.59	110.80
1	B	218	ILE	N-CA-C	7.87	121.98	111.44
2	C	138	ALA	N-CA-C	-7.78	103.59	113.23
1	B	380	ALA	N-CA-C	-7.77	101.79	111.11
1	A	292	THR	N-CA-C	7.73	120.62	108.79
1	A	442	ILE	CB-CA-C	-7.71	102.21	112.46
1	B	419	THR	N-CA-C	-7.70	95.04	108.20
1	A	78	PHE	CA-C-N	-7.62	111.73	122.71
1	A	78	PHE	C-N-CA	-7.62	111.73	122.71
2	C	146	HIS	N-CA-C	7.55	123.06	113.55
2	D	38	ALA	N-CA-C	7.53	126.84	110.80
1	A	52	ASN	N-CA-C	7.50	120.00	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	37	THR	N-CA-C	7.48	126.72	110.80
1	B	373	ILE	N-CA-C	-7.41	100.94	111.17
2	C	12	VAL	N-CA-C	7.40	119.00	108.42
1	B	78	PHE	N-CA-C	7.39	121.39	108.75
1	A	94	LYS	N-CA-C	7.38	120.45	108.41
1	B	418	ILE	CB-CA-C	-7.37	98.90	110.69
1	B	78	PHE	CA-C-N	-7.24	111.86	122.58
1	B	78	PHE	C-N-CA	-7.24	111.86	122.58
1	A	419	THR	N-CA-C	-7.18	95.28	107.99
1	B	345	THR	N-CA-C	7.17	122.47	113.43
1	A	418	ILE	N-CA-C	7.17	120.54	108.86
1	B	253	VAL	N-CA-C	7.13	118.16	108.17
2	D	131	SER	N-CA-C	7.13	118.74	110.97
2	C	173	ASP	N-CA-C	7.10	119.93	111.33
2	D	146	HIS	N-CA-C	7.05	122.56	113.88
1	A	320	PRO	N-CD-CG	-7.04	92.64	103.20
1	B	367	GLU	CA-CB-CG	7.01	128.13	114.10
2	C	113	VAL	CB-CA-C	-7.00	99.81	111.29
1	A	218	ILE	N-CA-C	6.96	123.54	113.16
1	B	325	ARG	N-CA-C	-6.95	103.91	112.88
1	A	274	ARG	N-CA-C	-6.93	104.70	113.43
1	A	102	ASP	N-CA-C	-6.91	104.73	113.72
2	C	168	CYS	N-CA-C	6.89	119.97	108.73
1	A	340	PHE	CB-CA-C	-6.83	100.36	110.95
1	B	102	ASP	N-CA-C	-6.82	105.24	113.97
1	A	315	PRO	N-CA-C	-6.82	104.45	113.65
1	B	432	LEU	N-CA-C	-6.81	96.30	110.80
1	B	349	ALA	N-CA-C	-6.78	104.88	113.02
1	A	443	LEU	CD1-CG-CD2	-6.74	95.98	110.80
1	A	42	GLU	N-CA-C	-6.72	105.08	113.55
1	B	81	VAL	CB-CA-C	-6.72	100.81	110.83
1	B	315	PRO	N-CA-C	-6.71	104.59	113.65
1	A	81	VAL	CB-CA-C	-6.70	100.62	110.81
2	C	151	MET	N-CA-C	6.70	118.69	109.18
1	B	211	GLN	CG-CD-NE2	6.70	126.45	116.40
1	A	1	MET	CB-CG-SD	6.69	132.77	112.70
1	B	150	GLN	CG-CD-NE2	6.68	126.42	116.40
1	A	15	LYS	CB-CG-CD	6.67	126.65	111.30
1	B	443	LEU	CD1-CG-CD2	-6.67	96.13	110.80
1	A	150	GLN	CG-CD-NE2	6.66	126.39	116.40
1	A	211	GLN	CG-CD-NE2	6.66	126.39	116.40
2	C	7	THR	CB-CA-C	-6.60	98.91	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	LEU	N-CA-C	6.57	120.53	109.76
2	D	128	ALA	N-CA-C	6.54	119.05	108.32
1	A	255	ILE	CB-CA-C	6.53	120.30	111.88
1	B	292	THR	N-CA-C	6.51	118.11	108.60
2	D	113	VAL	CB-CA-C	-6.47	100.67	111.29
1	A	395	LEU	N-CA-C	-6.45	103.15	111.02
1	A	78	PHE	N-CA-C	6.37	119.89	109.06
1	B	347	PRO	CB-CA-C	-6.33	103.66	111.64
2	D	102	LEU	CA-C-N	-6.30	114.93	123.12
2	D	102	LEU	C-N-CA	-6.30	114.93	123.12
1	B	57	GLY	CA-C-N	6.26	127.66	119.84
1	B	57	GLY	C-N-CA	6.26	127.66	119.84
1	A	97	ASP	N-CA-C	-6.25	105.75	113.19
1	B	1	MET	CB-CG-SD	6.23	131.39	112.70
1	A	442	ILE	N-CA-C	6.23	118.25	111.77
1	B	310	PHE	CB-CA-C	-6.19	103.57	111.86
1	B	272	VAL	CB-CA-C	6.16	121.39	111.29
1	B	330	VAL	CB-CA-C	-6.15	102.32	111.80
1	A	438	LEU	CA-CB-CG	-6.15	94.78	116.30
1	A	253	VAL	CB-CA-C	-6.13	101.55	110.63
2	D	7	THR	CB-CA-C	-6.13	99.69	109.80
1	B	327	PRO	N-CD-CG	-6.11	94.03	103.20
2	D	99	GLU	N-CA-C	6.11	119.12	111.24
1	A	326	LEU	CA-C-N	6.09	125.58	119.24
1	A	326	LEU	C-N-CA	6.09	125.58	119.24
1	A	96	VAL	CB-CA-C	-6.09	104.24	110.88
1	A	418	ILE	CB-CA-C	-6.09	100.95	110.69
1	B	442	ILE	CB-CA-C	-6.07	104.14	111.85
1	B	410	ALA	N-CA-C	6.06	118.66	111.33
1	B	253	VAL	CB-CA-C	-6.03	101.85	110.83
1	A	57	GLY	CA-C-N	5.99	127.32	119.84
1	A	57	GLY	C-N-CA	5.99	127.32	119.84
1	A	325	ARG	N-CA-C	-5.98	105.28	113.30
1	A	310	PHE	CB-CA-C	-5.98	103.85	111.86
2	D	20	MET	N-CA-C	5.95	118.62	108.02
1	B	369	THR	CB-CA-C	-5.93	97.27	110.19
1	B	355	TYR	CA-CB-CG	-5.89	103.30	113.90
1	B	104	THR	N-CA-C	-5.89	98.26	110.80
1	A	441	PHE	CB-CA-C	-5.88	100.90	110.79
1	B	293	LYS	CA-C-N	-5.87	112.75	122.32
1	B	293	LYS	C-N-CA	-5.87	112.75	122.32
1	B	79	ILE	N-CA-C	5.86	118.30	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	VAL	N-CA-C	5.86	117.03	108.53
1	B	441	PHE	CB-CA-C	-5.84	101.67	110.90
2	C	114	SER	CB-CA-C	-5.83	98.23	109.37
1	A	394	ARG	CG-CD-NE	5.82	124.80	112.00
1	B	267	SER	N-CA-C	5.79	117.68	111.36
1	A	380	ALA	N-CA-C	-5.79	104.32	111.33
1	A	103	LEU	N-CA-C	-5.76	106.30	113.15
1	B	321	GLU	CB-CG-CD	5.75	122.38	112.60
2	D	168	CYS	N-CA-C	5.75	118.11	108.96
1	B	353	VAL	CB-CA-C	-5.73	104.53	112.04
1	B	326	LEU	CA-CB-CG	-5.73	96.24	116.30
1	B	2	SER	N-CA-C	5.73	123.00	110.80
1	B	326	LEU	CA-C-N	5.72	125.19	119.24
1	B	326	LEU	C-N-CA	5.72	125.19	119.24
1	B	254	PHE	CA-C-N	5.72	129.63	122.48
1	B	254	PHE	C-N-CA	5.72	129.63	122.48
1	A	263	LYS	N-CA-C	5.71	121.63	110.56
1	A	16	HIS	N-CA-C	5.70	119.42	111.56
2	D	77	ASN	N-CA-CB	5.70	118.55	110.46
1	A	249	GLN	O-C-N	5.69	128.01	122.09
1	B	373	ILE	CB-CA-C	5.69	120.36	112.05
1	A	262	CYS	CA-C-N	-5.67	113.82	121.71
1	A	262	CYS	C-N-CA	-5.67	113.82	121.71
1	B	346	GLU	N-CA-C	5.67	122.34	109.81
1	A	324	GLY	N-CA-C	-5.66	105.76	115.61
2	C	117	GLY	N-CA-C	-5.63	107.22	115.72
1	B	358	LEU	N-CA-C	-5.63	104.83	110.97
1	B	263	LYS	N-CA-C	5.62	122.76	110.80
1	A	94	LYS	CA-C-N	5.61	131.01	122.65
1	A	94	LYS	C-N-CA	5.61	131.01	122.65
1	B	438	LEU	CA-CB-CG	-5.59	96.72	116.30
1	A	326	LEU	CA-CB-CG	-5.57	96.80	116.30
1	B	255	ILE	CB-CA-C	5.56	119.06	111.88
1	B	324	GLY	CA-C-O	5.56	124.10	119.04
1	A	289	THR	N-CA-C	-5.54	101.25	110.17
2	D	173	ASP	N-CA-C	5.53	118.02	111.33
1	A	131	ILE	CB-CA-C	-5.53	106.19	111.44
2	D	163	THR	N-CA-C	-5.51	105.19	111.14
1	A	293	LYS	CA-C-N	-5.50	113.35	122.32
1	A	293	LYS	C-N-CA	-5.50	113.35	122.32
1	B	412	ASP	N-CA-C	-5.49	106.26	113.12
2	C	61	PHE	N-CA-C	-5.49	99.10	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	PRO	N-CA-C	5.48	117.39	110.70
1	A	116	ILE	CB-CA-C	-5.47	102.31	111.29
1	A	412	ASP	N-CA-C	-5.46	106.29	113.12
1	B	36	ARG	CB-CG-CD	5.45	123.83	111.30
2	C	128	ALA	N-CA-C	5.43	117.22	108.32
2	C	14	HIS	N-CA-C	5.43	117.93	108.76
2	D	156	ILE	CB-CA-C	5.42	118.90	111.97
2	D	85	LEU	N-CA-C	-5.40	104.81	111.40
1	B	295	GLY	N-CA-C	5.38	119.47	112.68
1	A	295	GLY	CA-C-O	-5.38	118.52	122.23
2	C	77	ASN	N-CA-CB	5.37	118.09	110.46
1	B	36	ARG	CG-CD-NE	5.37	123.80	112.00
2	C	156	ILE	N-CA-C	-5.35	105.16	110.62
2	C	59	ASP	N-CA-C	-5.35	104.69	111.11
2	C	25	GLN	CA-C-N	-5.34	115.93	122.93
2	C	25	GLN	C-N-CA	-5.34	115.93	122.93
1	A	73	LEU	N-CA-C	-5.33	106.83	113.38
2	C	7	THR	CA-C-N	-5.33	114.21	122.09
2	C	7	THR	C-N-CA	-5.33	114.21	122.09
2	D	102	LEU	CB-CG-CD1	-5.32	94.73	110.70
1	A	33	ASN	N-CA-C	-5.30	104.96	111.75
1	A	137	PRO	N-CA-C	5.30	117.17	110.70
1	B	19	GLY	N-CA-C	5.30	121.44	111.80
1	A	45	ARG	N-CA-C	-5.29	105.68	111.82
2	C	111	LEU	N-CA-C	5.29	118.04	109.06
2	D	163	THR	CB-CA-C	5.28	119.25	110.90
2	D	117	GLY	N-CA-C	-5.27	107.94	115.64
2	C	32	VAL	CA-C-N	-5.27	116.24	123.14
2	C	32	VAL	C-N-CA	-5.27	116.24	123.14
1	A	393	ARG	N-CA-C	-5.26	105.23	110.97
1	A	2	SER	N-CA-C	5.25	121.99	110.80
1	A	69	ARG	N-CA-C	-5.25	104.47	112.04
2	C	50	LEU	CA-CB-CG	-5.25	97.92	116.30
1	A	417	ASN	N-CA-C	5.23	118.08	109.72
2	D	61	PHE	N-CA-C	-5.22	99.67	110.80
1	B	16	HIS	N-CA-C	5.21	118.75	111.56
2	C	131	SER	N-CA-C	5.21	117.37	111.02
1	B	333	GLN	CA-C-N	-5.19	112.77	121.39
1	B	333	GLN	C-N-CA	-5.19	112.77	121.39
1	B	367	GLU	CB-CA-C	5.18	118.61	109.80
1	A	310	PHE	CA-C-N	-5.16	113.33	122.26
1	A	310	PHE	C-N-CA	-5.16	113.33	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	39	ARG	N-CA-C	5.16	116.89	108.63
1	B	327	PRO	CB-CA-C	-5.16	104.48	113.20
2	D	172	ASN	CA-C-N	5.16	127.44	120.38
2	D	172	ASN	C-N-CA	5.16	127.44	120.38
1	A	73	LEU	CA-CB-CG	-5.15	98.28	116.30
2	C	99	GLU	N-CA-C	5.15	116.74	111.03
1	B	94	LYS	N-CA-C	5.14	117.29	108.90
1	A	58	PRO	N-CD-CG	-5.13	95.50	103.20
2	D	12	VAL	N-CA-C	5.12	116.38	108.44
1	A	410	ALA	N-CA-C	5.12	117.52	111.33
1	A	319	ILE	CB-CA-C	5.10	115.88	110.88
2	D	109	THR	N-CA-C	5.10	115.78	108.74
1	A	124	GLU	N-CA-C	-5.10	106.91	113.23
1	A	127	ALA	N-CA-C	-5.09	107.11	113.38
1	A	369	THR	CB-CA-C	-5.09	99.09	110.19
1	B	428	HIS	CA-C-N	-5.09	111.82	121.54
1	B	428	HIS	C-N-CA	-5.09	111.82	121.54
1	A	79	ILE	N-CA-C	5.08	115.97	108.45
2	C	39	ARG	N-CA-C	5.07	116.75	108.63
1	A	318	LEU	CA-CB-CG	-5.06	98.58	116.30
1	A	353	VAL	CB-CA-C	-5.06	105.41	112.04
1	B	314	LYS	N-CA-C	-5.06	100.03	108.23
2	D	137	LEU	CA-C-O	5.06	125.60	119.38
1	A	356	LYS	N-CA-C	-5.04	100.06	110.80
1	B	289	THR	N-CA-C	-5.03	103.02	110.46
1	A	30	ALA	N-CA-C	-5.02	107.29	113.41
2	D	165	GLY	CA-C-O	5.02	125.57	119.65

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

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Mol	Chain	Res	Type	Group
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	660	1
1	B	3223	0	3296	711	1
2	C	1358	0	1374	226	0
2	D	1358	0	1374	239	0
3	A	27	0	12	5	0
3	B	27	0	12	8	0
All	All	9215	0	9364	1813	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 98.

All (1813) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CE	1:B:110:MET:SD	2.10	1.40
1:B:168:LEU:CD1	1:B:219:LYS:CE	1.99	1.39
1:B:403:MET:CE	1:B:403:MET:SD	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
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:135:LEU:CG	1:B:171:LYS:HZ2	1.50	1.24
1:B:168:LEU:HD12	1:B:219:LYS:CD	1.68	1.23
2:D:9:ILE:CD1	2:D:53:PHE:O	1.87	1.22
2:C:106:ASN:ND2	2:C:109:THR:H	1.36	1.22
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	1.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:335:LEU:CD1	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
2:D:20:MET:HE1	2:D:51:ALA:C	1.78	1.07
1:B:403:MET:HE1	1:B:420:ILE:HD13	1.22	1.07
1:A:335:LEU:HD12	1:A:335:LEU:N	1.64	1.07
1:B:335:LEU:H	1:B:335:LEU:HD12	1.02	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
1:A:116:ILE:O	1:A:116:ILE:HG22	1.50	1.06
1:B:237:GLU:N	1:B:240:LYS:HE3	1.71	1.06
1:B:288:CYS:SG	1:B:299:THR:HG21	1.95	1.06
2:D:17:ARG:HG2	2:D:17:ARG:HH11	0.97	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
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
2:C:17:ARG:HG2	2:C:17:ARG:HH11	1.07	1.06
1:A:108:VAL:C	1:A:110:MET:H	1.58	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:130:ARG:HD3	1:B:225:LEU:HD11	1.34	1.05
1:B:168:LEU:CD1	1:B:219:LYS:CD	2.31	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:83:ALA:HB1	1:B:261:ILE:HD11	1.05	1.04
1:B:239:LEU:HD13	1:B:240:LYS:HD3	1.32	1.04
2:C:80:ARG:HG2	2:C:80:ARG:HH11	1.18	1.04
1:B:258:ILE:HD12	1:B:306:ALA:CB	1.72	1.04
1:A:438:LEU:HD21	1:A:442:ILE:HD12	1.35	1.04
1:B:237:GLU:H	1:B:240:LYS:HE3	0.87	1.04
1:A:403:MET:HE1	1:A:420:ILE:HD13	1.32	1.03
1:B:282:LEU:HB3	1:B:283:PRO:HD3	1.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:168:LEU:HD11	1:A:219:LYS:HD2	1.41	1.02
1:B:359:MET:CG	1:B:366:ILE:CD1	2.36	1.02
1:A:282:LEU:HB3	1:A:283:PRO:HD2	1.28	1.02
1:B:258:ILE:HD11	1:B:306:ALA:HB2	1.35	1.01
2:C:20:MET:HE3	2:C:41:VAL:HG13	1.40	1.01
1:A:361:THR:HG21	1:B:36:ARG:HG3	1.39	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:261:ILE:HD13	1:A:277:VAL:CG1	1.91	1.01
1:A:392:ALA:O	1:A:395:LEU:HD12	1.61	1.01
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
2:C:110:LEU:C	2:C:111:LEU:HD13	1.86	1.00
1:A:18:ILE:CD1	1:A:342:ARG:C	2.35	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: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:A:403:MET:HE3	1:A:406:ILE:HD12	1.41	0.99
1:B:18:ILE:HD12	1:B:343:ILE:CA	1.93	0.99
2:C:172:ASN:HD22	2:C:172:ASN:H	1.12	0.98
1:B:268:SER:CB	1:B:312:ILE:HG21	1.93	0.98
2:C:20:MET:HE1	2:C:51:ALA:C	1.88	0.98
1:A:61:VAL:HB	1:A:335:LEU:HD11	1.45	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: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:130:ARG:HD3	1:A:225:LEU:HD11	1.43	0.97
1:A:167:GLN:OE1	1:A:219:LYS:CD	2.11	0.97
2:D:80:ARG:HG2	2:D:80:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:ASN:HD21	2:D:109:THR:H	1.08	0.97
2:D:110:LEU:C	2:D:111:LEU:HD13	1.88	0.96
2:C:103:ILE:HG13	2:C:129:ILE:CD1	1.94	0.96
2:C:106:ASN:HD21	2:C:109:THR:H	1.03	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
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
1:A:135:LEU:CG	1:A:171:LYS:HZ2	1.71	0.95
1:B:322:LEU:CD1	1:B:326:LEU:CD1	2.45	0.95
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:H	1:A:335:LEU:HD12	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: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
2:C:20:MET:HE2	2:C:41:VAL:HG13	1.50	0.93
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:O	1:B:261:ILE:HG22	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
1:B:391:GLY:C	1:B:393:ARG:H	1.74	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:HH11	2:D:17:ARG:CG	1.81	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O	1:A:261:ILE:HG22	1.65	0.91
1:B:83:ALA:CB	1:B:261:ILE:HD11	1.96	0.91
1:B:168:LEU:HD11	1:B:219:LYS:HD2	1.47	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:108:VAL:C	1:B:110:MET:H	1.72	0.91
1:B:335:LEU:H	1:B:335:LEU:CD1	1.77	0.91
1:B:18:ILE:CD1	1:B:342:ARG:C	2.43	0.91
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:A:108:VAL:C	1:A:110:MET:N	2.24	0.90
1:B:235:ASN:N	1:B:236:PRO:HD3	1.85	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:355:TYR:O	1:A:356:LYS:C	2.15	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:A:390:ILE:HD12	1:A:394:ARG:NH1	1.86	0.89
1:A:391:GLY:C	1:A:393:ARG:H	1.75	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
1:B:135:LEU:HG	1:B:171:LYS:HZ2	1.34	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:135:LEU:CD2	1:B:171:LYS:CE	2.25	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:129:ILE:HG22	2:D:130:GLY:N	1.87	0.88
2:C:152:SER:O	2:C:156:ILE:HG13	1.73	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
1:B:355:TYR:O	1:B:356:LYS:C	2.16	0.88
2:D:17:ARG:HG2	2:D:17:ARG:NH1	1.76	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:O	1:A:442:ILE:CG2	2.20	0.87
1:A:431:ALA:HA	1:A:434:ALA:HB2	1.57	0.87
1:A:18:ILE:HD11	1:A:342:ARG:C	1.99	0.86
1:B:70:LEU:C	1:B:70:LEU:HD12	2.00	0.86
3:B:906:ADP:H5'1	3:B:906:ADP:C8	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
1:B:403:MET:HE3	1:B:406:ILE:HD12	1.55	0.86
2:D:106:ASN:HD21	2:D:109:THR:N	1.71	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
2:C:25:GLN:HB2	2:C:172:ASN:CG	2.01	0.86
1:B:442:ILE:CG2	1:B:442:ILE:O	2.24	0.86
1:A:167:GLN:CD	1:A:219:LYS:HE2	2.00	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:5:THR:HG23	1:B:8:GLU:HG3	1.56	0.86
1:A:18:ILE:HD11	1:A:342:ARG:O	1.75	0.85
1:A:268:SER:HB3	1:A:312:ILE:CG2	2.04	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:H	2:D:172:ASN:HD22	1.19	0.85
1:B:86:PHE:CD2	1:B:96:VAL:HG12	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:PHE:N	1:A:86:PHE:HD1	1.74	0.85
1:A:425:VAL:HG12	1:A:426:SER:N	1.90	0.85
1:A:79:ILE:HD11	1:A:102:ASP:O	1.75	0.85
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:A:403:MET:HE3	1:A:406:ILE:CD1	2.06	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:B:251:GLY:C	1:B:252:ILE:HG13	2.02	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
1:B:135:LEU:CD2	1:B:171:LYS:HZ1	0.82	0.84
1:B:359:MET:HG2	1:B:366:ILE:HD11	1.52	0.84
1:B:13:LEU:O	1:B:15:LYS:N	2.11	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:HD12	1:A:343:ILE:N	1.93	0.82
2:C:17:ARG:HG2	2:C:17:ARG:NH1	1.86	0.82
2:C:110:LEU:O	2:C:111:LEU:HD13	1.78	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:135:LEU:HD22	1:B:171:LYS:HZ3	1.31	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
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:B:73:LEU:HG	1:B:74:ALA:N	1.88	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:SER:O	1:A:29:ILE:N	2.13	0.81
1:A:237:GLU:N	1:A:240:LYS:HE3	1.94	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:A:251:GLY:C	1:A:252:ILE:HG13	2.05	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
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:13:LEU:C	1:B:15:LYS:H	1.88	0.80
1:A:391:GLY:C	1:A:393:ARG:N	2.36	0.80
1:B:359:MET:HG3	1:B:366:ILE:HD11	1.63	0.80
1:B:399:LEU:C	1:B:401:ARG:H	1.87	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:18:ILE:HD12	1:B:343:ILE:HA	1.58	0.79
1:B:108:VAL:C	1:B:110:MET:N	2.37	0.79
1:B:168:LEU:HD12	1:B:219:LYS:HE3	0.79	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:B:153:SER:C	1:B:155:ALA:H	1.90	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:27:VAL:HG23	1:B:70:LEU:HD23	1.63	0.79
1:B:391:GLY:O	1:B:393:ARG:N	2.16	0.79
1:B:259:ASP:HB3	1:B:310:PHE:CE2	2.18	0.79
2:D:20:MET:HE2	2:D:41:VAL:CG1	2.10	0.79
2:C:80:ARG:HG2	2:C:80:ARG:NH1	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:86:PHE:N	1:A:86:PHE:CD1	2.47	0.78
1:A:346:GLU:N	1:A:347:PRO:HD2	1.97	0.78
1:B:256:ASP:O	1:B:257:GLU:CB	2.31	0.78
2:D:129:ILE:CG2	2:D:130:GLY:N	2.46	0.78
2:C:103:ILE:HD11	2:C:129:ILE:HG13	1.63	0.78
2:C:112:LEU:CD2	2:C:113:VAL:H	1.95	0.78
1:B:336:THR:N	1:B:339:ASP:HB2	1.98	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:B:424:TYR:O	1:B:425:VAL:C	2.25	0.78
2:D:20:MET:HE1	2:D:52:GLY:N	1.98	0.78
1:A:18:ILE:HD13	1:A:342:ARG:CB	2.13	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
1:A:167:GLN:OE1	1:A:219:LYS:HG2	1.84	0.78
2:C:172:ASN:HD22	2:C:172:ASN:N	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:100:ILE:HD11	1:B:284:LEU:HD23	1.64	0.77
1:B:106:ALA:O	1:B:108:VAL:N	2.14	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:18:ILE:HD13	1:B:342:ARG:C	2.08	0.77
1:B:235:ASN:O	1:B:239:LEU:HD12	1.85	0.77
1:A:13:LEU:C	1:A:15:LYS:H	1.89	0.77
1:A:322:LEU:C	1:A:322:LEU:HD12	2.08	0.77
2:D:106:ASN:HD22	2:D:109:THR:H	1.31	0.77
2:C:114:SER:O	2:C:114:SER:OG	2.01	0.77
1:A:438:LEU:HD21	1:A:442:ILE:CD1	2.14	0.77
1:B:70:LEU:C	1:B:70:LEU:CD1	2.56	0.77
1:A:69:ARG:O	1:A:70:LEU:C	2.26	0.77
1:A:245:ASP:O	1:A:249:GLN:N	2.16	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:413:LEU:HD23	2.00	0.77
1:B:315:PRO:C	1:B:317:ASP:H	1.93	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:O	1:B:136:ILE:CG2	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:N	1:A:220:ASP:OD1	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: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:B:55:MET:HE1	1:B:63:LYS:HA	1.68	0.76
2:D:159:ALA:O	2:D:160:ALA:C	2.28	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
2:C:122:PRO:HG3	2:C:127:LEU:HG	1.68	0.76
1:B:399:LEU:C	1:B:401:ARG:N	2.43	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:B:375:ARG:O	1:B:376:ILE:C	2.29	0.75
1:A:135:LEU:CD2	1:A:171:LYS:CE	2.26	0.75
1:A:81:VAL:HG21	1:A:99:ILE:HG23	1.68	0.75
1:A:281:LEU:O	1:A:282:LEU:C	2.28	0.75
1:B:425:VAL:HG12	1:B:426:SER:N	2.01	0.75
1:A:86:PHE:HE2	1:A:96:VAL:HA	1.47	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: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:69:ARG:O	1:B:70:LEU:C	2.29	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:PHE:O	1:B:341:GLU:C	2.27	0.75
1:B:420:ILE:HG23	1:B:424:TYR:HD1	1.49	0.75
2:D:20:MET:HE3	2:D:41:VAL:HG13	1.69	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:34:ARG:O	1:A:35:TRP:C	2.30	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:5:THR:HG23	1:B:8:GLU:CG	2.18	0.74
1:B:86:PHE:N	1:B:86:PHE:HD1	1.84	0.74
1:B:375:ARG:HB2	1:B:425:VAL:HG11	1.68	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
1:A:257:GLU:O	1:A:258:ILE:C	2.31	0.74
2:C:57:VAL:HA	2:C:60:ALA:CB	2.16	0.74
1:A:130:ARG:O	1:A:173:ILE:HG21	1.87	0.74
1:B:98:SER:OG	1:B:99:ILE:N	2.21	0.74
1:B:237:GLU:HA	1:B:240:LYS:HG2	1.69	0.74
2:C:7:THR:HG22	2:C:23:ASP:OD2	1.88	0.74
2:C:104:VAL:O	2:C:110:LEU:HD23	1.87	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:A:4:MET:O	1:A:32:ARG:NH1	2.20	0.73
1:A:36:ARG:O	1:A:37:ARG:C	2.31	0.73
1:A:278:GLN:HE22	1:A:319:ILE:H	1.33	0.73
1:B:281:LEU:O	1:B:282:LEU:C	2.31	0.73
2:D:105:MET:HB3	2:D:110:LEU:CD2	2.18	0.73
1:B:292:THR:CG2	1:B:295:GLY:O	2.35	0.73
1:B:390:ILE:HG22	1:B:390:ILE:O	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:O	1:B:136:ILE:HG22	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:12:VAL:HG21	2:D:126:ILE:HG12	1.68	0.73
2:C:12:VAL:HG23	2:C:126:ILE:CG1	2.18	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
1:B:391:GLY:C	1:B:393:ARG:N	2.34	0.73
2:D:101:MET:HB3	2:D:112:LEU:HD21	1.70	0.73
2:D:134:ASN:O	2:D:135:TYR:C	2.31	0.73
1:B:135:LEU:CD2	1:B:171:LYS:HZ3	0.90	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
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:96:VAL:HG11	1:A:280:ASP:HB3	1.72	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:B:116:ILE:O	1:B:116:ILE:HG22	1.89	0.72
1:B:350:SER:HB3	1:B:353:VAL:CG2	2.19	0.72
1:A:13:LEU:C	1:A:15:LYS:N	2.45	0.72
1:A:41:ASN:OD1	1:A:44:LEU:HD12	1.89	0.72
1:A:106:ALA:O	1:A:110:MET:HB2	1.88	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:A:399:LEU:C	1:A:401:ARG:N	2.48	0.72
2:D:110:LEU:HD22	2:D:111:LEU:N	2.05	0.72
2:C:112:LEU:HD23	2:C:113:VAL: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:403:MET:HE3	1:B:420:ILE:HD13	1.70	0.72
1:B:428:HIS:C	1:B:429:LEU:HD12	2.15	0.72
1:B:336:THR:H	1:B:339:ASP:CB	2.03	0.71
2:D:43:LYS:NZ	2:D:179:GLU:O	2.21	0.71
2:D:152:SER:O	2:D:156:ILE:HG13	1.90	0.71
1:B:13:LEU:C	1:B:15:LYS:N	2.45	0.71
1:B:54:LEU:HD12	1:B:54:LEU:C	2.16	0.71
1:A:41:ASN:HD21	1:A:43:GLU:HB3	1.56	0.71
1:A:325:ARG:C	1:A:327:PRO:HD2	2.15	0.71
1:B:12:GLU:O	1:B:15:LYS:HB2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:16:HIS:HD2	1:B:69:ARG:HG2	1.54	0.71
1:B:424:TYR:CE2	1:B:428:HIS:CE1	2.79	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:A:18:ILE:HD12	1:A:343:ILE:CA	2.21	0.71
1:A:171:LYS:HD2	1:A:218:ILE:CD1	2.21	0.71
1:A:399:LEU:C	1:A:401:ARG:H	1.99	0.71
1:A:401:ARG:NH2	1:A:442:ILE:HG21	2.05	0.71
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:A:6:PRO:HD3	1:A:32:ARG:HD2	1.73	0.70
1:A:278:GLN:HE22	1:A:319:ILE:N	1.88	0.70
1:A:279:ARG:O	1:A:280:ASP:C	2.34	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:A:279:ARG:O	1:A:282:LEU:HB2	1.90	0.70
1:B:18:ILE:HD11	1:B:342:ARG:O	1.90	0.70
1:B:34:ARG:O	1:B:35:TRP:C	2.34	0.70
1:B:257:GLU:O	1:B:258:ILE:C	2.31	0.70
1:B:325:ARG:C	1:B:327:PRO:HD2	2.17	0.70
2:C:8:THR:HG21	2:C:132:GLY:H	1.55	0.70
2:C:129:ILE:CG2	2:C:130:GLY:N	2.54	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:B:235:ASN:C	1:B:239:LEU:HD12	2.16	0.70
1:A:310:PHE:CE1	1:A:315:PRO:CA	2.74	0.70
2:D:110:LEU:O	2:D:111:LEU:CD1	2.40	0.70
2:D:110:LEU:HD13	2:D:127:LEU:HD12	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:24:LYS:O	1:A:25:ARG:C	2.35	0.69
1:B:253:VAL:HG21	1:B:304:PHE:CE2	2.28	0.69
1:B:261:ILE:O	1:B:261:ILE:CG2	2.40	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
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: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
1:B:403:MET:HE3	1:B:420:ILE:CD1	2.20	0.69
2:C:57:VAL:O	2:C:61:PHE:HB2	1.93	0.69
2:C:60:ALA:O	2:C:61:PHE:C	2.35	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:D:112:LEU:CD2	2:D:113:VAL:H	2.05	0.68
2:C:8:THR:CG2	2:C:132:GLY:H	2.06	0.68
2:C:151:MET:HG3	2:C:156:ILE:HG12	1.75	0.68
1:B:279:ARG:O	1:B:280:ASP:C	2.35	0.68
2:C:20:MET:HE1	2:C:52:GLY:N	2.08	0.68
1:A:149:GLN:C	1:A:152:PRO:HD2	2.19	0.68
1:B:93:GLY:O	1:B:94:LYS:HD2	1.92	0.68
1:B:403:MET:HE3	1:B:406:ILE:CD1	2.23	0.68
2:C:112:LEU:HD22	2:C:113:VAL:N	2.07	0.68
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:O	1:A:390:ILE:HG22	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
1:A:167:GLN:CD	1:A:219:LYS:HG2	2.18	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
2:C:92:ASP:C	2:C:92:ASP:OD1	2.37	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:25:GLN:HB2	2:D:172:ASN:CG	2.18	0.68
1:A:153:SER:C	1:A:155:ALA:H	2.02	0.67
1:B:61:VAL:HB	1:B:335:LEU:CD1	2.24	0.67
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:A:70:LEU:C	1:A:70:LEU:HD12	2.20	0.67
1:B:322:LEU:O	1:B:324:GLY:N	2.28	0.67
2:C:94:VAL:HG12	2:C:95:LEU:HG	1.77	0.67
1:A:18:ILE:HD13	1:A:342:ARG:C	2.18	0.67
1:A:73:LEU:HG	1:A:74:ALA:N	1.99	0.67
2:D:114:SER:O	2:D:114:SER:OG	2.11	0.67
1:B:274:ARG:O	1:B:275:GLU:C	2.37	0.67
2:C:152:SER:O	2:C:156:ILE:CG1	2.42	0.67
1:A:418:ILE:CG2	1:A:419:THR:H	2.06	0.67
2:D:57:VAL:HA	2:D:60:ALA:CB	2.23	0.67
2:C:68:GLU:O	2:C:71:LEU:N	2.28	0.67
2:C:136:ALA:HB1	2:C:160:ALA:HB1	1.77	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:H8	3:A:905:ADP:H5'1	1.59	0.66
2:D:110:LEU:HD22	2:D:127:LEU:HD12	1.77	0.66
2:C:83:VAL:HG12	2:C:84:GLU:N	2.08	0.66
1:A:61:VAL:O	1:A:61:VAL:CG2	2.41	0.66
1:A:70:LEU:C	1:A:70:LEU:CD1	2.69	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
1:A:359:MET:HB3	1:A:366:ILE:CD1	2.25	0.66
1:A:5:THR:O	1:A:6:PRO:C	2.37	0.66
1:A:79:ILE:CD1	1:A:102:ASP:C	2.69	0.66
1:A:435:ASP:O	1:A:436:GLU:C	2.39	0.66
1:A:325:ARG:C	1:A:327:PRO:CD	2.69	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:237:GLU:N	1:B:240:LYS:CE	2.41	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:83:ALA:O	1:A:84:THR:C	2.39	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:282:LEU:HD11	1:B:321:GLU:HB3	1.78	0.66
2:D:110:LEU:CD2	2:D:111:LEU:N	2.59	0.66
2:C:95:LEU:HD23	2:C:98:LEU:HD12	1.76	0.66
2:D:152:SER:O	2:D:156:ILE:CG1	2.43	0.65
1:A:54:LEU:HD12	1:A:55:MET:N	2.11	0.65
1:A:350:SER:HB3	1:A:353:VAL:CG2	2.26	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
1:B:372:GLY:C	1:B:374:LYS:N	2.49	0.65
2:D:122:PRO:HG3	2:D:127:LEU:HG	1.77	0.65
2:C:9:ILE:HD12	2:C:53:PHE:O	1.95	0.65
2:C:103:ILE:HG13	2:C:129:ILE:HD11	1.76	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
1:A:428:HIS:C	1:A:429:LEU:HD12	2.21	0.65
2:D:13:GLN:HG3	2:D:105:MET:HE1	1.78	0.65
1:B:338:SER:O	1:B:339:ASP:C	2.40	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:338:SER:O	1:A:339:ASP:C	2.39	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
1:A:274:ARG:O	1:A:275:GLU:C	2.39	0.65
1:A:415:GLY:O	1:A:416:GLN:C	2.38	0.65
2:D:44:LEU:CB	2:D:49:VAL:CG2	2.75	0.65
2:D:60:ALA:O	2:D:61:PHE:C	2.40	0.65
1:B:36:ARG:O	1:B:37:ARG:C	2.40	0.65
1:B:415:GLY:O	1:B:416:GLN:C	2.39	0.65
2:C:132:GLY:O	2:C:133:GLY:C	2.40	0.65
1:A:23:ALA:O	1:A:24:LYS:C	2.39	0.64
2:D:103:ILE:HD11	2:D:129:ILE:HG13	1.78	0.64
1:A:54:LEU:HD12	1:A:54:LEU:C	2.22	0.64
1:A:100:ILE:HD12	1:A:290:VAL:HG21	1.78	0.64
1:A:394:ARG:O	1:A:395:LEU:C	2.38	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:315:PRO:O	1:B:317:ASP:N	2.30	0.64
1:B:432:LEU:H	1:B:434:ALA:H	1.46	0.64
1:B:438:LEU:O	1:B:439:SER:C	2.40	0.64
1:B:41:ASN:HD21	1:B:43:GLU:HB3	1.61	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
2:D:23:ASP:HB2	2:D:172:ASN:HD22	1.58	0.64
2:C:8:THR:HG21	2:C:132:GLY:N	2.12	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
1:B:35:TRP:O	1:B:36:ARG:C	2.41	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
2:C:58:ALA:O	2:C:59:ASP:C	2.41	0.64
1:A:77:PRO:HD2	1:A:251:GLY:CA	2.27	0.64
1:B:77:PRO:O	1:B:251:GLY:HA3	1.98	0.64
1:B:282:LEU:CB	1:B:283:PRO:HD3	2.18	0.64
2:D:25:GLN:OE1	2:D:172:ASN:HB3	1.96	0.64
2:D:86:ALA:O	2:D:87:LYS:C	2.41	0.64
2:C:138:ALA:O	2:C:142:ALA:HB2	1.96	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:A:390:ILE:HD11	1:B:323:GLN:CD	2.23	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
1:B:3:GLU:HG2	1:B:4:MET:H	1.64	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
2:D:153:ALA:O	2:D:154:SER:C	2.41	0.63
1:A:61:VAL:O	1:A:61:VAL:HG23	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:GLY:O	1:B:252:ILE:HG13	1.98	0.63
2:D:85:LEU:O	2:D:86:ALA:C	2.42	0.63
2:D:92:ASP:C	2:D:92:ASP:OD1	2.41	0.63
1:A:27:VAL:HG23	1:A:70:LEU:HD22	1.80	0.63
1:B:3:GLU:O	1:B:4:MET:CB	2.41	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:A:35:TRP:O	1:A:36:ARG:C	2.42	0.63
2:D:152:SER:O	2:D:156:ILE:CD1	2.46	0.63
2:C:95:LEU:O	2:C:98:LEU:HB2	1.97	0.63
2:C:105:MET:HE3	2:C:110:LEU:HG	1.81	0.63
1:A:12:GLU:O	1:A:15:LYS:HB2	1.99	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:135:LEU:HD21	1:B:171:LYS:HZ1	0.46	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
2:C:86:ALA:O	2:C:87:LYS:C	2.42	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:18:ILE:HD12	1:B:343:ILE:HG13	1.82	0.62
1:B:290:VAL:CG1	1:B:291:SER:N	2.63	0.62
2:D:81:ALA:O	2:D:82:ALA:C	2.43	0.62
1:A:88:GLU:OE2	1:A:91:TYR:C	2.42	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:A:227:GLU:C	1:A:229:GLU:H	2.08	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:B:432:LEU:O	1:B:435:ASP:N	2.33	0.62
1:B:379:ALA:O	1:B:380:ALA:C	2.43	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
2:D:172:ASN:ND2	2:D:172:ASN:O	2.32	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:224:LEU:O	1:B:225:LEU:C	2.42	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:ARG:HH21	1:B:442:ILE:HG22	1.62	0.62
2:D:12:VAL:HG23	2:D:125:GLY:O	2.00	0.62
2:C:54:ALA:HB3	2:C:100:ALA:HB1	1.81	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
1:A:31:LEU:HD22	1:A:70:LEU:HD11	1.81	0.61
1:B:435:ASP:O	1:B:436:GLU:C	2.42	0.61
2:D:67:PHE:HD2	2:D:85:LEU:HD22	1.63	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:C:153:ALA:O	2:C:154:SER:C	2.43	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:B:107:ALA:O	1:B:243:ALA:HB1	2.00	0.61
2:D:20:MET:CE	2:D:52:GLY:N	2.62	0.61
2:C:112:LEU:HB3	2:C:120:ILE:HB	1.82	0.61
1:A:390:ILE:CD1	1:B:323:GLN:NE2	2.63	0.61
1:B:315:PRO:O	1:B:318:LEU:HD12	2.00	0.61
2:D:7:THR:HG22	2:D:23:ASP:OD2	1.99	0.61
2:C:92:ASP:OD2	2:C:95:LEU:HD12	1.99	0.61
1:B:52:ASN:OD1	1:B:304:PHE:N	2.33	0.61
1:B:435:ASP:O	1:B:437:ASP:N	2.33	0.61
2:D:8:THR:HG21	2:D:132:GLY:N	2.16	0.61
1:B:135:LEU:HD21	1:B:171:LYS:NZ	1.14	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
2:C:159:ALA:O	2:C:160:ALA:C	2.42	0.61
1:A:20:GLN:HE22	1:A:332:LEU:CA	2.12	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
2:D:44:LEU:HB2	2:D:49:VAL:HG23	1.82	0.61
2:C:68:GLU:O	2:C:70:LYS:N	2.34	0.61
2:C:104:VAL:O	2:C:110:LEU:CD2	2.48	0.61
1:A:220:ASP:O	1:A:222:MET:N	2.33	0.61
1:B:83:ALA:O	1:B:84:THR:C	2.43	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
2:D:12:VAL:CG2	2:D:13:GLN:H	2.12	0.61
1:B:398:VAL:O	1:B:401:ARG:HB3	2.01	0.61
2:C:27:THR:HG21	2:C:170:TYR:HD2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:THR:O	2:C:166:GLU:HB3	2.01	0.61
1:A:26:SER:O	1:A:27:VAL:C	2.44	0.61
1:A:263:LYS:HE2	1:A:269:GLY:HA3	1.81	0.61
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:340:PHE:O	1:A:341:GLU:C	2.42	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:353:VAL:O	1:B:354:GLN:C	2.43	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: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:375:ARG:HA	1:B:378:GLU:HB2	1.83	0.60
2:D:79:LYS:O	2:D:82:ALA:HB3	2.01	0.60
2:C:110:LEU:HD22	2:C:127:LEU:HD12	1.83	0.60
1:A:26:SER:O	1:A:28:ALA:N	2.34	0.60
1:A:235:ASN:C	1:A:239:LEU:HD12	2.27	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: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
1:A:131:ILE:HG22	1:A:135:LEU:CD1	2.30	0.60
1:B:34:ARG:HE	1:B:250:HIS:CE1	2.19	0.60
1:B:307:SER:OG	1:B:308:GLY:N	2.35	0.60
1:B:441:PHE:N	1:B:441:PHE:HD2	1.99	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:225:LEU:O	1:A:226:ILE:C	2.45	0.60
1:A:235:ASN:H	1:A:236:PRO:HD3	1.64	0.60
1:B:52:ASN:CG	1:B:304:PHE:HB2	2.25	0.60
1:B:167:GLN:CD	1:B:219:LYS:HG2	2.27	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
1:B:425:VAL:HG12	1:B:426:SER:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:112:LEU:HD22	2:D:113:VAL:N	2.17	0.60
2:C:140:GLY:C	2:C:142:ALA:H	2.10	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
1:B:325:ARG:C	1:B:327:PRO:CD	2.75	0.59
2:D:13:GLN:HG3	2:D:105:MET:CE	2.32	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:A:353:VAL:O	1:A:354:GLN:C	2.45	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:408:TYR:HE1	1:B:6:PRO:HB3	1.67	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
2:C:21:SER:OG	2:C:157:ALA:HB1	2.02	0.59
1:A:424:TYR:O	1:A:425:VAL:C	2.46	0.59
1:B:55:MET:CE	1:B:63:LYS:HA	2.32	0.59
1:B:79:ILE:HD11	1:B:102:ASP:C	2.27	0.59
1:B:315:PRO:C	1:B:317:ASP:N	2.56	0.59
1:B:395:LEU:HD12	1:B:395:LEU:H	1.67	0.59
2:D:159:ALA:O	2:D:160:ALA:O	2.19	0.59
2:C:105:MET:HB3	2:C:110:LEU:CD2	2.32	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:78:LEU:O	2:C:79:LYS:C	2.45	0.59
1:A:17:ILE:HD13	1:A:66:ILE:HA	1.84	0.59
1:A:20:GLN:O	1:A:23:ALA:HB3	2.02	0.59
1:B:149:GLN:C	1:B:152:PRO:HD2	2.26	0.59
1:B:6:PRO:HD2	1:B:32:ARG:HD2	1.83	0.59
1:B:20:GLN:HE22	1:B:332:LEU:CB	2.16	0.59
2:C:101:MET:HB3	2:C:112:LEU:CD2	2.28	0.59
1:A:358:LEU:CD2	1:B:36:ARG:HB3	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:B:119:ASN:HB3	1:B:233:LEU:HD13	1.85	0.59
2:D:172:ASN:ND2	2:D:172:ASN:H	1.97	0.59
1:B:18:ILE:HD11	1:B:347:PRO:HD3	1.85	0.59
1:B:279:ARG:HG3	1:B:319:ILE:HD13	1.84	0.59
2:D:12:VAL:CG2	2:D:13:GLN:N	2.66	0.59
2:D:112:LEU:HD23	2:D:113:VAL:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:PHE:CE1	1:A:315:PRO:N	2.71	0.58
2:D:8:THR:HG21	2:D:132:GLY:H	1.67	0.58
2:D:110:LEU:CD2	2:D:111:LEU:H	2.15	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
2:D:132:GLY:O	2:D:133:GLY:C	2.45	0.58
1:A:55:MET:HE1	1:A:63:LYS:HA	1.86	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
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:D:23:ASP:CB	2:D:172:ASN:HD21	2.08	0.58
2:C:103:ILE:CG1	2:C:129:ILE:CD1	2.77	0.58
1:A:379:ALA:O	1:A:380:ALA:C	2.46	0.58
1:B:61:VAL:CB	1:B:335:LEU:HD11	2.29	0.58
2:D:44:LEU:O	2:D:49:VAL:HG22	2.02	0.58
2:D:54:ALA:HB3	2:D:100:ALA:HB1	1.86	0.58
2:C:43:LYS:NZ	2:C:179:GLU:O	2.26	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:125:GLU:HA	1:B:128:GLU:CD	2.29	0.58
1:B:285:VAL:HA	1:B:304:PHE:CE1	2.39	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
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
1:A:16:HIS:CD2	1:A:69:ARG:HG2	2.35	0.58
1:B:368:PHE:CB	1:B:373:ILE:HD11	2.34	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:B:135:LEU:CG	1:B:171:LYS:HZ3	1.83	0.57
1:B:145:GLN:C	1:B:147:GLU:H	2.12	0.57
2:D:105:MET:HE3	2:D:110:LEU:HG	1.86	0.57
2:C:13:GLN:HG3	2:C:105:MET:HE1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:134:ASN:OD1	2:C:134:ASN:N	2.36	0.57
1:A:276:GLY:O	1:A:279:ARG:N	2.37	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:394:ARG:O	1:B:395:LEU:C	2.48	0.57
1:B:424:TYR:O	1:B:425:VAL:O	2.22	0.57
2:C:83:VAL:O	2:C:86:ALA:N	2.37	0.57
2:C:140:GLY:O	2:C:142:ALA:N	2.37	0.57
1:A:315:PRO:C	1:A:317:ASP:H	2.13	0.57
1:B:249:GLN:O	1:B:250:HIS:HB3	2.02	0.57
1:B:322:LEU:C	1:B:324:GLY:H	2.13	0.57
1:B:17:ILE:HD13	1:B:66:ILE:HA	1.86	0.57
1:B:56:ILE:HD11	1:B:315:PRO:HG2	1.87	0.57
1:B:135:LEU:CD2	1:B:171:LYS:HZ2	1.23	0.57
1:B:298:LYS:CG	1:B:300:ASP:HB2	2.34	0.57
2:D:110:LEU:C	2:D:110:LEU:CD2	2.73	0.57
1:A:253:VAL:HG23	1:A:304:PHE:CE2	2.40	0.57
1:A:282:LEU:O	1:A:283:PRO:C	2.47	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:421:ASP:O	1:B:422:ALA:C	2.48	0.57
1:B:438:LEU:O	1:B:440:ARG:N	2.37	0.57
2:D:14:HIS:CE1	2:D:15:LYS:HE2	2.40	0.57
2:D:105:MET:HB3	2:D:110:LEU:HD21	1.86	0.57
2:D:110:LEU:C	2:D:110:LEU:HD22	2.28	0.57
1:A:322:LEU:C	1:A:322:LEU:CD1	2.68	0.57
1:B:403:MET:HE2	1:B:420:ILE:CD1	2.30	0.57
2:C:25:GLN:H	2:C:172:ASN:ND2	2.02	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
2:C:68:GLU:O	2:C:69:ALA:C	2.47	0.57
2:C:152:SER:HB3	2:C:155:GLU:CD	2.30	0.57
1:B:10:VAL:O	1:B:13:LEU:N	2.38	0.56
1:B:18:ILE:CD1	1:B:342:ARG:O	2.51	0.56
2:D:172:ASN:HD22	2:D:172:ASN:N	1.88	0.56
2:C:82:ALA:O	2:C:83:VAL:C	2.44	0.56
1:A:10:VAL:O	1:A:13:LEU:N	2.35	0.56
1:A:96:VAL:HG11	1:A:280:ASP:CB	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:TYR:HE2	1:B:25:ARG:CZ	2.18	0.56
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:163:THR:O	2:C:164:ALA:C	2.47	0.56
1:A:41:ASN:ND2	1:A:43:GLU:HB3	2.19	0.56
1:A:67:ALA:O	1:A:68:ARG:C	2.48	0.56
1:A:354:GLN:OE1	1:B:48:VAL:HG22	2.05	0.56
1:A:395:LEU:HD12	1:A:395:LEU:H	1.70	0.56
1:A:413:LEU:O	1:A:416:GLN:N	2.38	0.56
1:B:70:LEU:CD1	1:B:70:LEU:O	2.53	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:B:299:THR:OG1	1:B:300:ASP:N	2.36	0.56
1:B:322:LEU:HD12	1:B:326:LEU:HD12	1.85	0.56
1:A:25:ARG:O	1:A:26:SER:C	2.47	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:98:SER:O	1:B:99:ILE:C	2.49	0.56
1:B:336:THR:H	1:B:339:ASP:CG	2.13	0.56
1:B:399:LEU:O	1:B:402:LEU:N	2.38	0.56
2:C:110:LEU:C	2:C:110:LEU:HD22	2.31	0.56
1:A:366:ILE:CG2	1:A:420:ILE:HD12	2.36	0.56
1:B:41:ASN:OD1	1:B:44:LEU:HD12	2.04	0.56
1:B:322:LEU:O	1:B:326:LEU:HD12	2.06	0.56
2:D:83:VAL:HG12	2:D:84:GLU:N	2.19	0.56
1:A:285:VAL:HA	1:A:304:PHE:CE1	2.41	0.56
1:B:225:LEU:O	1:B:226:ILE:C	2.49	0.56
1:B:283:PRO:O	1:B:284:LEU:C	2.48	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:322:LEU:C	1:B:324:GLY:N	2.61	0.56
1:B:432:LEU:C	1:B:434:ALA:N	2.64	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
2:D:17:ARG:CG	2:D:17:ARG:NH1	2.52	0.56
2:D:108:ASP:CB	2:D:109:THR:HG22	2.36	0.56
1:B:16:HIS:CD2	1:B:69:ARG:HG2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:LEU:O	1:B:430:ASP:C	2.49	0.56
1:A:3:GLU:O	1:A:4:MET:CB	2.52	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:6:PRO:CD	1:A:32:ARG:CD	2.83	0.55
1:A:236:PRO:O	1:A:238:GLU:N	2.38	0.55
2:D:8:THR:CG2	2:D:132:GLY:N	2.69	0.55
2:C:17:ARG:HB3	2:C:153:ALA:HB3	1.88	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:349:ALA:O	1:B:350:SER:C	2.49	0.55
1:B:61:VAL:O	1:B:61:VAL:CG2	2.53	0.55
3:B:906:ADP:O5'	3:B:906:ADP:C2'	2.53	0.55
1:A:73:LEU:C	1:A:75:ASN:H	2.15	0.55
1:B:98:SER:O	1:B:101:ARG:N	2.40	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:418:ILE:HG23	1:A:419:THR:H	1.72	0.55
1:B:240:LYS:HB3	1:B:294:HIS:CD2	2.41	0.55
2:D:118:GLU:HG3	2:C:4:PHE:CD1	2.41	0.55
2:C:9:ILE:HD11	2:C:53:PHE:O	2.05	0.55
1:A:122:ARG:CZ	1:A:126:LEU:HD11	2.33	0.55
1:A:149:GLN:C	1:A:151:GLU:H	2.13	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:D:28:PHE:CG	2:D:29:GLY:N	2.75	0.55
2:C:35:LYS:HG2	2:C:36:HIS:N	2.21	0.55
1:A:344:LEU:HD11	1:A:376:ILE:HG22	1.88	0.55
1:B:251:GLY:C	1:B:252:ILE:CG1	2.76	0.55
1:B:399:LEU:O	1:B:400:GLU:C	2.49	0.55
1:A:18:ILE:CD1	1:A:343:ILE:HA	2.37	0.55
1:A:283:PRO:O	1:A:287:GLY:N	2.38	0.55
1:B:438:LEU:CD2	1:B:442:ILE:HD12	2.37	0.55
2:D:136:ALA:HB1	2:D:160:ALA:HB1	1.89	0.55
1:A:79:ILE:HD11	1:A:102:ASP:C	2.29	0.55
1:A:100:ILE:CG1	1:A:284:LEU:HD22	2.27	0.55
1:A:119:ASN:HB3	1:A:233:LEU:HD13	1.87	0.55
1:A:384:ASN:OD1	1:A:394:ARG:HD2	2.06	0.55
1:B:31:LEU:HD22	1:B:70:LEU:HD11	1.89	0.55
1:B:79:ILE:CD1	1:B:102:ASP:C	2.79	0.55
2:D:21:SER:OG	2:D:157:ALA:HB1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:PHE:CE2	1:A:99:ILE:HD11	2.42	0.55
1:B:86:PHE:CB	1:B:277:VAL:HG21	2.37	0.55
1:B:372:GLY:O	1:B:376:ILE:N	2.35	0.55
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
1:A:20:GLN:OE1	1:A:61:VAL:HG21	2.07	0.54
1:B:80:LYS:HA	1:B:254:PHE:O	2.07	0.54
1:B:299:THR:HA	1:B:302:ILE:HD12	1.89	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:A:16:HIS:C	1:A:17:ILE:HG13	2.32	0.54
1:A:277:VAL:O	1:A:278:GLN:C	2.49	0.54
1:A:360:ALA:HA	1:A:364:VAL:O	2.07	0.54
1:B:340:PHE:C	1:B:342:ARG:N	2.65	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
1:B:439:SER:O	1:B:440:ARG:C	2.46	0.54
2:D:39:ARG:HB2	2:D:39:ARG:CZ	2.37	0.54
2:C:143:LEU:O	2:C:147:ALA:N	2.32	0.54
1:A:219:LYS:C	1:A:220:ASP:O	2.49	0.54
1:A:259:ASP:HB3	1:A:310:PHE:CE2	2.42	0.54
1:B:61:VAL:O	1:B:61:VAL:HG23	2.07	0.54
2:C:72:GLU:C	2:C:74:TYR:N	2.66	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:N	1:B:413:LEU:CD2	2.62	0.54
1:A:246:ALA:O	1:A:247:VAL:C	2.49	0.54
1:A:247:VAL:O	1:A:248:GLU:C	2.49	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
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
1:B:100:ILE:HD12	1:B:290:VAL:CG2	2.21	0.54
1:B:282:LEU:O	1:B:283:PRO:C	2.51	0.54
2:D:60:ALA:O	2:D:61:PHE:O	2.25	0.54
2:D:129:ILE:CG2	2:D:130:GLY:H	2.20	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
1:A:349:ALA:O	1:A:350:SER:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:VAL:N	3:B:906:ADP:O2B	2.37	0.54
1:B:70:LEU:HA	1:B:73:LEU:HD21	1.90	0.54
2:D:112:LEU:HD22	2:D:113:VAL:H	1.71	0.54
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
1:B:149:GLN:C	1:B:151:GLU:H	2.16	0.53
1:B:282:LEU:CB	1:B:283:PRO:HD2	2.36	0.53
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:B:100:ILE:CD1	1:B:284:LEU:CD2	2.68	0.53
1:B:104:THR:HG22	1:B:247:VAL:HG21	1.90	0.53
1:B:253:VAL:HG23	1:B:304:PHE:CD2	2.43	0.53
1:B:257:GLU:O	1:B:259:ASP:N	2.40	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:69:ARG:O	1:B:73:LEU:HD23	2.09	0.53
1:B:70:LEU:HD12	1:B:71:ALA:HA	1.90	0.53
2:C:5:HIS:HB2	2:C:27:THR:HB	1.91	0.53
2:C:81:ALA:O	2:C:82:ALA:C	2.51	0.53
2:C:103:ILE:CG1	2:C:129:ILE:HD12	2.30	0.53
1:A:125:GLU:HA	1:A:128:GLU:CD	2.34	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:6:PRO:HD2	1:B:32:ARG:CD	2.39	0.53
1:B:7:ARG:O	1:B:8:GLU:C	2.51	0.53
1:B:153:SER:HA	1:B:156:ARG:HB3	1.90	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:18:ILE:HD11	1:B:342:ARG:C	2.25	0.53
1:B:54:LEU:C	1:B:54:LEU:CD1	2.82	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:A:421:ASP:O	1:A:422:ALA:C	2.51	0.53
1:B:79:ILE:CG2	1:B:80:LYS:N	2.72	0.53
1:B:368:PHE:HB2	1:B:373:ILE:HD11	1.91	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
1:A:88:GLU:HB2	1:A:92:VAL:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ALA:O	1:A:362:GLU:N	2.41	0.53
1:B:104:THR:HA	1:B:107:ALA:HB3	1.89	0.53
1:B:219:LYS:C	1:B:220:ASP:O	2.51	0.53
2:D:78:LEU:O	2:D:79:LYS:C	2.51	0.53
2:C:172:ASN:ND2	2:C:172:ASN:H	1.94	0.53
1:A:102:ASP:C	1:A:104:THR:H	2.16	0.52
1:A:355:TYR:OH	1:A:400:GLU:OE2	2.17	0.52
1:B:37:ARG:O	1:B:38:MET:C	2.51	0.52
2:D:112:LEU:HD13	2:D:120:ILE:HD12	1.90	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
1:A:320:PRO:O	1:A:321:GLU:C	2.53	0.52
1:B:322:LEU:O	1:B:323:GLN:C	2.52	0.52
1:B:408:TYR:C	1:B:410:ALA:H	2.17	0.52
2:D:23:ASP:CB	2:D:172:ASN:ND2	2.54	0.52
2:C:25:GLN:HB2	2:C:172:ASN:CB	2.38	0.52
1:A:84:THR:O	1:A:85:LYS:C	2.51	0.52
1:A:103:LEU:HD12	1:A:247:VAL:HG13	1.90	0.52
2:D:20:MET:HE1	2:D:51:ALA:O	2.08	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
2:C:12:VAL:HG22	2:C:13:GLN:N	2.24	0.52
2:C:110:LEU:C	2:C:110:LEU:CD2	2.72	0.52
1:A:55:MET:CE	1:A:63:LYS:HA	2.40	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: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: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:A:100:ILE:CD1	1:A:290:VAL:HG21	2.40	0.52
1:B:4:MET:HG2	1:B:8:GLU:HB2	1.91	0.52
1:B:128:GLU:C	1:B:130:ARG:H	2.17	0.52
1:B:244:ILE:O	1:B:245:ASP:C	2.51	0.52
1:B:336:THR:O	1:B:339:ASP:HB2	2.10	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:THR:O	1:B:340:PHE:HB2	2.09	0.52
2:C:27:THR:HG21	2:C:170:TYR:CE2	2.45	0.52
1:A:61:VAL:HB	1:A:335:LEU:CD1	2.28	0.52
1:A:394:ARG:HG2	1:A:398:VAL:HG23	1.92	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
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:276:GLY:O	1:A:277:VAL:C	2.52	0.52
1:A:342:ARG:O	1:A:347:PRO:HD2	2.10	0.52
1:B:3:GLU:HG2	1:B:4:MET:N	2.24	0.52
1:B:32:ARG:NH2	1:B:35:TRP:CZ3	2.77	0.52
1:B:413:LEU:O	1:B:414:SER:C	2.52	0.52
2:C:164:ALA:C	2:C:166:GLU:H	2.16	0.52
1:A:31:LEU:HD22	1:A:70:LEU:HD21	1.92	0.52
1:A:359:MET:HG2	1:A:366:ILE:HD13	1.85	0.52
3:A:905:ADP:C8	3:A:905:ADP:C5'	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:3:GLU:CG	1:A:4:MET:H	2.24	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:399:LEU:O	1:A:400:GLU:C	2.52	0.51
1:B:153:SER:C	1:B:155:ALA:N	2.59	0.51
2:D:80:ARG:HG2	2:D:80:ARG:NH1	2.05	0.51
1:A:82:GLU:OE1	1:A:256:ASP:HB3	2.11	0.51
1:A:224:LEU:O	1:A:225:LEU:C	2.53	0.51
1:A:251:GLY:O	1:A:252:ILE:HG13	2.09	0.51
1:B:131:ILE:CG2	1:B:135:LEU:HD11	2.29	0.51
2:D:163:THR:O	2:D:164:ALA:C	2.52	0.51
1:A:62:GLY:O	1:A:63:LYS:C	2.53	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
1:B:217:LYS:HB2	1:B:220:ASP:OD2	2.11	0.51
2:D:147:ALA:HB1	2:D:150:SER:HB3	1.92	0.51
2:C:104:VAL:HG22	2:C:111:LEU:HB2	1.93	0.51
1:A:237:GLU:N	1:A:240:LYS:CE	2.66	0.51
1:B:389:ASN:C	1:B:389:ASN:ND2	2.67	0.51
2:D:82:ALA:O	2:D:83:VAL:C	2.50	0.51
1:B:80:LYS:HG3	1:B:254:PHE:HD1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LYS:HD2	1:B:218:ILE:CD1	2.41	0.51
2:C:114:SER:O	2:C:116:THR:N	2.44	0.51
1:A:439:SER:O	1:A:440:ARG:C	2.54	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: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
2:C:178:GLU:HA	2:C:178:GLU:OE2	2.09	0.51
1:A:29:ILE:O	1:A:29:ILE:HG22	2.10	0.51
1:A:253:VAL:CG2	1:A:304:PHE:CD2	2.92	0.51
1:A:283:PRO:O	1:A:284:LEU:C	2.51	0.51
1:A:360:ALA:O	1:A:363:GLY:N	2.25	0.51
1:A:322:LEU:C	1:A:324:GLY:H	2.17	0.51
1:A:322:LEU:C	1:A:324:GLY:N	2.68	0.51
1:A:338:SER:O	1:A:340:PHE:N	2.43	0.51
1:B:418:ILE:HG23	1:B:419:THR:H	1.76	0.51
2:D:45:PHE:O	2:D:46:ASN:C	2.54	0.51
2:D:140:GLY:O	2:D:142:ALA:N	2.44	0.51
2:C:172:ASN:ND2	2:C:172:ASN:N	2.53	0.51
1:A:318:LEU:HB2	1:A:323:GLN:HG2	1.93	0.51
1:A:408:TYR:C	1:A:410:ALA:H	2.19	0.51
1:B:81:VAL:HG21	1:B:99:ILE:HG12	1.93	0.51
1:B:303:LEU:HG	1:B:304:PHE:N	2.25	0.51
1:B:375:ARG:CB	1:B:425:VAL:HG11	2.41	0.51
1:B:421:ASP:O	1:B:424:TYR:N	2.44	0.51
1:A:5:THR:CG2	1:A:8:GLU:HG3	2.28	0.50
1:A:246:ALA:O	1:A:247:VAL:O	2.29	0.50
1:A:315:PRO:C	1:A:317:ASP:N	2.68	0.50
1:B:12:GLU:HA	1:B:15:LYS:HD3	1.93	0.50
2:D:110:LEU:C	2:D:111:LEU:CD1	2.73	0.50
2:C:140:GLY:C	2:C:142:ALA:N	2.68	0.50
1:A:254:PHE:CZ	1:A:307:SER:HB2	2.46	0.50
1:A:268:SER:CB	1:A:312:ILE:CG2	2.75	0.50
2:D:39:ARG:HA	2:D:176:ILE:CD1	2.41	0.50
2:D:177:LEU:CD2	2:D:178:GLU:N	2.74	0.50
2:C:45:PHE:O	2:C:46:ASN:C	2.55	0.50
2:C:110:LEU:C	2:C:111:LEU:CD1	2.74	0.50
2:D:68:GLU:O	2:D:70:LYS:N	2.44	0.50
2:D:106:ASN:O	2:D:107:GLN:C	2.54	0.50
2:D:177:LEU:HD23	2:D:178:GLU:H	1.76	0.50
2:D:5:HIS:HB2	2:D:27:THR:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:MET:HG2	1:A:8:GLU:HB2	1.92	0.50
1:A:31:LEU:CD2	1:A:70:LEU:CD1	2.89	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: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: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:A:108:VAL:O	1:A:111:VAL:N	2.45	0.50
1:B:20:GLN:NE2	1:B:332:LEU:HB3	2.27	0.50
1:B:25:ARG:O	1:B:26:SER:C	2.54	0.50
1:B:87:THR:HG23	1:B:88:GLU:N	2.27	0.50
1:B:299:THR:HA	1:B:302:ILE:CD1	2.42	0.50
1:A:95:GLU:O	1:A:98:SER:HB3	2.11	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
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:251:GLY:C	1:A:252:ILE:CG1	2.78	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
1:B:212:LYS:HZ3	1:B:212:LYS:HB2	1.77	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: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:88:GLU:O	1:B:91:TYR:HA	2.12	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:O	1:B:330:VAL:CG2	2.58	0.49
3:B:906:ADP:C8	3:B:906:ADP:C5'	2.91	0.49
1:A:240:LYS:O	1:A:241:GLN:C	2.55	0.49
1:A:364:VAL:HG12	1:A:365:ASN:O	2.12	0.49
1:A:438:LEU:O	1:A:439:SER:C	2.55	0.49
1:A:390:ILE:O	1:A:390:ILE:CG2	2.60	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:B:106:ALA:C	1:B:108:VAL:N	2.68	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLN:HA	1:B:151:GLU:HB2	1.93	0.49
2:D:58:ALA:O	2:D:59:ASP:C	2.53	0.49
1:A:73:LEU:C	1:A:75:ASN:N	2.70	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:20:MET:HE2	2:C:41:VAL:CG1	2.33	0.49
2:C:44:LEU:HB2	2:C:49:VAL:CG2	2.43	0.49
1:B:5:THR:O	1:B:6:PRO:C	2.55	0.49
1:B:21:ASP:O	1:B:24:LYS:HG3	2.12	0.49
1:B:88:GLU:OE2	1:B:91:TYR:C	2.56	0.49
2:C:78:LEU:O	2:C:81:ALA:N	2.45	0.49
2:C:135:TYR:N	2:C:135:TYR:CD2	2.76	0.49
1:A:83:ALA:O	1:A:84:THR:O	2.31	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:429:LEU:O	1:A:430:ASP:C	2.55	0.49
2:C:20:MET:CE	2:C:52:GLY:N	2.75	0.49
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:17:ILE:CD1	1:B:66:ILE:HA	2.43	0.49
1:B:375:ARG:O	1:B:376:ILE:O	2.30	0.49
2:D:172:ASN:ND2	2:D:172:ASN:N	2.55	0.49
1:A:87:THR:HG23	1:A:88:GLU:N	2.28	0.49
1:A:145:GLN:C	1:A:147:GLU:H	2.20	0.49
1:A:310:PHE:HD1	1:A:314:LYS:CA	2.26	0.49
1:B:23:ALA:O	1:B:24:LYS:C	2.56	0.49
1:B:353:VAL:C	1:B:355:TYR:N	2.68	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:A:403:MET:O	1:A:404:GLU:C	2.56	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:D:114:SER:C	2:D:116:THR:H	2.20	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
2:D:41:VAL:HG12	2:D:178:GLU:HG3	1.95	0.48
2:C:62:THR:HG22	2:C:63:LEU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:72:GLU:O	2:C:73:GLU:C	2.56	0.48
1:A:375:ARG:CB	1:A:425:VAL:HG11	2.41	0.48
1:A:390:ILE:CD1	1:B:323:GLN:CD	2.86	0.48
1:B:55:MET:HE2	1:B:63:LYS:HB3	1.94	0.48
2:C:49:VAL:O	2:C:50:LEU:HD23	2.14	0.48
2:C:110:LEU:HD23	2:C:111:LEU:N	2.25	0.48
1:B:24:LYS:O	1:B:25:ARG:C	2.56	0.48
1:B:62:GLY:O	1:B:66:ILE:HG13	2.14	0.48
1:B:331:GLU:C	1:B:332:LEU:HD12	2.38	0.48
2:D:63:LEU:HD11	2:D:89:TRP:CE2	2.48	0.48
2:C:77:ASN:O	2:C:78:LEU:C	2.56	0.48
1:B:20:GLN:CD	1:B:332:LEU:HB3	2.38	0.48
1:B:48:VAL:O	1:B:301:HIS:HE1	1.97	0.48
1:B:286:GLU:HA	1:B:325:ARG:NH1	2.28	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:227:GLU:C	1:B:229:GLU:H	2.21	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
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
1:B:397:THR:O	1:B:398:VAL:C	2.57	0.48
2:D:68:GLU:O	2:D:69:ALA:C	2.56	0.48
2:D:104:VAL:O	2:D:110:LEU:CD2	2.62	0.48
2:D:110:LEU:HD23	2:D:110:LEU:HA	1.36	0.48
2:C:143:LEU:HA	2:C:143:LEU:HD23	1.38	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:A:132:LEU:HD21	1:A:160:ARG:HG3	1.95	0.48
1:A:403:MET:SD	1:A:403:MET:N	2.86	0.48
1:A:135:LEU:HD21	1:A:171:LYS:HZ2	1.10	0.47
1:A:336:THR:H	1:A:339:ASP:CG	2.21	0.47
2:D:26:VAL:HG12	2:D:26:VAL:O	2.13	0.47
2:C:44:LEU:CB	2:C:49:VAL:HG22	2.44	0.47
1:A:70:LEU:O	1:A:73:LEU:CD2	2.62	0.47
1:A:98:SER:O	1:A:99:ILE:C	2.57	0.47
1:A:236:PRO:C	1:A:238:GLU:N	2.72	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:A:282:LEU:O	1:A:285:VAL:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:GLY:O	1:A:416:GLN:O	2.32	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:B:377:ALA:O	1:B:378:GLU:C	2.56	0.47
1:A:246:ALA:O	1:A:250:HIS:N	2.47	0.47
1:A:135:LEU:CB	1:A:171:LYS:HZ3	2.28	0.47
2:D:17:ARG:HB3	2:D:153:ALA:HB3	1.97	0.47
2:D:174:GLN:H	2:D:174:GLN:HG2	1.52	0.47
1:A:224:LEU:O	1:A:227:GLU:N	2.47	0.47
1:B:18:ILE:HG23	1:B:342:ARG:HH21	1.79	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
1:B:340:PHE:O	1:B:342:ARG:N	2.47	0.47
1:B:391:GLY:O	1:B:392:ALA:C	2.56	0.47
1:B:406:ILE:CD1	1:B:420:ILE:HD11	2.45	0.47
2:D:8:THR:HG23	2:D:131:SER:N	2.29	0.47
1:A:45:ARG:HH21	1:A:46:HIS:CD2	2.33	0.47
1:A:302:ILE:HG22	1:A:303:LEU:N	2.29	0.47
1:A:408:TYR:HE1	1:B:6:PRO:CB	2.28	0.47
1:B:20:GLN:O	1:B:23:ALA:CB	2.62	0.47
1:B:37:ARG:HB3	1:B:38:MET:H	1.51	0.47
1:B:97:ASP:C	1:B:97:ASP:OD2	2.57	0.47
2:D:134:ASN:O	2:D:137:LEU:N	2.48	0.47
2:C:12:VAL:HG22	2:C:13:GLN:H	1.79	0.47
1:A:355:TYR:CE2	1:A:403:MET:HG2	2.49	0.47
1:A:372:GLY:C	1:A:376:ILE:HG13	2.39	0.47
1:B:18:ILE:HD13	1:B:342:ARG:CB	2.44	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: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:D:89:TRP:HD1	2:D:95:LEU:HB3	1.77	0.47
2:C:152:SER:O	2:C:156:ILE:CD1	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:CYS:O	1:B:299:THR:HG23	2.14	0.47
2:C:25:GLN:HB2	2:C:172:ASN:HB3	1.97	0.47
1:A:115:ALA:HB2	1:A:118:LYS:NZ	2.30	0.47
1:B:100:ILE:HG13	1:B:284:LEU:HD21	1.95	0.47
2:D:161:LEU:O	2:D:162:GLU:C	2.58	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:B:20:GLN:OE1	1:B:332:LEU:HB3	2.15	0.46
1:B:247:VAL:O	1:B:248:GLU:C	2.57	0.46
1:B:271:ASP:HB3	1:B:273:SER:HB3	1.97	0.46
1:A:31:LEU:CD2	1:A:70:LEU:HD13	2.46	0.46
1:A:150:GLN:O	1:A:153:SER:HB2	2.15	0.46
1:A:403:MET:CE	1:A:406:ILE:HD12	2.30	0.46
1:B:100:ILE:CD1	1:B:290:VAL:CG2	2.85	0.46
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
1:A:282:LEU:HD22	1:A:282:LEU:HA	1.58	0.46
1:A:375:ARG:O	1:A:376:ILE:C	2.59	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
1:A:6:PRO:HD2	1:A:32:ARG:CD	2.45	0.46
1:A:98:SER:O	1:A:101:ARG:HB3	2.15	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:424:TYR:CZ	1:A:428:HIS:NE2	2.75	0.46
1:B:4:MET:CG	1:B:8:GLU:HB2	2.45	0.46
1:B:6:PRO:HD3	1:B:32:ARG:CD	2.35	0.46
1:B:45:ARG:HH21	1:B:46:HIS:CD2	2.33	0.46
1:B:438:LEU:C	1:B:440:ARG:N	2.71	0.46
2:C:114:SER:C	2:C:116:THR:H	2.23	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: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: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:A:100:ILE:CD1	1:A:299:THR:HG21	2.45	0.46
1:A:128:GLU:C	1:A:130:ARG:H	2.23	0.46
1:A:441:PHE:HA	1:B:315:PRO:HD2	1.96	0.46
1:B:29:ILE:HG22	1:B:29:ILE:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLN:O	1:B:153:SER:HB2	2.14	0.46
2:D:72:GLU:C	2:D:74:TYR:N	2.74	0.46
2:C:8:THR:HG23	2:C:130:GLY:C	2.41	0.46
2:C:105:MET:HB3	2:C:110:LEU:HD21	1.97	0.46
1:A:20:GLN:OE1	1:A:332:LEU:HB3	2.16	0.46
1:A:83:ALA:CB	1:A:261:ILE:HD11	2.16	0.46
1:B:102:ASP:C	1:B:104:THR:H	2.23	0.46
1:B:284:LEU:HD23	1:B:284:LEU:HA	1.66	0.46
1:B:403:MET:HE3	1:B:420:ILE:HD11	1.96	0.46
2:D:143:LEU:HD12	2:D:156:ILE:HG23	1.97	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
1:A:338:SER:C	1:A:340:PHE:N	2.73	0.46
2:C:35:LYS:CD	2:C:38:ALA:H	2.28	0.46
2:C:95:LEU:HD23	2:C:98:LEU:CD1	2.45	0.46
2:C:103:ILE:HD11	2:C:129:ILE:CG1	2.41	0.46
1:A:66:ILE:HD12	1:A:332:LEU:HD21	1.97	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:B:116:ILE:O	1:B:117:GLU:HG3	2.16	0.46
2:D:110:LEU:HD23	2:D:111:LEU:H	1.81	0.46
2:D:140:GLY:C	2:D:142:ALA:N	2.74	0.46
2:C:25:GLN:HB2	2:C:172:ASN:ND2	2.31	0.46
2:C:51:ALA:HA	2:C:103:ILE:O	2.16	0.46
1:A:403:MET:HE3	1:A:420:ILE:CD1	2.43	0.46
1:B:221:ALA:N	1:B:224:LEU:HD13	2.31	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:263:LYS:O	1:A:264:ARG:C	2.58	0.45
1:A:315:PRO:O	1:A:317:ASP:N	2.49	0.45
1:B:350:SER:HG	1:B:352:THR:HG1	1.64	0.45
2:D:152:SER:HB3	2:D:155:GLU:OE2	2.17	0.45
2:C:33:VAL:O	2:C:33:VAL:HG12	2.16	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:A:432:LEU:C	1:A:434:ALA:N	2.75	0.45
1:B:36:ARG:O	1:B:37:ARG:O	2.34	0.45
1:B:135:LEU:CB	1:B:171:LYS:HZ3	2.26	0.45
1:B:252:ILE:HG12	1:B:303:LEU:HB3	1.98	0.45
1:B:320:PRO:O	1:B:321:GLU:C	2.60	0.45
2:C:44:LEU:CB	2:C:49:VAL:CG2	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ASP:HA	1:A:24:LYS:HG3	1.98	0.45
1:B:54:LEU:CD1	1:B:55:MET:N	2.73	0.45
1:B:355:TYR:CD2	1:B:359:MET:HE2	2.51	0.45
1:B:432:LEU:HB3	1:B:433:VAL:H	1.43	0.45
2:C:89:TRP:HZ3	2:C:113:VAL:O	2.00	0.45
2:C:89:TRP:CD2	2:C:115:GLY:HA2	2.52	0.45
2:D:114:SER:C	2:D:116:THR:N	2.74	0.45
2:D:140:GLY:C	2:D:142:ALA:H	2.24	0.45
1:B:40:LEU:HA	1:B:40:LEU:HD23	1.55	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
2:D:67:PHE:HD2	2:D:85:LEU:HD23	1.81	0.45
2:D:70:LYS:HZ1	2:D:84:GLU:HB3	1.81	0.45
2:D:89:TRP:NE1	2:D:95:LEU:HB3	2.31	0.45
2:C:39:ARG:CZ	2:C:39:ARG:HB2	2.47	0.45
2:C:137:LEU:O	2:C:141:ARG:HG3	2.16	0.45
1:A:31:LEU:HD22	1:A:70:LEU:CD2	2.46	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:391:GLY:O	1:A:392:ALA:C	2.59	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:271:ASP:C	1:A:273:SER:H	2.24	0.45
1:A:273:SER:O	1:A:273:SER:OG	2.33	0.45
1:B:70:LEU:HA	1:B:73:LEU:CD2	2.47	0.45
1:B:338:SER:C	1:B:340:PHE:N	2.73	0.45
1:B:128:GLU:C	1:B:130:ARG:N	2.75	0.45
1:B:372:GLY:O	1:B:373:ILE:C	2.60	0.45
2:D:26:VAL:O	2:D:26:VAL:HG13	2.17	0.45
2:D:39:ARG:HB2	2:D:39:ARG:NH1	2.32	0.45
2:D:89:TRP:CD1	2:D:95:LEU:CB	2.97	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:A:395:LEU:O	1:A:396:HIS:C	2.60	0.44
1:B:83:ALA:HB1	1:B:261:ILE:HD12	1.83	0.44
1:B:135:LEU:HD23	1:B:171:LYS:NZ	0.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:PRO:HG2	1:B:321:GLU:OE2	2.17	0.44
2:C:35:LYS:HD2	2:C:38:ALA:H	1.81	0.44
1:A:60:GLY:N	3:A:905:ADP:O2B	2.50	0.44
1:A:245:ASP:O	1:A:246:ALA:C	2.60	0.44
1:A:278:GLN:NE2	1:A:318:LEU:HB3	2.32	0.44
1:B:18:ILE:HD12	1:B:343:ILE:CB	2.45	0.44
1:B:34:ARG:O	1:B:35:TRP:O	2.35	0.44
1:B:104:THR:CG2	1:B:247:VAL:HG21	2.48	0.44
1:B:281:LEU:HA	1:B:281:LEU:HD22	1.25	0.44
1:B:298:LYS:HE2	1:B:300:ASP:CG	2.42	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:263:LYS:O	1:B:264:ARG:C	2.60	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: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: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: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
1:A:27:VAL:HA	1:A:53:ILE:CD1	2.48	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:D:152:SER:HB3	2:D:155:GLU:CD	2.43	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
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
2:D:160:ALA:O	2:D:163:THR:N	2.47	0.44
1:A:73:LEU:HD23	1:A:73:LEU:H	1.81	0.44
1:A:171:LYS:HD2	1:A:218:ILE:HD12	1.96	0.44
1:B:17:ILE:HG21	1:B:66:ILE:HG12	2.00	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
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:A:149:GLN:C	1:A:151:GLU:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:88:GLU:C	1:A:91:TYR:H	2.26	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
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
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
1:A:93:GLY:O	1:A:94:LYS:HD2	2.18	0.43
1:A:234:VAL:C	1:A:236:PRO:HD3	2.43	0.43
1:A:322:LEU:HD12	1:A:326:LEU:HD11	2.00	0.43
1:A:392:ALA:O	1:A:393:ARG:C	2.61	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
2:D:110:LEU:HD22	2:D:127:LEU:CD1	2.46	0.43
1:A:88:GLU:OE2	1:A:92:VAL:N	2.51	0.43
1:B:49:THR:O	1:B:50:PRO:C	2.61	0.43
1:B:246:ALA:O	1:B:247:VAL:C	2.60	0.43
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:D:89:TRP:HD1	2:D:95:LEU:CB	2.31	0.43
2:D:105:MET:HB3	2:D:110:LEU:CG	2.48	0.43
2:C:8:THR:C	2:C:9:ILE:HG13	2.43	0.43
2:C:159:ALA:O	2:C:162:GLU:HB2	2.17	0.43
1:A:79:ILE:HB	1:A:103:LEU:HD23	1.99	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:405:GLU:O	1:A:406:ILE:C	2.61	0.43
1:B:13:LEU:CD1	1:B:24:LYS:HB3	2.47	0.43
1:B:356:LYS:O	1:B:360:ALA:N	2.50	0.43
1:B:436:GLU:C	1:B:439:SER:HG	2.16	0.43
2:D:10:PHE:O	2:D:21:SER:N	2.51	0.43
1:A:37:ARG:O	1:A:38:MET:C	2.62	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:240:LYS:HB3	1:B:294:HIS:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:LEU:CB	2:D:49:VAL:HG22	2.47	0.43
1:B:48:VAL:HG12	1:B:49:THR:H	1.83	0.43
1:B:363:GLY:O	1:B:415:GLY:N	2.51	0.43
2:C:17:ARG:CG	2:C:17:ARG:NH1	2.57	0.43
2:C:70:LYS:O	2:C:74:TYR:HD1	2.01	0.43
2:C:174:GLN:H	2:C:174:GLN:HG2	1.56	0.43
1:A:13:LEU:O	1:A:14:ASP:C	2.58	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:16:HIS:C	1:B:17:ILE:HG13	2.44	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:304:PHE:C	1:A:305:ILE:HG13	2.43	0.43
1:B:13:LEU:O	1:B:14:ASP:C	2.62	0.43
1:B:224:LEU:O	1:B:227:GLU:N	2.51	0.43
2:C:137:LEU:HD21	2:C:141:ARG:NH1	2.33	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: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
1:B:111:VAL:HG21	1:B:243:ALA:HA	2.00	0.43
1:B:408:TYR:C	1:B:410:ALA:N	2.77	0.43
2:C:134:ASN:O	2:C:135:TYR:C	2.60	0.43
2:C:141:ARG:H	2:C:141:ARG:HG2	1.74	0.43
1:A:356:LYS:O	1:A:357:ALA:C	2.62	0.42
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
2:C:114:SER:C	2:C:116:THR:N	2.76	0.42
1:A:52:ASN:CG	1:A:304:PHE:HB2	2.44	0.42
1:A:128:GLU:C	1:A:130:ARG:N	2.76	0.42
1:A:136:ILE:O	1:A:136:ILE:CG2	2.67	0.42
1:B:31:LEU:CD2	1:B:70:LEU:HD13	2.49	0.42
1:B:167:GLN:HB2	1:B:168:LEU:H	1.58	0.42
1:B:313:ALA:C	1:B:314:LYS:HG3	2.44	0.42
1:B:438:LEU:C	1:B:438:LEU:HD23	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:92:ASP:CG	2:D:95:LEU:HD12	2.44	0.42
2:C:112:LEU:CD2	2:C:112:LEU:C	2.85	0.42
1:A:96:VAL:HG21	1:A:280:ASP:HB3	2.01	0.42
1:A:140:LYS:HE3	1:A:140:LYS:O	2.19	0.42
1:A:244:ILE:O	1:A:245:ASP:C	2.61	0.42
1:A:310:PHE:N	1:A:310:PHE:CD2	2.87	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:HE21	1:B:20:GLN:HB3	1.52	0.42
1:B:218:ILE:C	1:B:220:ASP:O	2.63	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:21:ASP:O	1:A:22:ASN:C	2.61	0.42
1:A:337:THR:O	1:A:340:PHE:HB2	2.19	0.42
1:A:360:ALA:C	1:A:362:GLU:N	2.77	0.42
1:B:271:ASP:O	1:B:274:ARG:HG2	2.20	0.42
2:D:53:PHE:CG	2:D:54:ALA:N	2.83	0.42
2:D:110:LEU:HD23	2:D:111:LEU:N	2.33	0.42
2:C:21:SER:HA	2:C:176:ILE:O	2.19	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
1:B:351:ILE:O	1:B:352:THR:C	2.61	0.42
2:D:28:PHE:O	2:D:29:GLY:O	2.38	0.42
2:C:92:ASP:CG	2:C:95:LEU:HD12	2.44	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:A:246:ALA:O	1:A:250:HIS:CA	2.68	0.42
1:A:377:ALA:O	1:A:378:GLU:C	2.63	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
2:C:9:ILE:HD13	2:C:53:PHE:O	2.09	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
1:B:348:ASN:C	1:B:350:SER:H	2.27	0.42
2:D:78:LEU:HD21	2:D:104:VAL:HG23	2.02	0.42
2:D:114:SER:HG	2:D:117:GLY:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:164:ALA:O	2:C:166:GLU:N	2.53	0.42
1:B:52:ASN:HB2	1:B:325:ARG:O	2.20	0.42
1:B:168:LEU:HD11	1:B:219:LYS:CD	2.18	0.42
2:C:44:LEU:O	2:C:49:VAL:HG22	2.20	0.42
2:C:68:GLU:C	2:C:70:LYS:N	2.76	0.42
1:A:268:SER:CB	1:A:312:ILE:HD13	2.50	0.41
1:A:302:ILE:CG2	1:A:303:LEU:N	2.83	0.41
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.89	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:27:VAL:CG2	1:A:70:LEU:CD2	2.84	0.41
1:A:32:ARG:O	1:A:36:ARG:HG3	2.19	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
1:A:284:LEU:HA	1:A:284:LEU:HD23	1.66	0.41
1:B:405:GLU:O	1:B:406:ILE:C	2.63	0.41
2:D:10:PHE:CE1	2:D:126:ILE:HG23	2.55	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
2:D:163:THR:O	2:D:166:GLU:HB3	2.19	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:HD13	1:A:432:LEU:HA	1.92	0.41
1:A:438:LEU:HD23	1:A:438:LEU:C	2.45	0.41
1:B:116:ILE:O	1:B:116:ILE:CG2	2.60	0.41
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
1:B:389:ASN:C	1:B:389:ASN:HD22	2.29	0.41
1:B:403:MET:O	1:B:404:GLU:C	2.63	0.41
2:C:121:GLU:HA	2:C:122:PRO:HD3	1.92	0.41
1:A:160:ARG:HG2	1:A:160:ARG:HH11	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:67:ALA:O	1:B:68:ARG:C	2.63	0.41
1:B:355:TYR:HD2	1:B:403:MET:HG2	1.81	0.41
2:D:159:ALA:HA	2:D:162:GLU:HB2	2.02	0.41
2:C:63:LEU:HD11	2:C:89:TRP:CZ2	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:THR:O	1:B:85:LYS:C	2.64	0.41
2:D:51:ALA:HA	2:D:103:ILE:O	2.21	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
1:A:40:LEU:HA	1:A:40:LEU:HD23	1.53	0.41
1:A:79:ILE:HD12	1:A:103:LEU:HA	2.01	0.41
1:A:136:ILE:O	1:A:136:ILE:HG22	2.20	0.41
1:A:428:HIS:O	1:A:429:LEU:HD12	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
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:392:ALA:O	1:B:393:ARG:C	2.62	0.41
2:C:78:LEU:HD21	2:C:104:VAL:HG23	2.02	0.41
1:A:103:LEU:O	1:A:247:VAL:HG22	2.20	0.41
1:A:168:LEU:HD12	1:A:219:LYS:CG	2.42	0.41
1:B:5:THR:O	1:B:8:GLU:N	2.54	0.41
1:B:42:GLU:O	1:B:43:GLU:C	2.62	0.41
1:B:88:GLU:C	1:B:91:TYR:H	2.29	0.41
1:B:374:LYS:O	1:B:378:GLU:HG3	2.21	0.41
2:D:62:THR:HG22	2:D:63:LEU:N	2.33	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
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
1:A:145:GLN:C	1:A:146:THR:HG23	2.46	0.41
1:A:217:LYS:HB2	1:A:220:ASP:OD2	2.21	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
1:B:332:LEU:N	1:B:332:LEU:CD1	2.81	0.41
2:D:68:GLU:O	2:D:71:LEU:HB2	2.21	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:9:ILE:CG2	1:B:28:ALA:HB2	2.51	0.41
1:B:18:ILE:HD12	1:B:343:ILE:HG12	1.96	0.41
1:B:31:LEU:CD2	1:B:70:LEU:CD1	2.97	0.41
1:B:153:SER:HA	1:B:157:GLN:H	1.86	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:89:TRP:CD2	2:D:115:GLY:HA2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:PRO:CD	1:A:32:ARG:HD3	2.50	0.41
1:A:55:MET:HE2	1:A:63:LYS:HB3	2.03	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
2:D:25:GLN:HB2	2:D:172:ASN:HB3	2.03	0.41
2:C:102:LEU:HA	2:C:102:LEU:HD23	1.79	0.41
1:A:319:ILE:HG23	1:A:320:PRO:HD2	2.03	0.40
1:A:401:ARG:O	1:A:402:LEU:C	2.63	0.40
1:B:26:SER:O	1:B:27:VAL:C	2.64	0.40
1:B:86:PHE:HB3	1:B:277:VAL:HG21	2.03	0.40
1:B:103:LEU:CD1	1:B:247:VAL:HG13	2.48	0.40
1:B:244:ILE:C	1:B:246:ALA:N	2.75	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:A:227:GLU:C	1:A:229:GLU:N	2.77	0.40
1:B:10:VAL:O	1:B:13:LEU:CB	2.64	0.40
1:B:79:ILE:HD12	1:B:103:LEU:N	2.36	0.40
1:B:401:ARG:O	1:B:401:ARG:HD3	2.21	0.40
2:D:177:LEU:HD23	2:D:177:LEU:HA	1.77	0.40
2:C:53:PHE:CE2	2:C:55:GLY:HA3	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:A:259:ASP:HB3	1:A:310:PHE:CD2	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:408:TYR:HB2	1:B:29:ILE:CD1	2.51	0.40
1:B:56:ILE:HD11	1:B:315:PRO:CG	2.50	0.40
2:D:72:GLU:O	2:D:73:GLU:C	2.64	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:266:GLU:HB3	2:D:66:LYS:HE3	2.03	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:72:LYS:O	1:B:72:LYS:HG2	2.21	0.40
1:B:79:ILE:CG1	1:B:103:LEU:HD23	2.52	0.40
1:B:263:LYS:HD2	1:B:272:VAL:CG1	2.48	0.40
1:B:406:ILE:HD13	1:B:420:ILE:HD11	2.02	0.40
2:C:25:GLN:N	2:C:172:ASN:OD1	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry 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	1
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	11
2	D	178/181 (98%)	145 (82%)	20 (11%)	13 (7%)	1	11
All	All	1164/1248 (93%)	755 (65%)	215 (18%)	194 (17%)	0	2

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	210 (60%)	140 (40%)	0	1
1	B	350/377 (93%)	205 (59%)	145 (41%)	0	0
2	C	138/139 (99%)	88 (64%)	50 (36%)	0	1
2	D	138/139 (99%)	88 (64%)	50 (36%)	0	1
All	All	976/1032 (95%)	591 (61%)	385 (39%)	0	1

All (385) 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	8	GLU
1	A	11	SER
1	A	12	GLU
1	A	14	ASP
1	A	15	LYS
1	A	16	HIS

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Mol	Chain	Res	Type
1	A	21	ASP
1	A	24	LYS
1	A	27	VAL
1	A	33	ASN
1	A	38	MET
1	A	39	GLN
1	A	42	GLU
1	A	43	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
1	A	104	THR
1	A	108	VAL
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

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Mol	Chain	Res	Type
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	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
1	A	267	SER
1	A	273	SER
1	A	274	ARG
1	A	277	VAL
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

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Mol	Chain	Res	Type
1	A	311	GLN
1	A	314	LYS
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	364	VAL
1	A	369	THR
1	A	371	SER
1	A	374	LYS
1	A	375	ARG
1	A	382	GLN
1	A	385	GLU
1	A	388	GLU
1	A	389	ASN
1	A	393	ARG
1	A	394	ARG
1	A	399	LEU
1	A	402	LEU
1	A	403	MET
1	A	404	GLU
1	A	407	SER
1	A	411	SER
1	A	413	LEU
1	A	414	SER
1	A	416	GLN
1	A	419	THR
1	A	421	ASP
1	A	425	VAL
1	A	427	LYS
1	A	428	HIS
1	A	432	LEU
1	A	433	VAL
1	A	436	GLU
1	A	437	ASP

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Mol	Chain	Res	Type
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	8	GLU
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	26	SER
1	B	27	VAL
1	B	33	ASN
1	B	36	ARG
1	B	38	MET
1	B	39	GLN
1	B	42	GLU
1	B	43	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
1	B	89	VAL

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Mol	Chain	Res	Type
1	B	94	LYS
1	B	97	ASP
1	B	98	SER
1	B	103	LEU
1	B	104	THR
1	B	108	VAL
1	B	109	LYS
1	B	112	ARG
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	148	GLN
1	B	149	GLN
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	239	LEU
1	B	240	LYS

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Mol	Chain	Res	Type
1	B	247	VAL
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	272	VAL
1	B	274	ARG
1	B	275	GLU
1	B	277	VAL
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	330	VAL
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	364	VAL
1	B	369	THR
1	B	371	SER
1	B	374	LYS
1	B	375	ARG
1	B	382	GLN
1	B	385	GLU
1	B	388	GLU
1	B	389	ASN

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Mol	Chain	Res	Type
1	B	393	ARG
1	B	394	ARG
1	B	399	LEU
1	B	402	LEU
1	B	403	MET
1	B	404	GLU
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	433	VAL
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	21	SER
2	D	26	VAL
2	D	30	GLN
2	D	32	VAL
2	D	33	VAL
2	D	36	HIS
2	D	42	ARG
2	D	44	LEU
2	D	48	LYS
2	D	61	PHE
2	D	62	THR
2	D	63	LEU
2	D	71	LEU
2	D	74	TYR

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Mol	Chain	Res	Type
2	D	78	LEU
2	D	80	ARG
2	D	83	VAL
2	D	85	LEU
2	D	90	ARG
2	D	92	ASP
2	D	94	VAL
2	D	98	LEU
2	D	102	LEU
2	D	104	VAL
2	D	106	ASN
2	D	107	GLN
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	33	VAL
2	C	36	HIS
2	C	42	ARG

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Mol	Chain	Res	Type
2	C	44	LEU
2	C	48	LYS
2	C	49	VAL
2	C	61	PHE
2	C	62	THR
2	C	63	LEU
2	C	65	GLU
2	C	71	LEU
2	C	74	TYR
2	C	78	LEU
2	C	80	ARG
2	C	83	VAL
2	C	85	LEU
2	C	90	ARG
2	C	94	VAL
2	C	98	LEU
2	C	99	GLU
2	C	101	MET
2	C	102	LEU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	20	GLN
1	A	33	ASN
1	A	39	GLN
1	A	75	ASN
1	A	114	GLN
1	A	119	ASN
1	A	241	GLN
1	A	278	GLN
1	A	301	HIS
1	A	417	ASN
1	B	20	GLN
1	B	75	ASN
1	B	114	GLN
1	B	119	ASN
1	B	250	HIS
1	B	278	GLN
1	B	323	GLN
1	B	417	ASN
2	D	36	HIS
2	D	106	ASN
2	D	172	ASN
2	D	174	GLN
2	C	13	GLN
2	C	14	HIS
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 oligosaccharides 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	A	905	-	28,29,29	1.54	5 (17%)	43,45,45	2.30	17 (39%)
3	ADP	B	906	-	28,29,29	1.39	4 (14%)	43,45,45	1.77	14 (32%)

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	A	905	-	-	2/16/32/32	0/3/3/3
3	ADP	B	906	-	-	4/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	905	ADP	PA-O3A	5.38	1.65	1.59
3	B	906	ADP	PA-O3A	4.08	1.63	1.59
3	A	905	ADP	C2-N3	2.92	1.39	1.33
3	B	906	ADP	C2-N1	2.91	1.39	1.33
3	A	905	ADP	O4'-C4'	-2.47	1.39	1.45
3	B	906	ADP	C2-N3	2.39	1.38	1.33
3	A	905	ADP	C8-N7	2.30	1.36	1.31
3	A	905	ADP	C2-N1	2.27	1.38	1.33
3	B	906	ADP	C8-N7	2.03	1.35	1.31

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	905	ADP	C5-C4-N3	-5.38	119.30	126.72
3	A	905	ADP	N3-C2-N1	-5.19	120.73	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	905	ADP	N9-C8-N7	-4.69	107.28	113.94
3	A	905	ADP	C5-N7-C8	4.41	110.38	103.45
3	B	906	ADP	C5-C4-N3	-4.01	121.19	126.72
3	A	905	ADP	N3-C4-N9	3.92	133.83	127.17
3	A	905	ADP	O4'-C1'-N9	3.79	115.37	108.09
3	A	905	ADP	C2-N3-C4	3.63	120.69	111.83
3	B	906	ADP	N3-C2-N1	-3.41	123.42	128.58
3	A	905	ADP	O3B-PB-O2B	3.28	120.08	107.80
3	B	906	ADP	C2'-C3'-C4'	-3.13	96.56	102.61
3	B	906	ADP	C5-N7-C8	3.11	108.34	103.45
3	A	905	ADP	C4-C5-N7	-3.08	107.06	110.58
3	B	906	ADP	N9-C8-N7	-3.05	109.61	113.94
3	A	905	ADP	C5-C6-N6	-2.93	116.04	123.29
3	A	905	ADP	O2A-PA-O3A	2.80	114.83	107.27
3	B	906	ADP	O2'-C2'-C1'	2.64	119.19	110.10
3	A	905	ADP	C4-N9-C8	2.53	108.40	105.74
3	A	905	ADP	C2'-C1'-N9	-2.51	107.08	113.30
3	B	906	ADP	O3B-PB-O3A	2.50	113.03	104.64
3	B	906	ADP	C6-C5-C4	2.44	120.51	117.18
3	B	906	ADP	N3-C4-N9	2.40	131.25	127.17
3	A	905	ADP	C2'-C3'-C4'	2.32	107.09	102.61
3	B	906	ADP	O3B-PB-O2B	2.30	116.41	107.80
3	B	906	ADP	C4-C5-N7	-2.29	107.96	110.58
3	B	906	ADP	O5'-PA-O1A	-2.17	100.32	108.94
3	A	905	ADP	O4'-C1'-C2'	2.11	111.12	106.62
3	B	906	ADP	O2A-PA-O5'	2.09	117.03	107.57
3	A	905	ADP	C6-C5-C4	2.02	119.94	117.18
3	A	905	ADP	O2'-C2'-C3'	2.02	118.30	111.82
3	B	906	ADP	C2-N3-C4	2.02	116.76	111.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

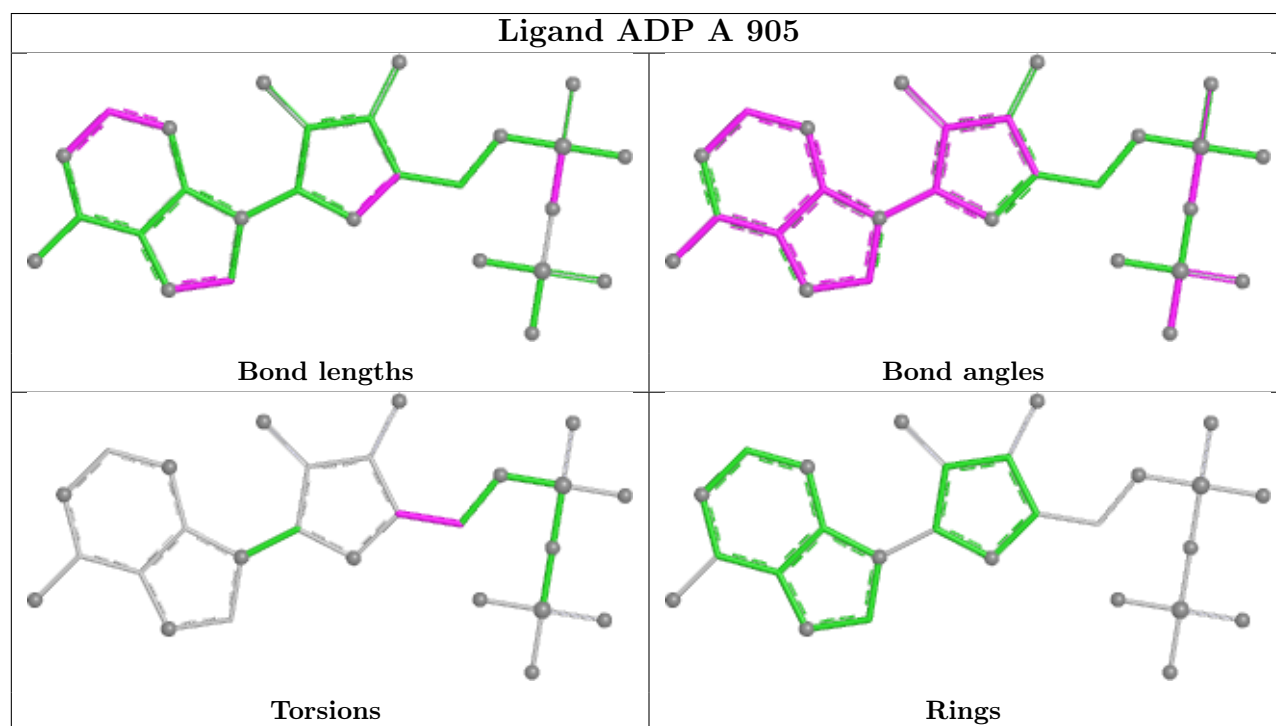
Mol	Chain	Res	Type	Atoms
3	A	905	ADP	O4'-C4'-C5'-O5'
3	A	905	ADP	C3'-C4'-C5'-O5'
3	B	906	ADP	O4'-C4'-C5'-O5'
3	B	906	ADP	C3'-C4'-C5'-O5'
3	B	906	ADP	C5'-O5'-PA-O3A
3	B	906	ADP	PA-O3A-PB-O2B

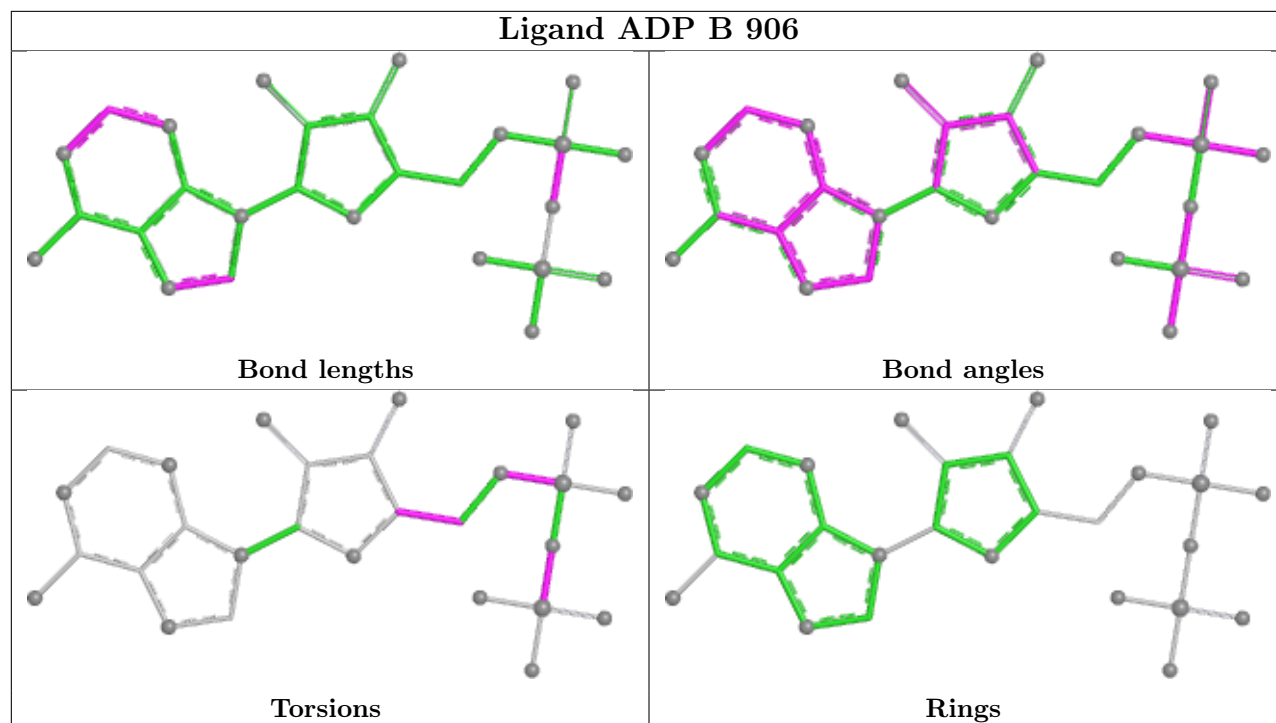
There are no ring outliers.

2 monomers are involved in 13 short contacts:

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

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	408/443 (92%)	1.61	110 (26%) 1 4	16, 55, 94, 96	0
1	B	408/443 (92%)	1.27	85 (20%) 2 6	16, 55, 93, 95	0
2	C	180/181 (99%)	0.16	1 (0%) 85 72	3, 23, 45, 55	0
2	D	180/181 (99%)	0.22	1 (0%) 85 72	3, 23, 45, 55	0
All	All	1176/1248 (94%)	1.06	197 (16%) 4 8	3, 45, 93, 96	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	ALA	11.4
1	A	89	VAL	9.6
1	B	89	VAL	9.1
1	A	147	GLU	8.3
1	A	131	ILE	8.1
1	A	159	PHE	8.0
1	B	146	THR	7.9
1	A	149	GLN	7.8
1	A	129	GLU	7.0
1	A	213	ALA	6.8
1	A	163	LEU	6.8
1	A	90	GLY	6.7
1	A	142	ASN	6.5
1	A	154	ALA	6.4
1	A	220	ASP	6.4
1	A	173	ILE	6.3
1	A	218	ILE	6.3
1	B	91	TYR	6.1
1	A	166	GLY	6.1
1	B	145	GLN	6.1
1	A	133	ASP	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	90	GLY	6.0
1	A	158	ALA	5.6
1	A	167	GLN	5.6
1	B	267	SER	5.4
1	A	91	TYR	5.4
1	A	140	LYS	5.4
1	A	216	LEU	5.3
1	A	161	LYS	5.2
1	A	128	GLU	5.2
1	A	228	GLU	5.2
1	B	92	VAL	5.1
1	B	222	MET	5.1
1	A	152	PRO	5.0
1	A	132	LEU	5.0
1	B	151	GLU	4.9
1	A	212	LYS	4.9
1	A	174	GLU	4.9
1	A	134	VAL	4.9
1	A	137	PRO	4.8
1	B	147	GLU	4.8
1	A	169	ASP	4.8
1	A	171	LYS	4.8
1	A	222	MET	4.6
1	A	170	ASP	4.6
1	A	145	GLN	4.5
1	A	224	LEU	4.5
1	A	157	GLN	4.5
1	A	146	THR	4.5
1	B	266	GLU	4.5
1	A	225	LEU	4.4
1	B	148	GLN	4.3
1	A	139	ALA	4.3
1	B	125	GLU	4.2
1	B	265	GLY	4.2
1	B	165	GLU	4.2
1	A	172	GLU	4.1
1	B	138	PRO	4.1
1	B	174	GLU	4.1
1	A	214	ARG	4.0
1	B	38	MET	4.0
1	B	270	PRO	4.0
1	B	171	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	124	GLU	3.9
1	A	92	VAL	3.9
1	A	155	ALA	3.9
1	A	164	ARG	3.9
1	A	138	PRO	3.8
1	A	265	GLY	3.8
1	B	234	VAL	3.7
1	B	269	GLY	3.7
1	A	153	SER	3.7
1	B	210	LYS	3.7
1	A	151	GLU	3.7
1	A	136	ILE	3.7
1	A	211	GLN	3.7
1	A	148	GLN	3.6
1	A	165	GLU	3.6
1	B	1	MET	3.6
1	A	130	ARG	3.6
1	B	144	GLY	3.6
1	B	127	ALA	3.5
1	B	128	GLU	3.5
1	A	49	THR	3.5
1	B	163	LEU	3.5
1	B	294	HIS	3.4
1	B	169	ASP	3.4
1	B	129	GLU	3.4
1	A	160	ARG	3.4
1	A	162	LYS	3.4
1	A	123	ALA	3.4
1	B	216	LEU	3.4
1	A	294	HIS	3.3
1	B	88	GLU	3.3
1	B	166	GLY	3.3
1	B	173	ILE	3.3
1	A	267	SER	3.3
1	B	172	GLU	3.3
1	B	271	ASP	3.3
1	A	1	MET	3.3
1	B	212	LYS	3.3
1	A	141	ASN	3.2
1	B	240	LYS	3.2
1	A	144	GLY	3.2
1	A	135	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	126	LEU	3.2
1	A	84	THR	3.2
1	B	152	PRO	3.2
1	A	143	TRP	3.1
1	A	121	TYR	3.1
1	B	130	ARG	3.1
1	B	211	GLN	3.1
1	B	139	ALA	3.1
1	A	271	ASP	3.0
1	B	236	PRO	3.0
1	A	223	LYS	3.0
1	A	210	LYS	2.9
1	A	113	VAL	2.9
1	B	137	PRO	2.9
1	A	272	VAL	2.9
1	B	150	GLN	2.9
1	A	88	GLU	2.8
1	B	117	GLU	2.8
1	A	156	ARG	2.8
1	B	160	ARG	2.8
1	A	219	LYS	2.8
1	A	125	GLU	2.8
1	B	136	ILE	2.8
1	A	269	GLY	2.8
1	B	143	TRP	2.8
1	B	367	GLU	2.7
1	A	110	MET	2.7
1	B	161	LYS	2.7
1	B	95	GLU	2.7
1	B	268	SER	2.7
1	B	121	TYR	2.6
1	B	142	ASN	2.6
1	A	248	GLU	2.6
1	B	214	ARG	2.6
1	A	150	GLN	2.6
1	A	263	LYS	2.5
2	D	48	LYS	2.5
1	B	2	SER	2.5
1	A	2	SER	2.5
1	A	231	ALA	2.5
1	B	437	ASP	2.5
1	A	3	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	133	ASP	2.5
1	B	162	LYS	2.5
1	A	117	GLU	2.4
1	B	118	LYS	2.4
1	A	112	ARG	2.4
1	A	120	ARG	2.4
1	B	213	ALA	2.4
1	B	33	ASN	2.4
1	A	270	PRO	2.4
1	B	245	ASP	2.4
1	A	122	ARG	2.4
1	A	39	GLN	2.4
1	A	229	GLU	2.3
1	B	217	LYS	2.3
1	A	168	LEU	2.3
1	B	157	GLN	2.3
1	A	109	LYS	2.3
1	A	215	LYS	2.3
1	B	231	ALA	2.3
1	A	217	LYS	2.3
1	B	244	ILE	2.3
1	A	127	ALA	2.3
1	B	131	ILE	2.3
1	B	223	LYS	2.3
1	B	272	VAL	2.3
1	B	156	ARG	2.3
1	A	237	GLU	2.3
1	A	87	THR	2.3
1	A	367	GLU	2.2
1	B	227	GLU	2.2
1	B	348	ASN	2.2
1	A	319	ILE	2.2
1	A	390	ILE	2.2
1	B	66	ILE	2.2
1	B	122	ARG	2.2
1	B	238	GLU	2.2
1	A	268	SER	2.2
1	B	296	MET	2.2
1	B	170	ASP	2.1
1	A	100	ILE	2.1
1	B	159	PHE	2.1
1	B	239	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	111	VAL	2.1
1	B	218	ILE	2.1
1	A	258	ILE	2.0
1	A	241	GLN	2.0
1	A	419	THR	2.0
1	B	369	THR	2.0
1	B	34	ARG	2.0
2	C	48	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

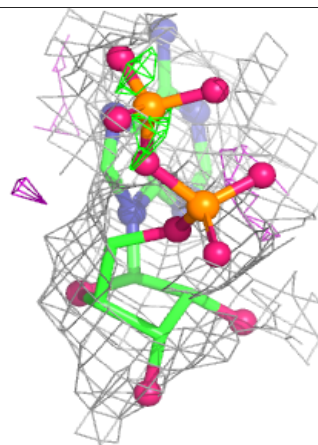
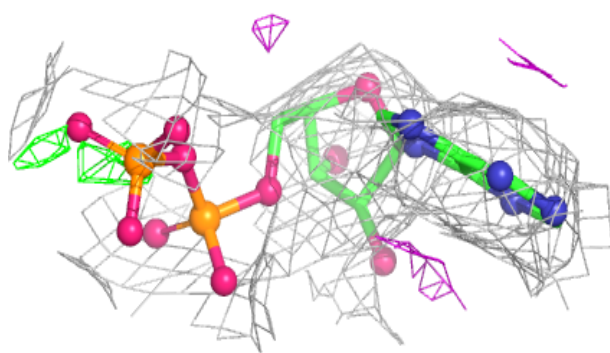
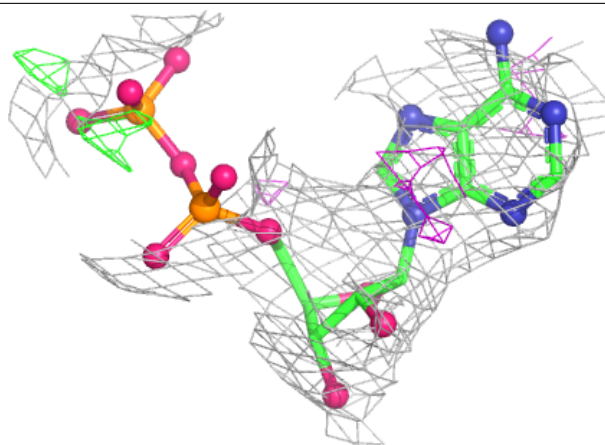
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADP	B	906	27/27	0.91	0.21	79,89,97,98	0
3	ADP	A	905	27/27	0.93	0.20	85,101,106,106	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.

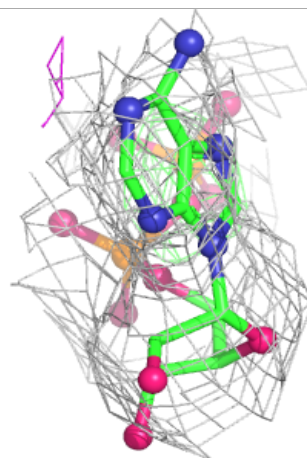
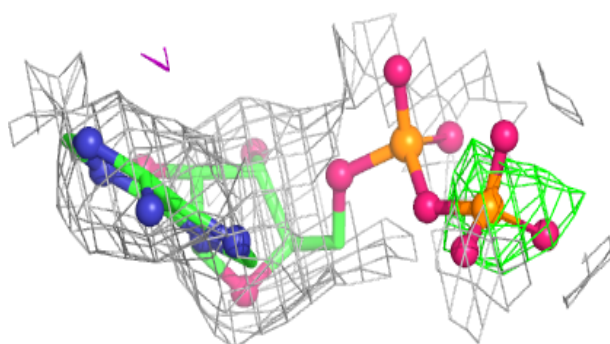
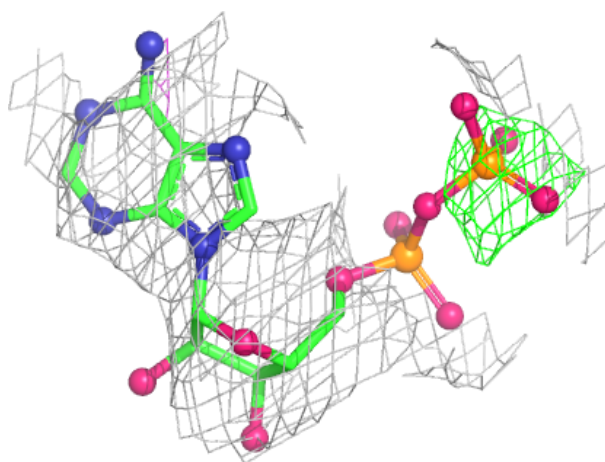
Electron density around ADP B 906:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.