



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:07 AM UTC

PDB ID : 2VYF / pdb_00002vyf
Title : Crystal Structure of the DnaC
Authors : Lo, Y.H.; Tsai, K.L.; Sun, Y.J.; Hsiao, C.D.
Deposited on : 2008-07-23
Resolution : 3.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

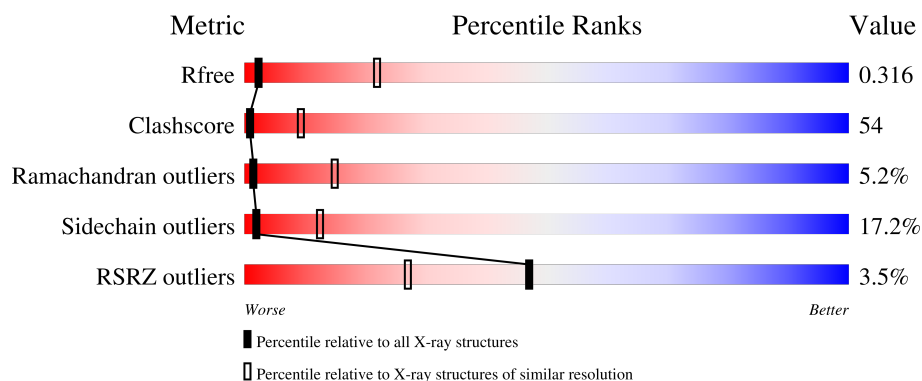
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

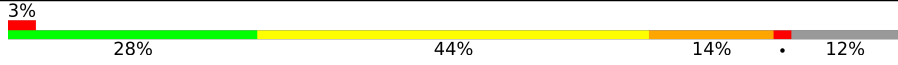
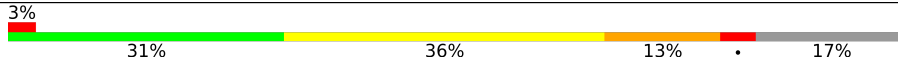
The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	454	
1	B	454	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5946 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 REPLICATIVE DNA HELICASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	4
			3062	1912	539	599	12			
1	B	377	Total	C	N	O	S	0	0	6
			2880	1798	506	564	12			

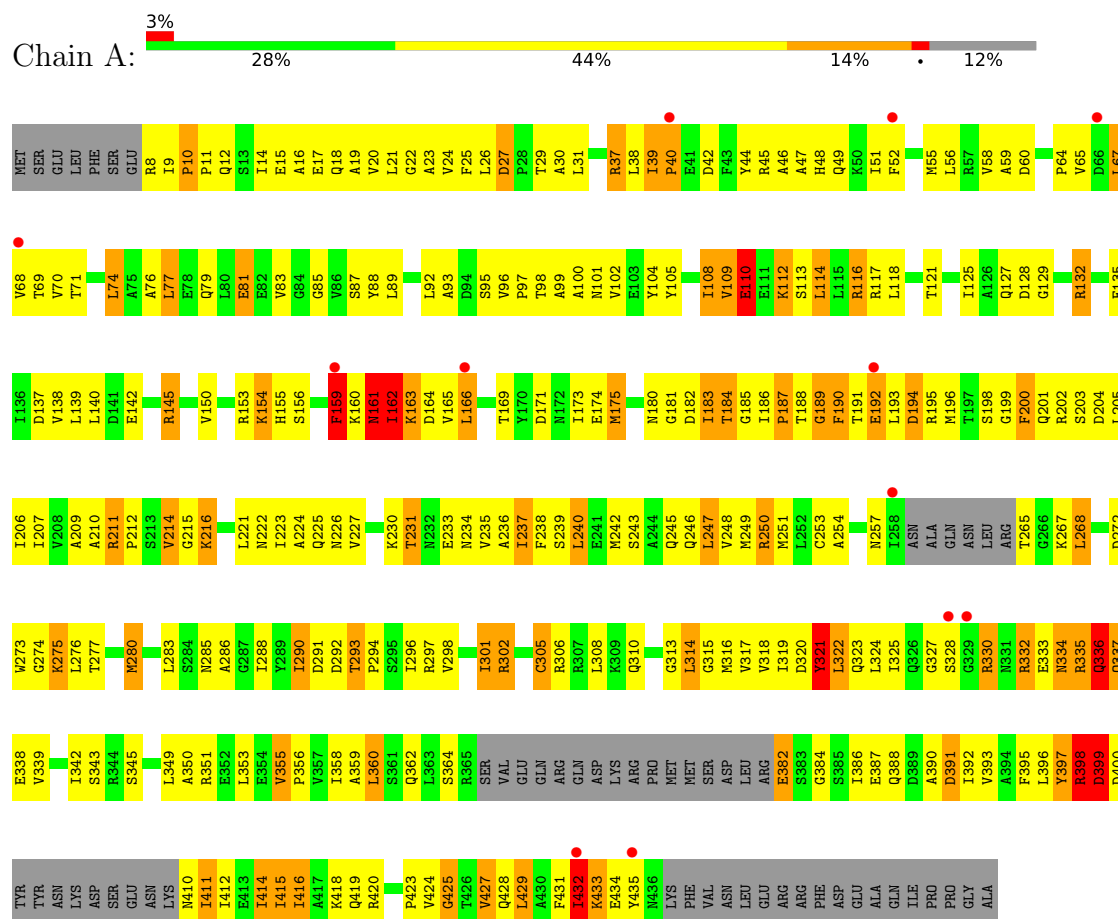
- Molecule 2 is GOLD ION (CCD ID: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Au	0	0
			2	2		
2	B	2	Total	Au	0	0
			2	2		

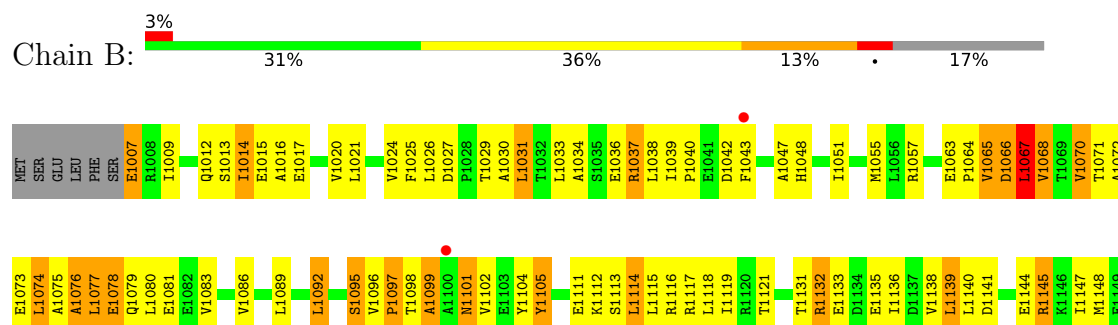
3 Residue-property plots

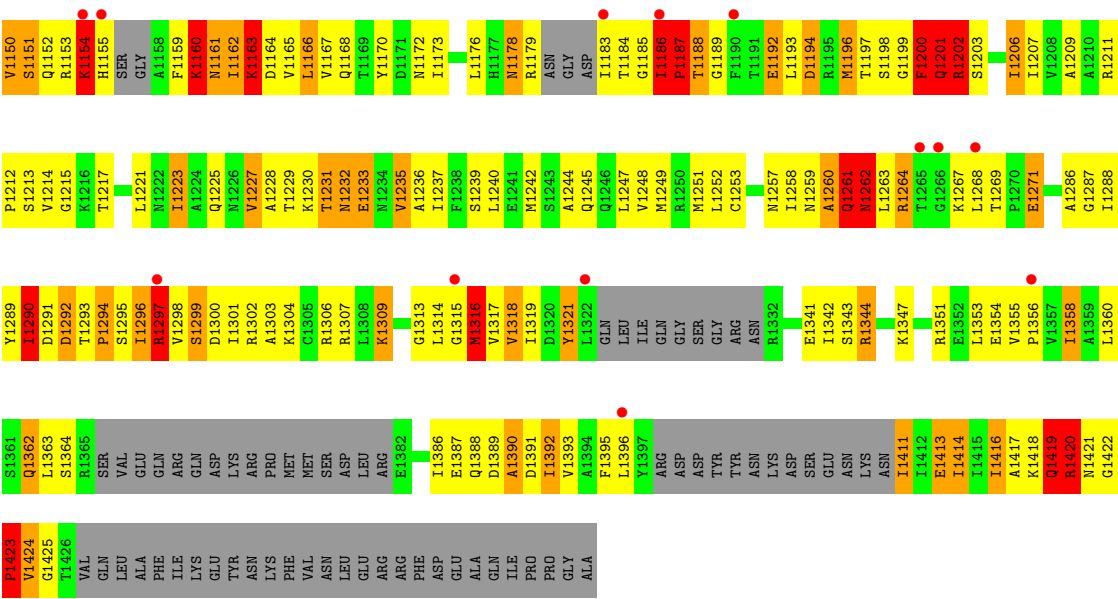
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: REPLICATIVE DNA HELICASE



• Molecule 1: REPLICATIVE DNA HELICASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	176.97 Å 176.97 Å 108.82 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.87 – 3.60 24.87 – 3.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (24.87-3.60) 91.7 (24.87-3.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.64 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.293 , 0.324 0.291 , 0.316	Depositor DCC
R_{free} test set	1770 reflections (7.86%)	wwPDB-VP
Wilson B-factor (Å ²)	142.8	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 102.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5946	wwPDB-VP
Average B, all atoms (Å ²)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.52	4/3096 (0.1%)	1.19	35/4184 (0.8%)
1	B	0.59	7/2908 (0.2%)	1.44	54/3930 (1.4%)
All	All	0.56	11/6004 (0.2%)	1.31	89/8114 (1.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	399	ASP	C-N	-6.25	1.24	1.33
1	B	1154	LYS	C-N	-5.88	1.25	1.33
1	A	435	TYR	C-N	-5.82	1.25	1.33
1	B	1321	TYR	C-N	-5.79	1.25	1.33
1	B	1178	ASN	C-N	-5.79	1.25	1.33
1	A	364	SER	C-N	-5.78	1.25	1.33
1	B	1396	LEU	C-N	-5.74	1.25	1.33
1	A	257	ASN	C-N	-5.66	1.25	1.33
1	B	1364	SER	C-N	-5.65	1.25	1.33
1	B	1425	GLY	C-N	-5.44	1.25	1.33
1	B	1227	VAL	C-O	-5.35	1.18	1.24

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1260	ALA	N-CA-C	16.99	135.79	110.30
1	B	1419	GLN	N-CA-C	14.65	131.68	110.14
1	B	1297	ARG	N-CA-C	11.87	136.08	110.80
1	A	293	THR	CA-C-N	11.62	131.74	119.89
1	A	293	THR	C-N-CA	11.62	131.74	119.89
1	B	1163	LYS	N-CA-C	-11.58	98.73	111.36
1	A	268	LEU	N-CA-C	11.10	126.89	110.46
1	B	1066	ASP	N-CA-C	10.67	124.51	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1420	ARG	N-CA-C	-10.55	101.45	114.75
1	B	1262	ASN	N-CA-C	-10.52	93.41	109.41
1	B	1201	GLN	N-CA-C	10.52	125.60	110.14
1	B	1065	VAL	N-CA-C	10.20	125.35	113.42
1	B	1151	SER	N-CA-C	10.09	123.72	111.40
1	B	1316	MET	N-CA-C	-9.23	94.19	109.24
1	B	1390	ALA	CA-C-N	8.97	138.68	121.54
1	B	1390	ALA	C-N-CA	8.97	138.68	121.54
1	B	1013	SER	N-CA-C	8.93	123.96	112.89
1	B	1202	ARG	N-CA-C	8.91	129.79	110.80
1	A	425	GLY	N-CA-C	8.79	122.71	111.37
1	B	1422	GLY	CA-C-N	8.71	130.73	119.84
1	B	1422	GLY	C-N-CA	8.71	130.73	119.84
1	B	1073	GLU	N-CA-C	-8.49	101.97	111.14
1	B	1267	LYS	N-CA-C	-8.49	101.64	112.93
1	B	1299	SER	N-CA-C	8.25	120.05	111.14
1	A	114	LEU	N-CA-C	-8.16	101.97	111.03
1	B	1416	ILE	CA-C-N	8.04	136.90	121.54
1	B	1416	ILE	C-N-CA	8.04	136.90	121.54
1	B	1411	ILE	N-CA-C	7.99	133.36	111.00
1	B	1065	VAL	CB-CA-C	-7.61	102.59	110.88
1	B	1067	LEU	N-CA-C	7.49	126.74	110.80
1	A	79	GLN	N-CA-C	-7.46	104.21	113.38
1	B	1424	VAL	N-CA-C	7.28	118.36	108.17
1	B	1249	MET	N-CA-C	-7.22	103.49	111.36
1	A	328	SER	N-CA-C	7.05	120.08	110.35
1	B	1150	VAL	N-CA-C	7.02	117.62	110.82
1	B	1068	VAL	N-CA-C	-7.01	105.01	111.67
1	A	267	LYS	N-CA-C	-6.87	105.68	112.97
1	B	1138	VAL	N-CA-C	6.84	116.97	110.74
1	B	1012	GLN	N-CA-C	6.80	120.57	109.76
1	A	59	ALA	N-CA-C	-6.79	105.00	113.28
1	B	1200	PHE	N-CA-C	-6.75	96.42	110.80
1	A	175	MET	N-CA-C	-6.57	105.08	113.23
1	A	267	LYS	CB-CA-C	-6.36	101.44	111.17
1	B	1079	GLN	N-CA-C	-6.35	103.86	113.89
1	A	285	ASN	N-CA-C	-6.32	104.39	111.28
1	B	1132	ARG	N-CA-C	6.29	118.96	108.20
1	A	10	PRO	CA-C-N	6.22	127.61	119.84
1	A	10	PRO	C-N-CA	6.22	127.61	119.84
1	A	391	ASP	N-CA-C	-6.22	104.75	112.90
1	B	1160	LYS	CA-C-N	6.17	133.32	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1160	LYS	C-N-CA	6.17	133.32	121.54
1	A	109	VAL	N-CA-C	-6.11	105.10	111.58
1	B	1290	ILE	CB-CG1-CD1	-6.09	101.01	113.80
1	B	1193	LEU	N-CA-C	6.08	117.91	111.28
1	A	65	VAL	N-CA-C	6.07	117.20	107.73
1	B	1391	ASP	N-CA-C	-6.00	98.01	110.80
1	A	215	GLY	N-CA-C	-5.98	107.24	114.66
1	B	1313	GLY	N-CA-C	-5.95	99.08	113.18
1	B	1423	PRO	N-CA-C	5.91	124.65	112.47
1	A	162	ILE	CG1-CB-CG2	-5.85	93.16	110.70
1	B	1186	ILE	CA-C-N	5.83	127.13	119.84
1	B	1186	ILE	C-N-CA	5.83	127.13	119.84
1	B	1131	THR	N-CA-C	5.77	120.70	113.43
1	A	327	GLY	N-CA-C	-5.75	99.56	113.18
1	A	411	ILE	N-CA-C	5.72	116.99	109.21
1	B	1392	ILE	CB-CA-C	-5.70	103.69	111.33
1	A	253	CYS	N-CA-C	-5.66	105.63	112.54
1	B	1014	ILE	N-CA-C	5.61	121.00	109.34
1	A	433	LYS	N-CA-C	5.55	118.17	111.40
1	A	286	ALA	CB-CA-C	-5.52	110.22	116.63
1	A	273	TRP	N-CA-C	-5.44	105.46	111.71
1	A	110	GLU	N-CA-C	-5.37	105.43	111.28
1	B	1099	ALA	N-CA-C	5.34	118.86	111.71
1	A	222	ASN	N-CA-C	-5.30	105.42	111.14
1	A	159	PHE	CA-C-N	-5.23	113.70	122.17
1	A	159	PHE	C-N-CA	-5.23	113.70	122.17
1	B	1297	ARG	CA-C-N	-5.19	112.62	121.97
1	B	1297	ARG	C-N-CA	-5.19	112.62	121.97
1	A	27	ASP	CA-C-N	-5.15	113.40	119.84
1	A	27	ASP	C-N-CA	-5.15	113.40	119.84
1	B	1201	GLN	CA-C-N	5.15	131.38	121.54
1	B	1201	GLN	C-N-CA	5.15	131.38	121.54
1	B	1034	ALA	N-CA-C	-5.12	105.61	111.14
1	B	1140	LEU	N-CA-C	-5.12	105.88	111.82
1	A	355	VAL	CA-C-N	-5.11	115.09	120.66
1	A	355	VAL	C-N-CA	-5.11	115.09	120.66
1	B	1076	ALA	N-CA-C	-5.02	103.85	110.43
1	A	39	ILE	CA-C-N	5.01	126.11	119.84
1	A	39	ILE	C-N-CA	5.01	126.11	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3062	0	3098	362	2
1	B	2880	0	2922	306	2
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	5946	0	6020	646	2

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 54.

All (646) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:HD3	1:A:212:PRO:CD	1.49	1.41
1:A:297:ARG:HH22	1:B:1154:LYS:N	1.15	1.39
1:A:145:ARG:HB3	1:A:145:ARG:NH2	1.35	1.37
1:B:1145:ARG:NH2	1:B:1145:ARG:HB2	1.41	1.34
1:A:297:ARG:NH2	1:B:1154:LYS:H	1.24	1.33
1:B:1076:ALA:O	1:B:1077:LEU:HD22	1.35	1.21
1:A:211:ARG:CD	1:A:212:PRO:HD3	1.71	1.19
1:B:1290:ILE:N	1:B:1290:ILE:HD12	1.38	1.18
1:A:193:LEU:HD13	1:A:200:PHE:CZ	1.80	1.17
1:B:1201:GLN:H	1:B:1201:GLN:NE2	1.41	1.17
1:A:332:ARG:HD3	1:A:332:ARG:C	1.71	1.14
1:B:1227:VAL:O	1:B:1231:THR:CG2	1.98	1.11
1:A:186:ILE:HD11	1:A:231:THR:HB	1.17	1.11
1:B:1227:VAL:O	1:B:1231:THR:HG22	1.51	1.10
1:A:193:LEU:HD13	1:A:200:PHE:HZ	1.10	1.09
1:A:240:LEU:H	1:A:240:LEU:HD23	1.16	1.09
1:A:214:VAL:HG21	1:A:216:LYS:HE3	1.29	1.09
1:A:81:GLU:OE1	1:A:81:GLU:HA	1.53	1.08
1:A:211:ARG:CD	1:A:212:PRO:CD	2.27	1.08
1:A:214:VAL:CG2	1:A:216:LYS:HE3	1.82	1.08
1:B:1196:MET:HG2	1:B:1416:ILE:HD12	1.25	1.07
1:A:192:GLU:HG2	1:A:193:LEU:N	1.69	1.04
1:A:414:ILE:HD13	1:A:427:VAL:O	1.57	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLU:HG2	1:A:193:LEU:H	0.92	1.04
1:A:398:ARG:NE	1:A:398:ARG:HA	1.74	1.03
1:A:99:ALA:O	1:A:102:VAL:HG23	1.59	1.02
1:B:1231:THR:CG2	1:B:1233:GLU:H	1.72	1.02
1:B:1413:GLU:HA	1:B:1413:GLU:OE2	1.53	1.02
1:A:210:ALA:HB2	1:A:216:LYS:HD3	1.41	1.01
1:B:1211:ARG:HG2	1:B:1363:LEU:O	1.58	1.01
1:B:1201:GLN:H	1:B:1201:GLN:HE21	1.02	1.00
1:B:1203:SER:HB3	1:B:1354:GLU:HA	1.44	1.00
1:A:332:ARG:HD3	1:A:332:ARG:O	1.60	0.99
1:A:298:VAL:HA	1:A:301:ILE:HD13	1.43	0.98
1:B:1393:VAL:O	1:B:1417:ALA:HB3	1.63	0.98
1:A:332:ARG:NH2	1:A:336:GLN:H	1.62	0.97
1:A:145:ARG:HB3	1:A:145:ARG:HH21	1.15	0.97
1:A:333:GLU:OE1	1:A:337:GLN:HG3	1.64	0.97
1:B:1201:GLN:HE21	1:B:1201:GLN:N	1.60	0.97
1:B:1145:ARG:CB	1:B:1145:ARG:HH21	1.78	0.97
1:A:414:ILE:HD12	1:A:429:LEU:HD21	1.44	0.96
1:A:305:CYS:SG	1:A:317:VAL:HG21	2.05	0.96
1:B:1290:ILE:HD12	1:B:1290:ILE:H	1.19	0.94
1:B:1161:ASN:O	1:B:1163:LYS:N	2.01	0.93
1:A:145:ARG:HB3	1:A:145:ARG:CZ	1.96	0.93
1:A:414:ILE:HD12	1:A:429:LEU:CD2	1.98	0.93
1:A:171:ASP:HA	1:A:174:GLU:HG2	1.50	0.93
1:B:1261:GLN:HE22	1:B:1264:ARG:HB2	1.31	0.93
1:B:1392:ILE:HD11	1:B:1420:ARG:HB2	1.49	0.93
1:A:297:ARG:NH2	1:B:1154:LYS:N	1.94	0.92
1:A:214:VAL:HG21	1:A:216:LYS:CE	2.00	0.91
1:B:1201:GLN:HG2	1:B:1202:ARG:HG2	1.53	0.91
1:B:1211:ARG:HG3	1:B:1363:LEU:HB2	1.55	0.89
1:B:1024:VAL:HG21	1:B:1055:MET:HE3	1.53	0.89
1:B:1253:CYS:SG	1:B:1260:ALA:HB2	2.12	0.89
1:B:1299:SER:HA	1:B:1302:ARG:HE	1.38	0.88
1:A:160:LYS:O	1:A:161:ASN:O	1.91	0.88
1:B:1299:SER:O	1:B:1302:ARG:HG3	1.72	0.88
1:A:145:ARG:NH2	1:A:145:ARG:CB	2.31	0.87
1:B:1007:GLU:CD	1:B:1007:GLU:O	2.17	0.87
1:B:1039:ILE:HG23	1:B:1040:PRO:HD2	1.56	0.87
1:B:1290:ILE:N	1:B:1290:ILE:CD1	2.28	0.87
1:A:46:ALA:O	1:A:49:GLN:HG2	1.75	0.87
1:A:211:ARG:CD	1:A:212:PRO:HD2	2.03	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ILE:CD1	1:A:429:LEU:HD21	2.06	0.86
1:A:235:VAL:CG1	1:A:288:ILE:HG12	2.05	0.86
1:A:211:ARG:HH11	1:A:212:PRO:HG2	1.38	0.86
1:A:192:GLU:CG	1:A:193:LEU:H	1.73	0.85
1:B:1145:ARG:HB2	1:B:1145:ARG:HH21	1.11	0.85
1:B:1185:GLY:HA3	1:B:1201:GLN:HB3	1.56	0.85
1:A:332:ARG:HH22	1:A:336:GLN:N	1.74	0.85
1:A:332:ARG:HH22	1:A:336:GLN:H	0.88	0.85
1:A:411:ILE:HD11	1:A:428:GLN:HB2	1.58	0.84
1:B:1145:ARG:NH2	1:B:1145:ARG:CB	2.32	0.84
1:B:1392:ILE:HD12	1:B:1392:ILE:H	1.41	0.84
1:A:121:THR:O	1:A:125:ILE:HD13	1.77	0.83
1:B:1416:ILE:O	1:B:1424:VAL:HG22	1.78	0.83
1:B:1211:ARG:CG	1:B:1363:LEU:O	2.27	0.83
1:A:296:ILE:HG23	1:A:301:ILE:HD11	1.60	0.83
1:B:1145:ARG:HB2	1:B:1145:ARG:CZ	2.07	0.82
1:B:1201:GLN:NE2	1:B:1201:GLN:N	2.20	0.82
1:B:1231:THR:CG2	1:B:1232:ASN:N	2.42	0.82
1:B:1231:THR:HG21	1:B:1233:GLU:HB2	1.61	0.82
1:A:399:ASP:CG	1:A:400:ASP:N	2.38	0.82
1:B:1067:LEU:O	1:B:1071:THR:HB	1.80	0.81
1:B:1200:PHE:H	1:B:1201:GLN:HE21	1.28	0.81
1:B:1184:THR:HB	1:B:1201:GLN:CD	2.06	0.81
1:A:297:ARG:NH2	1:B:1153:ARG:HA	1.96	0.81
1:B:1236:ALA:HB3	1:B:1317:VAL:HG22	1.62	0.81
1:A:236:ALA:HB3	1:A:317:VAL:HG22	1.61	0.81
1:B:1231:THR:HG22	1:B:1233:GLU:H	1.46	0.80
1:A:40:PRO:HD3	1:A:56:LEU:HD11	1.62	0.80
1:A:216:LYS:HG3	1:A:360:LEU:HB3	1.64	0.80
1:B:1024:VAL:HG23	1:B:1031:LEU:HB2	1.64	0.80
1:A:240:LEU:H	1:A:240:LEU:CD2	1.94	0.80
1:B:1200:PHE:HE1	1:B:1206:ILE:HG21	1.46	0.79
1:A:297:ARG:HH12	1:B:1154:LYS:HB3	1.48	0.79
1:A:301:ILE:O	1:A:305:CYS:HB2	1.82	0.79
1:A:188:THR:HG21	1:A:192:GLU:OE2	1.82	0.79
1:A:186:ILE:CD1	1:A:231:THR:HB	2.08	0.78
1:A:166:LEU:O	1:A:169:THR:HG22	1.83	0.78
1:A:235:VAL:HG13	1:A:288:ILE:HG12	1.64	0.78
1:B:1231:THR:CG2	1:B:1233:GLU:N	2.47	0.78
1:A:210:ALA:CB	1:A:216:LYS:HD3	2.13	0.78
1:A:316:MET:HB2	1:A:356:PRO:HG2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASP:CA	1:A:174:GLU:HG2	2.13	0.77
1:B:1309:LYS:CG	1:B:1314:LEU:HB2	2.15	0.77
1:B:1315:GLY:O	1:B:1355:VAL:HG23	1.83	0.77
1:A:211:ARG:HD2	1:A:212:PRO:HD2	1.65	0.77
1:A:382:GLU:N	1:A:382:GLU:OE2	2.17	0.77
1:A:424:VAL:HG22	1:A:425:GLY:H	1.50	0.77
1:A:22:GLY:O	1:A:26:LEU:HD23	1.85	0.76
1:A:297:ARG:HH21	1:B:1153:ARG:HA	1.47	0.76
1:A:211:ARG:HH11	1:A:212:PRO:CG	1.99	0.75
1:A:414:ILE:HD13	1:A:414:ILE:H	1.47	0.75
1:A:21:LEU:HG	1:A:92:LEU:HD21	1.66	0.75
1:B:1047:ALA:HB1	1:B:1083:VAL:HG13	1.69	0.75
1:A:302:ARG:HH12	1:A:349:LEU:HB2	1.51	0.75
1:B:1067:LEU:HA	1:B:1070:VAL:HG13	1.66	0.75
1:A:223:ILE:HG22	1:A:316:MET:HE1	1.67	0.75
1:A:192:GLU:HG2	1:A:193:LEU:HG	1.68	0.74
1:A:211:ARG:NH1	1:A:212:PRO:HG2	2.02	0.74
1:B:1200:PHE:H	1:B:1201:GLN:NE2	1.84	0.74
1:A:101:ASN:HB2	1:A:104:TYR:HD1	1.51	0.74
1:A:24:VAL:HG11	1:A:55:MET:SD	2.27	0.74
1:A:12:GLN:HE21	1:A:14:ILE:HG23	1.50	0.74
1:B:1414:ILE:HD13	1:B:1414:ILE:H	1.51	0.74
1:A:145:ARG:HH21	1:A:145:ARG:CB	1.99	0.73
1:B:1068:VAL:HA	1:B:1071:THR:HG22	1.68	0.73
1:A:290:ILE:HD13	1:A:291:ASP:N	2.03	0.73
1:A:237:ILE:HG12	1:A:318:VAL:HB	1.70	0.73
1:A:414:ILE:HD11	1:A:427:VAL:HG23	1.70	0.73
1:B:1076:ALA:C	1:B:1077:LEU:HD22	2.12	0.73
1:B:1014:ILE:HA	1:B:1017:GLU:HB2	1.71	0.73
1:B:1021:LEU:O	1:B:1024:VAL:HG12	1.88	0.72
1:B:1037:ARG:HH11	1:B:1037:ARG:HB2	1.55	0.72
1:A:416:ILE:HD13	1:A:419:GLN:NE2	2.05	0.72
1:B:1231:THR:HG22	1:B:1232:ASN:N	2.04	0.72
1:A:25:PHE:HZ	1:A:89:LEU:HD12	1.55	0.71
1:B:1262:ASN:O	1:B:1263:LEU:HB2	1.90	0.71
1:B:1314:LEU:HG	1:B:1315:GLY:H	1.56	0.70
1:B:1203:SER:HB2	1:B:1351:ARG:HA	1.73	0.70
1:A:211:ARG:HD3	1:A:212:PRO:HD3	0.75	0.70
1:A:315:GLY:O	1:A:356:PRO:HD2	1.91	0.70
1:B:1227:VAL:O	1:B:1231:THR:HG21	1.91	0.69
1:A:414:ILE:CD1	1:A:429:LEU:CD2	2.67	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:THR:HG21	1:A:150:VAL:HG21	1.75	0.69
1:B:1309:LYS:HG2	1:B:1314:LEU:HB2	1.72	0.69
1:A:162:ILE:HG22	1:A:162:ILE:O	1.93	0.69
1:A:349:LEU:C	1:A:349:LEU:HD23	2.18	0.68
1:B:1196:MET:HG2	1:B:1416:ILE:CD1	2.16	0.68
1:B:1066:ASP:C	1:B:1067:LEU:HD13	2.17	0.68
1:B:1290:ILE:H	1:B:1290:ILE:CD1	2.00	0.68
1:B:1392:ILE:HA	1:B:1418:LYS:O	1.93	0.68
1:B:1231:THR:HG23	1:B:1233:GLU:N	2.09	0.68
1:A:145:ARG:CZ	1:A:145:ARG:CB	2.67	0.67
1:A:216:LYS:HD2	1:A:360:LEU:HB3	1.76	0.67
1:A:22:GLY:HA3	1:A:92:LEU:O	1.93	0.67
1:A:187:PRO:HG2	1:A:194:ASP:OD1	1.95	0.67
1:A:297:ARG:O	1:A:301:ILE:HD12	1.95	0.67
1:B:1051:ILE:HD11	1:B:1083:VAL:HG11	1.75	0.67
1:A:16:ALA:CB	1:A:108:ILE:HD11	2.24	0.67
1:B:1161:ASN:CB	1:B:1164:ASP:HB2	2.24	0.67
1:A:67:LEU:HD13	1:A:67:LEU:H	1.59	0.67
1:A:238:PHE:HE1	1:A:301:ILE:HA	1.58	0.67
1:A:297:ARG:NH2	1:B:1153:ARG:CA	2.58	0.67
1:B:1217:THR:O	1:B:1221:LEU:HD23	1.94	0.67
1:B:1344:ARG:O	1:B:1344:ARG:HG2	1.94	0.67
1:B:1057:ARG:HH22	1:B:1077:LEU:HD11	1.61	0.66
1:A:414:ILE:CD1	1:A:427:VAL:O	2.39	0.66
1:B:1188:THR:HB	1:B:1223:ILE:CD1	2.26	0.66
1:A:214:VAL:HG23	1:A:216:LYS:HE3	1.71	0.66
1:A:67:LEU:HD13	1:A:67:LEU:N	2.11	0.66
1:A:160:LYS:O	1:A:160:LYS:HG3	1.96	0.66
1:A:265:THR:N	1:A:268:LEU:HD13	2.10	0.66
1:B:1221:LEU:HD12	1:B:1251:MET:SD	2.36	0.66
1:A:185:GLY:O	1:A:186:ILE:HG13	1.96	0.66
1:B:1161:ASN:HB2	1:B:1164:ASP:HB2	1.78	0.65
1:A:113:SER:HA	1:A:116:ARG:HB3	1.78	0.65
1:A:162:ILE:O	1:A:162:ILE:CG2	2.44	0.65
1:B:1185:GLY:CA	1:B:1201:GLN:HB3	2.25	0.65
1:A:297:ARG:HH21	1:B:1153:ARG:CA	2.10	0.65
1:A:169:THR:O	1:A:173:ILE:HG12	1.96	0.65
1:A:414:ILE:CD1	1:A:427:VAL:HG23	2.27	0.65
1:B:1024:VAL:HG11	1:B:1055:MET:SD	2.36	0.65
1:A:397:TYR:O	1:A:398:ARG:HB2	1.97	0.65
1:A:431:PHE:C	1:A:432:ILE:HG13	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1039:ILE:O	1:B:1042:ASP:HB2	1.97	0.65
1:B:1067:LEU:HA	1:B:1070:VAL:CG1	2.26	0.65
1:A:105:TYR:O	1:A:109:VAL:HG23	1.97	0.64
1:A:193:LEU:HD13	1:A:200:PHE:CE1	2.32	0.64
1:A:393:VAL:HG22	1:A:418:LYS:H	1.61	0.64
1:A:99:ALA:O	1:A:102:VAL:CG2	2.41	0.64
1:A:322:LEU:O	1:A:325:ILE:HD13	1.97	0.64
1:B:1211:ARG:O	1:B:1213:SER:N	2.26	0.64
1:B:1192:GLU:O	1:B:1196:MET:HB2	1.98	0.64
1:A:101:ASN:HB2	1:A:104:TYR:CD1	2.31	0.64
1:B:1038:LEU:C	1:B:1039:ILE:HD12	2.22	0.64
1:A:183:ILE:CD1	1:A:184:THR:OG1	2.46	0.64
1:B:1299:SER:HA	1:B:1302:ARG:NE	2.10	0.64
1:A:51:ILE:HG22	1:A:55:MET:HE3	1.78	0.64
1:A:45:ARG:HD3	1:A:48:HIS:CD2	2.33	0.63
1:A:391:ASP:C	1:A:392:ILE:HD12	2.23	0.63
1:A:19:ALA:O	1:A:96:VAL:HG22	1.98	0.63
1:B:1321:TYR:CE1	1:B:1362:GLN:HG2	2.32	0.63
1:A:188:THR:HG21	1:A:192:GLU:CD	2.23	0.63
1:A:110:GLU:O	1:A:114:LEU:HB2	1.98	0.63
1:A:117:ARG:NH1	1:A:153:ARG:HD2	2.13	0.63
1:B:1024:VAL:CG2	1:B:1031:LEU:HB2	2.28	0.63
1:B:1141:ASP:O	1:B:1144:GLU:HG2	1.98	0.63
1:B:1162:ILE:O	1:B:1166:LEU:HD23	1.98	0.63
1:A:85:GLY:O	1:A:89:LEU:HD23	1.98	0.62
1:A:322:LEU:C	1:A:322:LEU:HD13	2.23	0.62
1:A:24:VAL:CG2	1:A:31:LEU:HB2	2.29	0.62
1:B:1298:VAL:HG13	1:B:1299:SER:N	2.13	0.62
1:A:297:ARG:NH1	1:B:1154:LYS:HB3	2.14	0.62
1:B:1253:CYS:SG	1:B:1260:ALA:CB	2.87	0.62
1:B:1170:TYR:O	1:B:1173:ILE:HG22	2.00	0.62
1:B:1014:ILE:HD12	1:B:1015:GLU:N	2.15	0.62
1:B:1014:ILE:HD12	1:B:1015:GLU:H	1.65	0.62
1:B:1225:GLN:O	1:B:1229:THR:HG22	2.00	0.62
1:A:38:LEU:C	1:A:39:ILE:HD12	2.24	0.62
1:A:40:PRO:HD3	1:A:56:LEU:CD1	2.29	0.62
1:A:192:GLU:CG	1:A:193:LEU:N	2.44	0.62
1:A:240:LEU:HD23	1:A:240:LEU:N	2.00	0.62
1:A:416:ILE:O	1:A:416:ILE:HG13	1.99	0.62
1:A:187:PRO:HG2	1:A:194:ASP:CG	2.24	0.62
1:A:192:GLU:HA	1:A:427:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1299:SER:CA	1:B:1302:ARG:HE	2.10	0.62
1:B:1268:LEU:C	1:B:1268:LEU:HD12	2.24	0.61
1:A:238:PHE:CE1	1:A:301:ILE:HA	2.35	0.61
1:A:382:GLU:N	1:A:382:GLU:CD	2.58	0.61
1:B:1188:THR:HB	1:B:1223:ILE:HD13	1.83	0.61
1:A:216:LYS:CG	1:A:360:LEU:HB3	2.30	0.61
1:A:171:ASP:HA	1:A:174:GLU:CG	2.28	0.61
1:A:183:ILE:HD12	1:A:184:THR:OG1	1.99	0.61
1:B:1068:VAL:O	1:B:1071:THR:HG22	2.01	0.61
1:B:1258:ILE:O	1:B:1260:ALA:N	2.34	0.61
1:B:1152:GLN:HA	1:B:1152:GLN:NE2	2.16	0.61
1:B:1211:ARG:HG3	1:B:1363:LEU:CB	2.30	0.61
1:A:398:ARG:HA	1:A:398:ARG:HE	1.61	0.60
1:A:247:LEU:HD22	1:A:290:ILE:HG13	1.83	0.60
1:A:428:GLN:O	1:A:429:LEU:HD13	2.01	0.60
1:A:185:GLY:HA3	1:A:199:GLY:O	2.01	0.60
1:A:297:ARG:HH12	1:B:1154:LYS:CB	2.14	0.60
1:A:102:VAL:HA	1:A:105:TYR:HD1	1.66	0.60
1:A:237:ILE:HD13	1:A:237:ILE:C	2.26	0.60
1:B:1057:ARG:NH2	1:B:1077:LEU:HD11	2.17	0.60
1:B:1113:SER:HA	1:B:1116:ARG:CZ	2.31	0.60
1:A:387:GLU:HG3	1:A:388:GLN:N	2.16	0.60
1:A:297:ARG:NH2	1:B:1153:ARG:C	2.60	0.60
1:A:321:TYR:HB3	1:A:324:LEU:HG	1.82	0.59
1:B:1007:GLU:CD	1:B:1007:GLU:C	2.70	0.59
1:B:1321:TYR:CZ	1:B:1362:GLN:HG2	2.37	0.59
1:B:1392:ILE:CD1	1:B:1420:ARG:HB2	2.28	0.59
1:A:52:PHE:O	1:A:56:LEU:HG	2.01	0.59
1:A:21:LEU:CG	1:A:92:LEU:HD21	2.31	0.59
1:A:214:VAL:HG13	1:A:214:VAL:O	2.01	0.59
1:B:1068:VAL:CA	1:B:1071:THR:HG22	2.31	0.59
1:A:24:VAL:HG23	1:A:31:LEU:HB2	1.83	0.59
1:A:113:SER:O	1:A:116:ARG:HG2	2.01	0.59
1:B:1039:ILE:CG2	1:B:1040:PRO:HD2	2.29	0.59
1:A:335:ARG:H	1:A:335:ARG:HD2	1.68	0.59
1:A:207:ILE:HD13	1:A:359:ALA:HB3	1.84	0.59
1:A:227:VAL:HG12	1:A:227:VAL:O	2.02	0.59
1:B:1015:GLU:HG2	1:B:1016:ALA:N	2.17	0.59
1:A:239:SER:HA	1:A:320:ASP:HB3	1.84	0.59
1:A:296:ILE:HG12	1:A:301:ILE:HD12	1.83	0.59
1:A:225:GLN:HA	1:A:288:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1016:ALA:O	1:B:1020:VAL:HG23	2.03	0.59
1:A:25:PHE:CZ	1:A:89:LEU:HD12	2.38	0.59
1:A:332:ARG:NH2	1:A:336:GLN:N	2.43	0.58
1:A:188:THR:O	1:A:194:ASP:OD1	2.20	0.58
1:A:415:ILE:HD13	1:A:415:ILE:C	2.29	0.58
1:A:319:ILE:O	1:A:360:LEU:HG	2.03	0.58
1:A:190:PHE:HA	1:A:194:ASP:CG	2.29	0.58
1:A:24:VAL:HA	1:A:30:ALA:HB3	1.85	0.58
1:B:1289:TYR:C	1:B:1290:ILE:HD12	2.22	0.58
1:B:1162:ILE:HA	1:B:1165:VAL:HB	1.86	0.57
1:B:1347:LYS:HD2	1:B:1389:ASP:HB3	1.86	0.57
1:A:70:VAL:O	1:A:74:LEU:HB2	2.04	0.57
1:A:216:LYS:CD	1:A:360:LEU:HB3	2.34	0.57
1:A:183:ILE:HD13	1:A:183:ILE:C	2.28	0.57
1:B:1168:GLN:O	1:B:1172:ASN:HB2	2.04	0.57
1:A:320:ASP:O	1:A:321:TYR:HB2	2.03	0.57
1:A:12:GLN:OE1	1:A:44:TYR:CE1	2.57	0.57
1:A:392:ILE:HG13	1:A:419:GLN:HA	1.87	0.57
1:B:1068:VAL:HA	1:B:1071:THR:CG2	2.35	0.57
1:B:1144:GLU:O	1:B:1148:MET:HG2	2.05	0.57
1:B:1261:GLN:NE2	1:B:1264:ARG:HD3	2.19	0.57
1:B:1413:GLU:OE2	1:B:1413:GLU:CA	2.37	0.57
1:A:81:GLU:OE1	1:A:81:GLU:CA	2.41	0.57
1:B:1147:ILE:O	1:B:1150:VAL:HG12	2.05	0.57
1:A:429:LEU:N	1:A:429:LEU:HD22	2.19	0.57
1:B:1063:GLU:HB3	1:B:1064:PRO:HD2	1.86	0.57
1:A:12:GLN:NE2	1:A:14:ILE:HG23	2.18	0.57
1:A:51:ILE:O	1:A:55:MET:HG2	2.05	0.57
1:B:1314:LEU:HG	1:B:1315:GLY:N	2.18	0.57
1:A:132:ARG:HH11	1:A:135:GLU:H	1.51	0.56
1:A:67:LEU:H	1:A:67:LEU:HD22	1.71	0.56
1:A:183:ILE:O	1:A:184:THR:HG23	2.04	0.56
1:A:214:VAL:CG2	1:A:216:LYS:CE	2.66	0.56
1:B:1086:VAL:HA	1:B:1089:LEU:HD12	1.87	0.56
1:B:1392:ILE:HD12	1:B:1392:ILE:N	2.18	0.56
1:A:104:TYR:O	1:A:108:ILE:HG23	2.05	0.56
1:A:250:ARG:HA	1:A:250:ARG:NE	2.20	0.56
1:B:1228:ALA:HB2	1:B:1235:VAL:HG12	1.86	0.56
1:A:398:ARG:CG	1:A:412:ILE:HA	2.36	0.56
1:B:1207:ILE:HD13	1:B:1386:ILE:HB	1.88	0.56
1:A:211:ARG:HH11	1:A:212:PRO:CD	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1070:VAL:O	1:B:1074:LEU:HB2	2.07	0.55
1:B:1154:LYS:O	1:B:1154:LYS:HD3	2.06	0.55
1:A:159:PHE:O	1:A:159:PHE:CD2	2.59	0.55
1:B:1164:ASP:O	1:B:1167:VAL:HB	2.07	0.55
1:B:1196:MET:CG	1:B:1416:ILE:HD12	2.18	0.55
1:A:27:ASP:OD2	1:A:29:THR:HB	2.07	0.55
1:A:265:THR:HA	1:A:268:LEU:HD22	1.87	0.55
1:A:414:ILE:CG1	1:A:427:VAL:HG23	2.37	0.55
1:A:248:VAL:HG21	1:B:1165:VAL:HG11	1.89	0.55
1:A:358:ILE:HD12	1:A:358:ILE:H	1.71	0.55
1:A:97:PRO:HB2	1:B:1066:ASP:OD2	2.07	0.55
1:B:1319:ILE:O	1:B:1360:LEU:HD13	2.07	0.55
1:B:1025:PHE:CD1	1:B:1067:LEU:HB3	2.42	0.54
1:B:1392:ILE:H	1:B:1392:ILE:CD1	2.19	0.54
1:B:1416:ILE:HB	1:B:1423:PRO:O	2.07	0.54
1:B:1024:VAL:HG13	1:B:1025:PHE:N	2.22	0.54
1:B:1118:LEU:HA	1:B:1121:THR:HG22	1.89	0.54
1:B:1211:ARG:HG2	1:B:1212:PRO:CD	2.37	0.54
1:B:1229:THR:HG23	1:B:1230:LYS:N	2.23	0.54
1:A:175:MET:HG2	1:A:423:PRO:HG3	1.88	0.54
1:A:200:PHE:HD2	1:A:206:ILE:HG12	1.72	0.54
1:A:358:ILE:HD12	1:A:358:ILE:N	2.22	0.54
1:A:412:ILE:HG12	1:A:431:PHE:HB2	1.89	0.54
1:A:231:THR:HG23	1:A:233:GLU:H	1.71	0.54
1:A:185:GLY:O	1:A:186:ILE:CG1	2.56	0.54
1:A:237:ILE:HG23	1:A:290:ILE:HG12	1.88	0.54
1:A:171:ASP:C	1:A:174:GLU:HG2	2.33	0.54
1:B:1096:VAL:HG12	1:B:1098:THR:O	2.08	0.54
1:A:338:GLU:O	1:A:342:ILE:HD13	2.07	0.54
1:A:333:GLU:O	1:A:333:GLU:HG2	2.07	0.54
1:A:209:ALA:HB3	1:A:395:PHE:CD1	2.43	0.54
1:A:118:LEU:O	1:A:121:THR:HG22	2.08	0.53
1:A:414:ILE:HG12	1:A:427:VAL:HG23	1.91	0.53
1:B:1186:ILE:N	1:B:1186:ILE:HD12	2.23	0.53
1:A:206:ILE:N	1:A:206:ILE:HD12	2.22	0.53
1:B:1117:ARG:HH12	1:B:1155:HIS:N	2.06	0.53
1:B:1207:ILE:CD1	1:B:1386:ILE:HB	2.39	0.53
1:A:180:ASN:HB3	1:A:195:ARG:NH1	2.23	0.53
1:A:302:ARG:NH1	1:A:349:LEU:HB2	2.23	0.53
1:B:1183:ILE:HD12	1:B:1183:ILE:O	2.07	0.53
1:A:205:LEU:HD11	1:A:207:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LYS:HG3	1:A:360:LEU:HD13	1.89	0.53
1:A:77:LEU:HD13	1:A:77:LEU:N	2.24	0.53
1:B:1163:LYS:C	1:B:1163:LYS:HD3	2.34	0.53
1:B:1245:GLN:HA	1:B:1248:VAL:HG22	1.91	0.53
1:A:298:VAL:HA	1:A:301:ILE:CD1	2.30	0.53
1:A:207:ILE:CD1	1:A:359:ALA:HB3	2.39	0.53
1:A:332:ARG:HH12	1:A:339:VAL:HB	1.73	0.53
1:B:1200:PHE:CE1	1:B:1206:ILE:HG21	2.35	0.53
1:B:1300:ASP:O	1:B:1304:LYS:HG3	2.08	0.53
1:A:296:ILE:CG2	1:A:301:ILE:HD11	2.37	0.52
1:A:272:ASP:HB3	1:A:275:LYS:HB2	1.92	0.52
1:B:1051:ILE:HD11	1:B:1083:VAL:CG1	2.39	0.52
1:A:68:VAL:HA	1:A:71:THR:CG2	2.38	0.52
1:A:280:MET:HE3	1:B:1166:LEU:HD12	1.92	0.52
1:B:1288:ILE:N	1:B:1288:ILE:HD12	2.25	0.52
1:A:382:GLU:C	1:A:384:GLY:H	2.17	0.52
1:B:1291:ASP:OD2	1:B:1304:LYS:NZ	2.42	0.52
1:B:1390:ALA:HB1	1:B:1393:VAL:CG2	2.39	0.52
1:B:1196:MET:HE3	1:B:1196:MET:HA	1.91	0.52
1:B:1197:THR:HG23	1:B:1199:GLY:O	2.10	0.52
1:A:64:PRO:O	1:A:69:THR:HG21	2.10	0.52
1:A:242:MET:HE2	1:A:247:LEU:HA	1.92	0.52
1:A:418:LYS:HE2	1:A:420:ARG:HG2	1.92	0.52
1:B:1025:PHE:HB3	1:B:1067:LEU:HD12	1.91	0.52
1:B:1152:GLN:HA	1:B:1152:GLN:HE21	1.75	0.52
1:A:288:ILE:O	1:B:1162:ILE:HG22	2.10	0.51
1:A:302:ARG:NH2	1:A:349:LEU:HA	2.24	0.51
1:A:315:GLY:O	1:A:355:VAL:HB	2.10	0.51
1:B:1237:ILE:HG23	1:B:1290:ILE:HG23	1.92	0.51
1:A:397:TYR:O	1:A:398:ARG:CB	2.58	0.51
1:B:1231:THR:HG23	1:B:1232:ASN:N	2.18	0.51
1:A:424:VAL:HG22	1:A:425:GLY:N	2.22	0.51
1:B:1136:ILE:HA	1:B:1139:LEU:HD13	1.93	0.51
1:B:1247:LEU:HD12	1:B:1248:VAL:N	2.25	0.51
1:B:1184:THR:HG22	1:B:1201:GLN:HG3	1.92	0.51
1:B:1290:ILE:HG22	1:B:1291:ASP:N	2.25	0.51
1:B:1200:PHE:O	1:B:1200:PHE:CD1	2.63	0.51
1:A:210:ALA:HB2	1:A:216:LYS:HB3	1.93	0.51
1:A:398:ARG:HG3	1:A:411:ILE:O	2.11	0.51
1:B:1154:LYS:HD3	1:B:1154:LYS:C	2.36	0.51
1:B:1024:VAL:HA	1:B:1030:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ASN:O	1:A:230:LYS:HB2	2.11	0.50
1:A:46:ALA:O	1:A:47:ALA:C	2.53	0.50
1:A:296:ILE:HG12	1:A:301:ILE:CD1	2.42	0.50
1:B:1026:LEU:HD12	1:B:1099:ALA:HB2	1.93	0.50
1:B:1133:GLU:OE2	1:B:1136:ILE:HD11	2.11	0.50
1:B:1198:SER:O	1:B:1201:GLN:NE2	2.45	0.50
1:B:1353:LEU:O	1:B:1354:GLU:C	2.53	0.50
1:A:236:ALA:O	1:A:317:VAL:HA	2.11	0.50
1:A:193:LEU:CD1	1:A:200:PHE:HZ	2.02	0.50
1:B:1229:THR:HA	1:B:1286:ALA:HB2	1.93	0.50
1:A:431:PHE:O	1:A:432:ILE:HG13	2.12	0.50
1:B:1007:GLU:O	1:B:1007:GLU:OE1	2.29	0.50
1:A:9:ILE:HG23	1:A:9:ILE:O	2.11	0.50
1:B:1299:SER:O	1:B:1302:ARG:CG	2.54	0.50
1:A:297:ARG:HG3	1:B:1153:ARG:NH1	2.26	0.50
1:A:290:ILE:HD13	1:A:290:ILE:C	2.36	0.50
1:A:67:LEU:O	1:A:71:THR:HG22	2.11	0.49
1:A:127:GLN:C	1:A:129:GLY:H	2.20	0.49
1:B:1066:ASP:HB2	1:B:1067:LEU:HD13	1.94	0.49
1:B:1163:LYS:O	1:B:1166:LEU:HB2	2.12	0.49
1:B:1037:ARG:HH11	1:B:1037:ARG:CB	2.22	0.49
1:B:1239:SER:OG	1:B:1242:MET:HG2	2.12	0.49
1:B:1231:THR:HG22	1:B:1232:ASN:H	1.75	0.49
1:B:1414:ILE:HD13	1:B:1414:ILE:N	2.25	0.49
1:A:290:ILE:O	1:B:1160:LYS:HB2	2.12	0.49
1:A:24:VAL:CG1	1:A:25:PHE:N	2.76	0.49
1:A:26:LEU:HD21	1:A:93:ALA:O	2.12	0.49
1:A:183:ILE:HG23	1:A:184:THR:N	2.27	0.49
1:B:1290:ILE:HG22	1:B:1291:ASP:H	1.77	0.49
1:A:139:LEU:HA	1:A:142:GLU:HB3	1.93	0.49
1:A:308:LEU:HD23	1:A:308:LEU:C	2.38	0.49
1:B:1236:ALA:O	1:B:1317:VAL:HG13	2.12	0.49
1:A:243:SER:OG	1:A:246:GLN:HB2	2.12	0.49
1:A:308:LEU:HD23	1:A:308:LEU:O	2.11	0.49
1:B:1170:TYR:HA	1:B:1173:ILE:HG22	1.95	0.49
1:A:132:ARG:HH12	1:A:138:VAL:HG21	1.77	0.49
1:A:432:ILE:HD12	1:A:433:LYS:N	2.28	0.49
1:B:1211:ARG:CG	1:B:1363:LEU:HB2	2.36	0.49
1:A:16:ALA:O	1:A:19:ALA:HB3	2.13	0.48
1:B:1043:PHE:CD2	1:B:1048:HIS:HB3	2.48	0.48
1:A:251:MET:O	1:A:254:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ILE:O	1:B:1162:ILE:CG2	2.61	0.48
1:A:51:ILE:HD11	1:A:83:VAL:HB	1.95	0.48
1:A:183:ILE:HD13	1:A:183:ILE:O	2.13	0.48
1:A:216:LYS:HD2	1:A:360:LEU:CB	2.42	0.48
1:B:1244:ALA:N	1:B:1292:ASP:OD2	2.46	0.48
1:A:21:LEU:O	1:A:24:VAL:HG12	2.14	0.48
1:A:237:ILE:HG23	1:A:237:ILE:O	2.13	0.48
1:B:1178:ASN:OD1	1:B:1179:ARG:N	2.46	0.48
1:B:1297:ARG:O	1:B:1301:ILE:HG13	2.13	0.48
1:A:332:ARG:NH2	1:A:335:ARG:HA	2.29	0.48
1:A:349:LEU:HD21	1:A:353:LEU:HD22	1.95	0.48
1:B:1200:PHE:O	1:B:1200:PHE:CG	2.66	0.48
1:B:1207:ILE:HD12	1:B:1390:ALA:HB2	1.94	0.48
1:B:1231:THR:CG2	1:B:1233:GLU:HB2	2.40	0.48
1:A:238:PHE:CE1	1:A:301:ILE:HG13	2.49	0.48
1:A:108:ILE:HD12	1:A:108:ILE:O	2.14	0.48
1:A:166:LEU:O	1:A:166:LEU:HD22	2.13	0.48
1:A:192:GLU:CG	1:A:193:LEU:HG	2.41	0.48
1:A:338:GLU:OE2	1:A:338:GLU:N	2.47	0.48
1:B:1089:LEU:O	1:B:1092:LEU:HB2	2.14	0.48
1:B:1214:VAL:HG12	1:B:1214:VAL:O	2.13	0.47
1:B:1231:THR:O	1:B:1232:ASN:CB	2.62	0.47
1:B:1188:THR:HB	1:B:1223:ILE:HD11	1.96	0.47
1:B:1199:GLY:O	1:B:1200:PHE:CB	2.61	0.47
1:A:161:ASN:HD21	1:A:164:ASP:HB2	1.80	0.47
1:A:166:LEU:HD22	1:A:166:LEU:C	2.39	0.47
1:B:1132:ARG:O	1:B:1132:ARG:HG3	2.13	0.47
1:B:1411:ILE:C	1:B:1411:ILE:HD12	2.40	0.47
1:A:14:ILE:O	1:A:18:GLN:HG3	2.14	0.47
1:B:1184:THR:CG2	1:B:1201:GLN:HG3	2.45	0.47
1:B:1067:LEU:HD13	1:B:1067:LEU:N	2.29	0.47
1:B:1203:SER:HA	1:B:1355:VAL:O	2.15	0.47
1:A:56:LEU:O	1:A:60:ASP:HB2	2.15	0.47
1:A:117:ARG:CZ	1:A:153:ARG:HD2	2.44	0.47
1:A:88:TYR:HE1	1:A:92:LEU:HD13	1.78	0.47
1:A:332:ARG:C	1:A:332:ARG:CD	2.60	0.47
1:A:386:ILE:HG13	1:A:387:GLU:N	2.30	0.47
1:B:1112:LYS:HD3	1:B:1112:LYS:N	2.30	0.47
1:B:1207:ILE:CD1	1:B:1390:ALA:HB2	2.45	0.47
1:B:1117:ARG:HG3	1:B:1150:VAL:HG23	1.95	0.47
1:B:1150:VAL:HG13	1:B:1151:SER:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PHE:CE1	1:A:70:VAL:HG21	2.50	0.47
1:A:183:ILE:HD13	1:A:184:THR:OG1	2.14	0.47
1:A:293:THR:HG23	1:A:293:THR:O	2.14	0.47
1:A:302:ARG:HH22	1:A:349:LEU:HA	1.79	0.47
1:A:334:ASN:O	1:A:335:ARG:C	2.58	0.47
1:B:1039:ILE:O	1:B:1042:ASP:N	2.42	0.47
1:A:415:ILE:HG23	1:A:415:ILE:O	2.15	0.46
1:B:1119:ILE:C	1:B:1119:ILE:HD12	2.39	0.46
1:A:76:ALA:C	1:A:77:LEU:HD13	2.40	0.46
1:A:249:MET:HE1	1:A:276:LEU:HD11	1.97	0.46
1:A:333:GLU:OE1	1:A:337:GLN:CG	2.51	0.46
1:A:349:LEU:C	1:A:349:LEU:CD2	2.88	0.46
1:B:1076:ALA:C	1:B:1078:GLU:N	2.72	0.46
1:B:1386:ILE:HG13	1:B:1387:GLU:N	2.31	0.46
1:A:314:LEU:HB3	1:A:315:GLY:H	1.42	0.46
1:B:1200:PHE:N	1:B:1201:GLN:NE2	2.59	0.46
1:A:39:ILE:O	1:A:42:ASP:N	2.33	0.46
1:A:240:LEU:CD2	1:A:240:LEU:N	2.68	0.46
1:B:1223:ILE:O	1:B:1227:VAL:HG23	2.15	0.46
1:B:1235:VAL:HG23	1:B:1316:MET:O	2.16	0.46
1:A:132:ARG:HD2	1:A:132:ARG:HA	1.57	0.46
1:A:188:THR:OG1	1:A:189:GLY:N	2.49	0.46
1:A:214:VAL:HG21	1:A:216:LYS:NZ	2.30	0.46
1:B:1303:ALA:O	1:B:1307:ARG:HG3	2.16	0.46
1:A:248:VAL:HG21	1:B:1165:VAL:CG1	2.46	0.46
1:B:1298:VAL:O	1:B:1302:ARG:HG2	2.16	0.46
1:B:1362:GLN:N	1:B:1362:GLN:OE1	2.48	0.46
1:A:68:VAL:HA	1:A:71:THR:HG22	1.96	0.46
1:A:159:PHE:CD2	1:A:159:PHE:N	2.84	0.46
1:A:200:PHE:CD2	1:A:206:ILE:HG12	2.51	0.46
1:B:1227:VAL:O	1:B:1231:THR:CB	2.63	0.46
1:A:51:ILE:O	1:A:55:MET:HE3	2.15	0.46
1:A:294:PRO:HG2	1:B:1388:GLN:CD	2.42	0.46
1:B:1039:ILE:HG23	1:B:1040:PRO:CD	2.38	0.46
1:A:322:LEU:HD12	1:A:323:GLN:NE2	2.31	0.45
1:A:396:LEU:CD2	1:A:414:ILE:HG22	2.46	0.45
1:B:1111:GLU:O	1:B:1115:LEU:HD23	2.16	0.45
1:A:205:LEU:HD12	1:A:390:ALA:HA	1.98	0.45
1:A:183:ILE:HG22	1:A:198:SER:HB2	1.98	0.45
1:B:1033:LEU:O	1:B:1036:GLU:HB3	2.16	0.45
1:B:1298:VAL:CG1	1:B:1299:SER:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:THR:C	1:A:100:ALA:N	2.71	0.45
1:B:1390:ALA:CB	1:B:1393:VAL:CG2	2.94	0.45
1:A:171:ASP:O	1:A:174:GLU:HG2	2.17	0.45
1:A:221:LEU:HD12	1:A:221:LEU:C	2.42	0.45
1:A:238:PHE:CE2	1:B:1159:PHE:HE1	2.34	0.45
1:B:1309:LYS:HG3	1:B:1314:LEU:HB2	1.96	0.45
1:A:98:THR:O	1:A:100:ALA:O	2.34	0.45
1:A:137:ASP:O	1:A:140:LEU:HB3	2.17	0.45
1:A:293:THR:HA	1:A:294:PRO:HD3	1.68	0.45
1:A:316:MET:CB	1:A:356:PRO:HG2	2.42	0.45
1:B:1076:ALA:C	1:B:1078:GLU:H	2.24	0.45
1:A:234:ASN:HB2	1:A:313:GLY:O	2.16	0.45
1:B:1043:PHE:HD2	1:B:1048:HIS:HB3	1.82	0.45
1:B:1297:ARG:HG3	1:B:1297:ARG:HH11	1.82	0.45
1:B:1353:LEU:HB3	1:B:1355:VAL:HG12	1.97	0.45
1:A:21:LEU:HD12	1:A:21:LEU:HA	1.85	0.44
1:A:23:ALA:N	1:A:96:VAL:HG21	2.32	0.44
1:A:322:LEU:C	1:A:325:ILE:HD13	2.41	0.44
1:A:274:GLY:O	1:A:277:THR:N	2.48	0.44
1:A:306:ARG:HG2	1:A:310:GLN:OE1	2.16	0.44
1:B:1024:VAL:CG1	1:B:1025:PHE:N	2.81	0.44
1:A:24:VAL:HG13	1:A:25:PHE:N	2.32	0.44
1:A:154:LYS:HE2	1:A:156:SER:O	2.18	0.44
1:A:206:ILE:O	1:A:207:ILE:HD13	2.18	0.44
1:B:1221:LEU:HD23	1:B:1221:LEU:H	1.82	0.44
1:A:37:ARG:HH22	1:A:156:SER:HB2	1.82	0.44
1:A:127:GLN:C	1:A:129:GLY:N	2.75	0.44
1:A:140:LEU:HD23	1:A:140:LEU:C	2.42	0.44
1:B:1184:THR:HB	1:B:1201:GLN:CG	2.47	0.44
1:A:292:ASP:O	1:A:293:THR:C	2.61	0.44
1:A:332:ARG:CZ	1:A:335:ARG:HA	2.48	0.44
1:B:1197:THR:O	1:B:1198:SER:C	2.60	0.44
1:B:1318:VAL:HA	1:B:1358:ILE:O	2.18	0.44
1:A:186:ILE:HG13	1:A:186:ILE:O	2.17	0.44
1:A:342:ILE:O	1:A:345:SER:HB2	2.18	0.44
1:B:1392:ILE:HD11	1:B:1420:ARG:CB	2.35	0.44
1:B:1068:VAL:C	1:B:1071:THR:HG22	2.43	0.44
1:A:166:LEU:C	1:A:166:LEU:HD13	2.42	0.44
1:A:410:ASN:O	1:A:431:PHE:N	2.42	0.44
1:B:1161:ASN:HB3	1:B:1164:ASP:HB2	1.99	0.44
1:A:162:ILE:HG23	1:A:162:ILE:HD12	1.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1227:VAL:HG21	1:B:1316:MET:SD	2.58	0.44
1:B:1206:ILE:O	1:B:1358:ILE:HA	2.18	0.43
1:B:1187:PRO:HG3	1:B:1194:ASP:HA	1.99	0.43
1:A:185:GLY:C	1:A:186:ILE:CG1	2.91	0.43
1:B:1027:ASP:OD1	1:B:1029:THR:N	2.49	0.43
1:A:25:PHE:HZ	1:A:89:LEU:CD1	2.27	0.43
1:B:1211:ARG:HG2	1:B:1212:PRO:HD3	1.99	0.43
1:B:1287:GLY:C	1:B:1288:ILE:HD12	2.43	0.43
1:A:245:GLN:HG2	1:B:1419:GLN:NE2	2.33	0.43
1:A:398:ARG:HG3	1:A:412:ILE:HA	2.00	0.43
1:B:1293:THR:O	1:B:1294:PRO:C	2.61	0.43
1:B:1240:LEU:N	1:B:1240:LEU:HD12	2.34	0.43
1:B:1261:GLN:NE2	1:B:1264:ARG:HB2	2.15	0.43
1:A:37:ARG:NH2	1:A:156:SER:HB2	2.34	0.43
1:B:1057:ARG:HH22	1:B:1077:LEU:CD1	2.30	0.43
1:B:1114:LEU:O	1:B:1117:ARG:HB3	2.19	0.43
1:A:330:ARG:H	1:A:330:ARG:HG2	1.41	0.43
1:B:1314:LEU:CG	1:B:1315:GLY:H	2.27	0.43
1:B:1298:VAL:HG13	1:B:1299:SER:H	1.80	0.42
1:A:254:ALA:HA	1:A:434:GLU:HG3	2.01	0.42
1:B:1009:ILE:HG23	1:B:1009:ILE:O	2.18	0.42
1:B:1033:LEU:HA	1:B:1036:GLU:HB2	2.01	0.42
1:A:387:GLU:HG3	1:A:388:GLN:H	1.81	0.42
1:A:38:LEU:O	1:A:39:ILE:HD12	2.19	0.42
1:A:277:THR:HA	1:A:280:MET:HB2	2.01	0.42
1:A:414:ILE:HD13	1:A:414:ILE:N	2.26	0.42
1:B:1072:ALA:O	1:B:1075:ALA:HB3	2.19	0.42
1:B:1209:ALA:HB3	1:B:1395:PHE:HD2	1.84	0.42
1:A:161:ASN:HB2	1:A:162:ILE:H	1.63	0.42
1:A:351:ARG:C	1:A:353:LEU:H	2.28	0.42
1:A:22:GLY:O	1:A:26:LEU:CD2	2.63	0.42
1:A:163:LYS:HG3	1:A:164:ASP:N	2.31	0.42
1:A:325:ILE:N	1:A:325:ILE:HD12	2.34	0.42
1:B:1296:ILE:HG23	1:B:1297:ARG:N	2.35	0.42
1:A:10:PRO:HA	1:A:11:PRO:HD3	1.68	0.42
1:B:1101:ASN:O	1:B:1105:TYR:HB2	2.20	0.42
1:B:1261:GLN:HE22	1:B:1264:ARG:CB	2.18	0.42
1:A:39:ILE:O	1:A:42:ASP:HB2	2.18	0.42
1:B:1185:GLY:H	1:B:1199:GLY:HA3	1.85	0.42
1:B:1215:GLY:C	1:B:1217:THR:H	2.28	0.42
1:A:112:LYS:HD3	1:A:112:LYS:HA	1.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PHE:CE1	1:A:56:LEU:HD11	2.55	0.41
1:A:132:ARG:HH11	1:A:135:GLU:N	2.18	0.41
1:A:183:ILE:HG21	1:A:201:GLN:CD	2.45	0.41
1:A:382:GLU:C	1:A:384:GLY:N	2.79	0.41
1:A:424:VAL:HG13	1:A:425:GLY:N	2.35	0.41
1:A:190:PHE:O	1:A:191:THR:C	2.62	0.41
1:A:414:ILE:HG12	1:A:414:ILE:O	2.19	0.41
1:B:1042:ASP:OD1	1:B:1154:LYS:HE2	2.21	0.41
1:A:398:ARG:NE	1:A:398:ARG:CA	2.62	0.41
1:B:1188:THR:OG1	1:B:1189:GLY:N	2.51	0.41
1:B:1342:ILE:HG13	1:B:1343:SER:N	2.35	0.41
1:A:17:GLU:OE2	1:A:44:TYR:N	2.51	0.41
1:A:227:VAL:O	1:A:227:VAL:CG1	2.67	0.41
1:B:1066:ASP:HB2	1:B:1067:LEU:CD1	2.51	0.41
1:A:202:ARG:C	1:A:204:ASP:H	2.28	0.41
1:A:203:SER:HA	1:A:350:ALA:O	2.20	0.41
1:B:1092:LEU:O	1:B:1095:SER:HB2	2.21	0.41
1:B:1166:LEU:HD13	1:B:1166:LEU:HA	1.91	0.41
1:B:1184:THR:HB	1:B:1201:GLN:OE1	2.19	0.41
1:B:1212:PRO:HD3	1:B:1363:LEU:O	2.20	0.41
1:B:1268:LEU:C	1:B:1268:LEU:CD1	2.93	0.41
1:B:1065:VAL:O	1:B:1070:VAL:HG12	2.21	0.41
1:B:1080:LEU:C	1:B:1080:LEU:HD13	2.45	0.41
1:B:1237:ILE:CG2	1:B:1290:ILE:HG13	2.51	0.41
1:B:1114:LEU:HD12	1:B:1114:LEU:HA	1.82	0.41
1:B:1209:ALA:HB3	1:B:1395:PHE:CD2	2.56	0.41
1:B:1269:THR:HG22	1:B:1271:GLU:HG3	2.03	0.41
1:A:298:VAL:O	1:A:301:ILE:HB	2.21	0.41
1:B:1025:PHE:HE1	1:B:1070:VAL:HG11	1.87	0.41
1:B:1039:ILE:HD12	1:B:1039:ILE:N	2.35	0.41
1:B:1096:VAL:HA	1:B:1097:PRO:HD3	1.85	0.41
1:B:1248:VAL:O	1:B:1252:LEU:HD13	2.22	0.41
1:A:251:MET:HE3	1:A:283:LEU:HD21	2.02	0.40
1:B:1086:VAL:O	1:B:1089:LEU:HB2	2.21	0.40
1:B:1199:GLY:O	1:B:1200:PHE:HB3	2.21	0.40
1:B:1245:GLN:HA	1:B:1248:VAL:CG2	2.50	0.40
1:A:221:LEU:O	1:A:224:ALA:HB3	2.22	0.40
1:A:343:SER:HB2	1:A:386:ILE:HG22	2.03	0.40
1:B:1104:TYR:CD1	1:B:1104:TYR:N	2.89	0.40
1:B:1211:ARG:C	1:B:1213:SER:N	2.80	0.40
1:B:1314:LEU:HD23	1:B:1355:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1321:TYR:CE1	1:B:1362:GLN:CG	3.03	0.40
1:B:1021:LEU:HD23	1:B:1021:LEU:HA	1.90	0.40
1:B:1101:ASN:N	1:B:1101:ASN:HD22	2.18	0.40
1:B:1039:ILE:CG2	1:B:1040:PRO:CD	2.96	0.40
1:B:1074:LEU:HB3	1:B:1080:LEU:HD23	2.02	0.40
1:B:1392:ILE:HG12	1:B:1421:ASN:HD21	1.87	0.40
1:A:108:ILE:HD12	1:A:108:ILE:C	2.46	0.40
1:B:1211:ARG:HG2	1:B:1212:PRO:HD2	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LYS:O	1:B:1307:ARG:NH1[2_655]	1.77	0.43
1:A:87:SER:OG	1:B:1163:LYS:NZ[4_665]	1.89	0.31

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	390/454 (86%)	319 (82%)	54 (14%)	17 (4%)	2	18
1	B	365/454 (80%)	305 (84%)	38 (10%)	22 (6%)	1	13
All	All	755/908 (83%)	624 (83%)	92 (12%)	39 (5%)	1	15

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	PRO
1	A	161	ASN
1	A	190	PHE
1	A	192	GLU

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Mol	Chain	Res	Type
1	A	211	ARG
1	A	334	ASN
1	A	398	ARG
1	B	1067	LEU
1	B	1161	ASN
1	B	1162	ILE
1	B	1188	THR
1	B	1200	PHE
1	B	1202	ARG
1	B	1297	ARG
1	B	1423	PRO
1	A	187	PRO
1	A	189	GLY
1	A	200	PHE
1	A	335	ARG
1	A	336	GLN
1	B	1078	GLU
1	B	1097	PRO
1	B	1187	PRO
1	B	1259	ASN
1	B	1261	GLN
1	B	1296	ILE
1	B	1186	ILE
1	B	1295	SER
1	A	321	TYR
1	A	432	ILE
1	B	1232	ASN
1	B	1257	ASN
1	B	1294	PRO
1	B	1356	PRO
1	B	1135	GLU
1	B	1264	ARG
1	A	314	LEU
1	A	181	GLY
1	A	214	VAL

5.3.2 Protein sidechains ⓘ

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	332/388 (86%)	272 (82%)	60 (18%)	2	11
1	B	313/388 (81%)	262 (84%)	51 (16%)	2	15
All	All	645/776 (83%)	534 (83%)	111 (17%)	2	12

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	15	GLU
1	A	20	VAL
1	A	37	ARG
1	A	58	VAL
1	A	67	LEU
1	A	74	LEU
1	A	77	LEU
1	A	81	GLU
1	A	95	SER
1	A	108	ILE
1	A	110	GLU
1	A	112	LYS
1	A	116	ARG
1	A	128	ASP
1	A	132	ARG
1	A	145	ARG
1	A	154	LYS
1	A	155	HIS
1	A	159	PHE
1	A	161	ASN
1	A	162	ILE
1	A	163	LYS
1	A	165	VAL
1	A	166	LEU
1	A	182	ASP
1	A	183	ILE
1	A	184	THR
1	A	194	ASP
1	A	196	MET
1	A	216	LYS
1	A	231	THR
1	A	237	ILE
1	A	240	LEU

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Mol	Chain	Res	Type
1	A	247	LEU
1	A	250	ARG
1	A	275	LYS
1	A	280	MET
1	A	290	ILE
1	A	301	ILE
1	A	302	ARG
1	A	305	CYS
1	A	321	TYR
1	A	322	LEU
1	A	330	ARG
1	A	332	ARG
1	A	336	GLN
1	A	337	GLN
1	A	360	LEU
1	A	362	GLN
1	A	382	GLU
1	A	397	TYR
1	A	398	ARG
1	A	399	ASP
1	A	414	ILE
1	A	415	ILE
1	A	416	ILE
1	A	427	VAL
1	A	429	LEU
1	A	432	ILE
1	B	1007	GLU
1	B	1031	LEU
1	B	1037	ARG
1	B	1067	LEU
1	B	1070	VAL
1	B	1074	LEU
1	B	1077	LEU
1	B	1081	GLU
1	B	1092	LEU
1	B	1095	SER
1	B	1101	ASN
1	B	1102	VAL
1	B	1105	TYR
1	B	1114	LEU
1	B	1139	LEU
1	B	1145	ARG

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Mol	Chain	Res	Type
1	B	1154	LYS
1	B	1160	LYS
1	B	1163	LYS
1	B	1166	LEU
1	B	1176	LEU
1	B	1187	PRO
1	B	1192	GLU
1	B	1194	ASP
1	B	1196	MET
1	B	1200	PHE
1	B	1201	GLN
1	B	1202	ARG
1	B	1206	ILE
1	B	1223	ILE
1	B	1231	THR
1	B	1233	GLU
1	B	1235	VAL
1	B	1261	GLN
1	B	1262	ASN
1	B	1271	GLU
1	B	1290	ILE
1	B	1292	ASP
1	B	1297	ARG
1	B	1306	ARG
1	B	1309	LYS
1	B	1316	MET
1	B	1318	VAL
1	B	1341	GLU
1	B	1344	ARG
1	B	1358	ILE
1	B	1362	GLN
1	B	1413	GLU
1	B	1414	ILE
1	B	1419	GLN
1	B	1420	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	18	GLN
1	A	49	GLN

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Mol	Chain	Res	Type
1	A	79	GLN
1	A	101	ASN
1	A	161	ASN
1	A	172	ASN
1	A	222	ASN
1	A	245	GLN
1	A	336	GLN
1	A	419	GLN
1	A	428	GLN
1	B	1012	GLN
1	B	1101	ASN
1	B	1127	GLN
1	B	1152	GLN
1	B	1177	HIS
1	B	1201	GLN
1	B	1222	ASN
1	B	1225	GLN
1	B	1234	ASN
1	B	1259	ASN
1	B	1261	GLN
1	B	1262	ASN
1	B	1285	ASN
1	B	1334	ASN
1	B	1336	GLN
1	B	1419	GLN
1	B	1421	ASN

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

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	398/454 (87%)	0.26	12 (3%)	52 30	112, 165, 187, 187	0
1	B	377/454 (83%)	0.27	15 (3%)	42 24	96, 175, 187, 187	0
All	All	775/908 (85%)	0.27	27 (3%)	47 27	96, 171, 187, 187	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	GLU	5.1
1	B	1265	THR	4.0
1	B	1396	LEU	3.9
1	B	1322	LEU	3.7
1	A	435	TYR	3.4
1	B	1297	ARG	3.4
1	A	328	SER	3.3
1	A	40	PRO	3.2
1	B	1268	LEU	2.8
1	B	1266	GLY	2.7
1	B	1154	LYS	2.6
1	A	52	PHE	2.5
1	A	329	GLY	2.5
1	A	432	ILE	2.4
1	A	159	PHE	2.4
1	B	1183	ILE	2.4
1	B	1043	PHE	2.3
1	A	66	ASP	2.3
1	A	166	LEU	2.1
1	B	1315	GLY	2.1
1	A	258	ILE	2.1
1	B	1190	PHE	2.1
1	B	1155	HIS	2.1
1	B	1100	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1186	ILE	2.0
1	B	1356	PRO	2.0
1	A	68	VAL	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(Å ²)	Q<0.9
2	AU	B	2426	1/1	0.95	0.16	186,186,186,186	0
2	AU	A	1437	1/1	0.98	0.03	186,186,186,186	0
2	AU	B	2427	1/1	0.98	0.12	186,186,186,186	0
2	AU	A	1436	1/1	0.99	0.05	186,186,186,186	0

6.5 Other polymers [i](#)

There are no such residues in this entry.