



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:28 PM UTC

PDB ID : 4II7 / pdb_00004ii7
Title : Archaeellum Assembly ATPase FlaI
Authors : Reindl, S.; Williams, G.J.; Tainer, J.A.
Deposited on : 2012-12-20
Resolution : 3.59 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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:

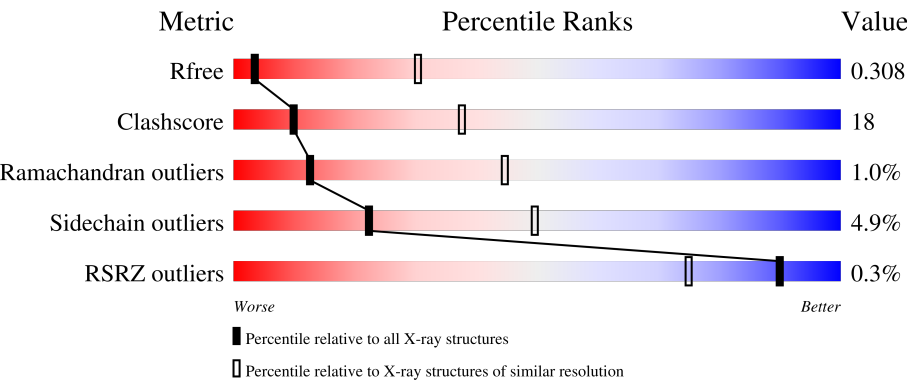
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	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	513	62%31%5%.
1	B	513	59%35%..
1	C	513	67%30%..
1	D	513	68%27%..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16239 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.

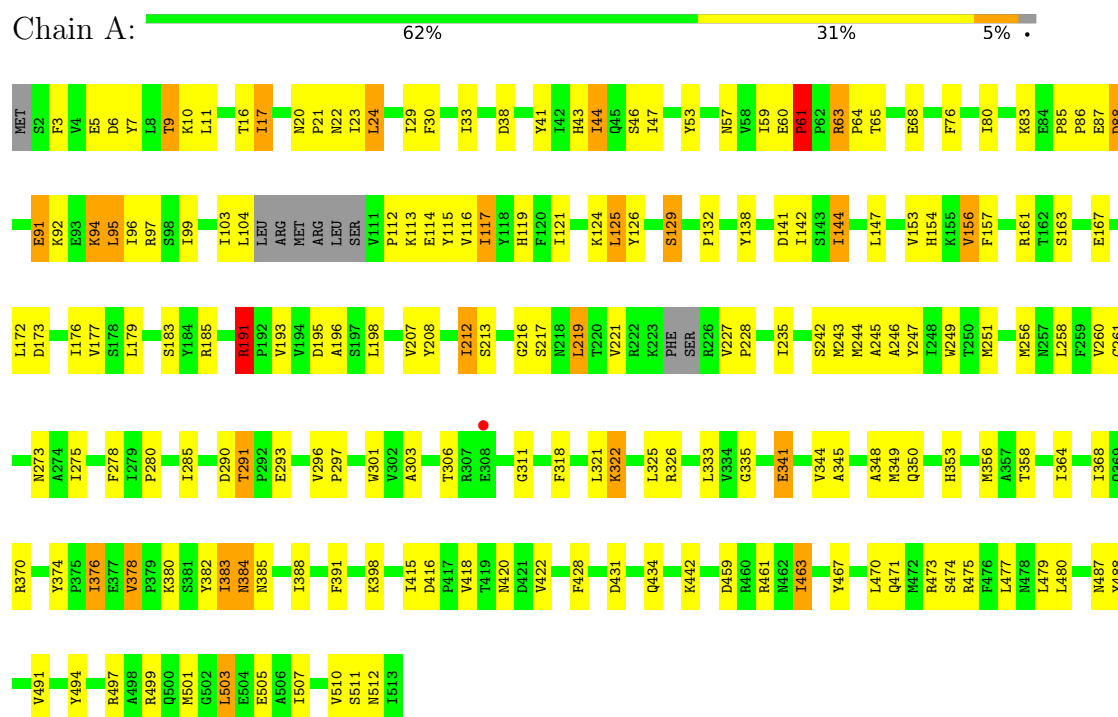
- Molecule 1 is a protein called FlaI ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			4064	2608	679	764	13			
1	B	500	Total	C	N	O	S	0	1	0
			4042	2597	681	750	14			
1	C	510	Total	C	N	O	S	3	0	0
			4116	2640	691	771	14			
1	D	498	Total	C	N	O	S	3	1	0
			4017	2580	673	751	13			

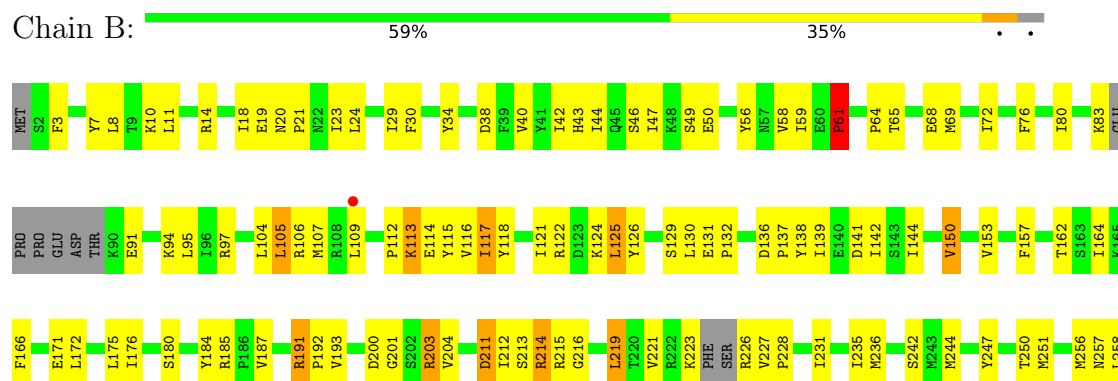
3 Residue-property plots

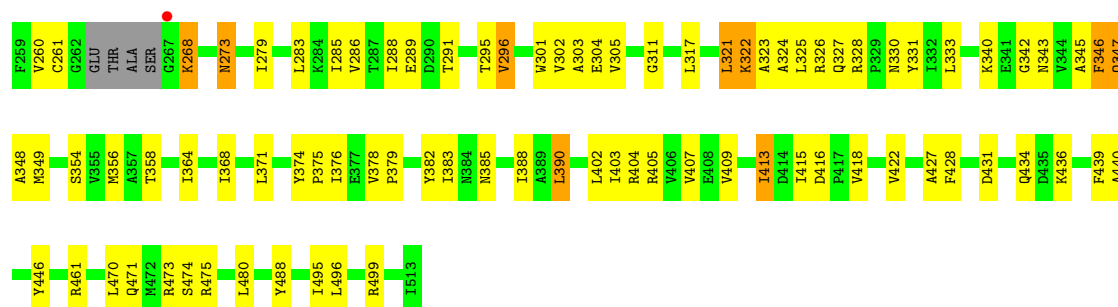
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



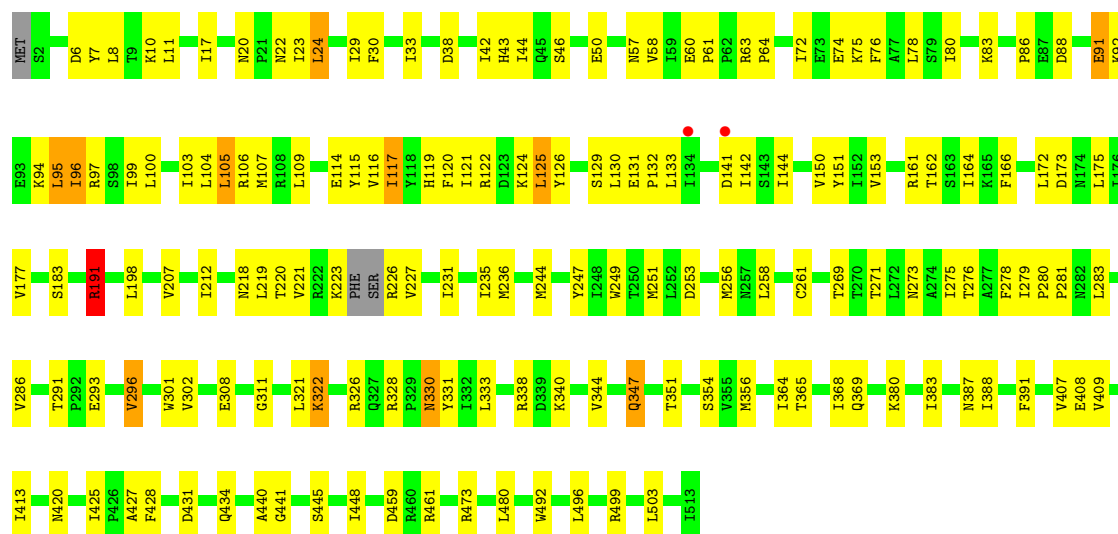
• Molecule 1: FlaI ATPase





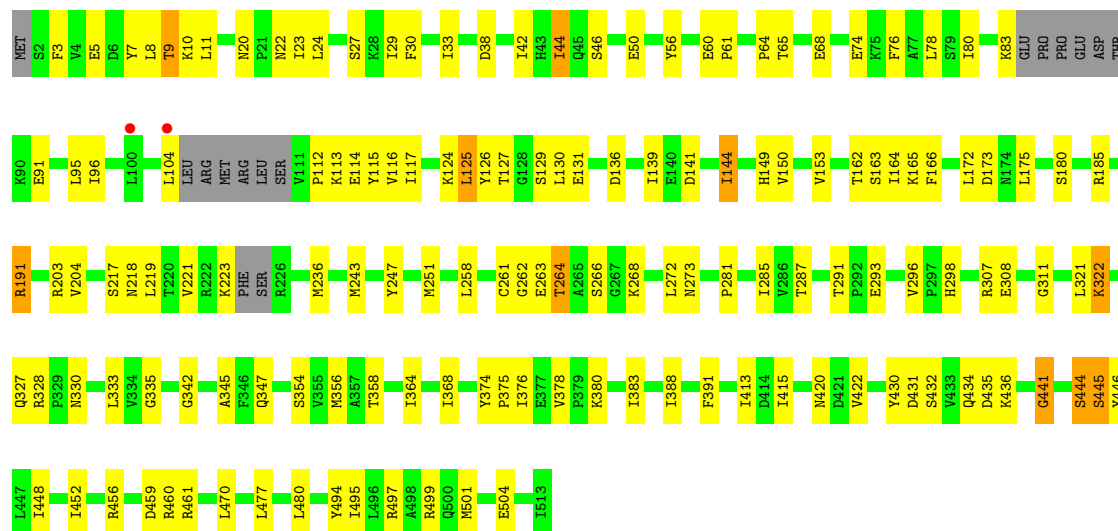
● Molecule 1: FlaI ATPase

Chain C: 67% 30% ..



● Molecule 1: FlaI ATPase

Chain D: 68% 27% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	130.02Å 130.02Å 311.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.92 – 3.59 49.92 – 3.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.92-3.59) 94.5 (49.92-3.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.243 , 0.306 0.256 , 0.308	Depositor DCC
R_{free} test set	1990 reflections (5.73%)	wwPDB-VP
Wilson B-factor (Å ²)	121.1	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 5.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.059 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16239	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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

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	0.76	0/4146	1.18	25/5619 (0.4%)
1	B	0.76	0/4121	1.18	26/5578 (0.5%)
1	C	0.61	0/4199	1.03	9/5690 (0.2%)
1	D	0.62	0/4096	1.03	14/5547 (0.3%)
All	All	0.69	0/16562	1.11	74/22434 (0.3%)

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	ARG	N-CA-C	-9.20	101.37	112.59
1	A	345	ALA	N-CA-C	-8.50	101.60	111.03
1	A	280	PRO	CA-C-N	7.49	127.20	119.56
1	A	280	PRO	C-N-CA	7.49	127.20	119.56
1	B	191	ARG	CA-C-N	7.40	128.04	120.04
1	B	191	ARG	C-N-CA	7.40	128.04	120.04
1	D	144	ILE	CA-C-N	7.11	126.82	119.64
1	D	144	ILE	C-N-CA	7.11	126.82	119.64
1	D	264	THR	CB-CA-C	-7.10	99.94	110.16
1	C	330	ASN	N-CA-C	-7.02	104.85	113.41
1	B	291	THR	CB-CA-C	-6.91	100.97	110.16
1	A	291	THR	CA-C-N	6.75	128.28	119.84
1	A	291	THR	C-N-CA	6.75	128.28	119.84
1	A	47	ILE	CB-CA-C	-6.61	104.32	111.59
1	B	289	GLU	N-CA-C	6.37	119.10	109.23
1	A	38	ASP	N-CA-C	-6.28	101.81	110.35
1	B	328	ARG	CA-C-N	-6.23	113.87	120.66
1	B	328	ARG	C-N-CA	-6.23	113.87	120.66
1	A	144	ILE	CA-C-N	6.21	127.17	120.83
1	A	144	ILE	C-N-CA	6.21	127.17	120.83
1	D	328	ARG	CA-C-N	-6.21	114.38	120.52
1	D	328	ARG	C-N-CA	-6.21	114.38	120.52
1	D	191	ARG	CA-C-N	6.17	126.70	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	191	ARG	C-N-CA	6.17	126.70	120.04
1	C	328	ARG	CA-C-N	-6.16	113.95	120.66
1	C	328	ARG	C-N-CA	-6.16	113.95	120.66
1	A	63	ARG	CA-C-N	6.02	125.96	119.76
1	A	63	ARG	C-N-CA	6.02	125.96	119.76
1	B	413	ILE	CB-CA-C	-6.00	106.61	111.71
1	B	346	PHE	N-CA-C	-5.97	105.07	112.90
1	B	383	ILE	N-CA-C	5.97	116.63	110.36
1	A	260	VAL	CB-CA-C	-5.97	105.88	112.68
1	D	441	GLY	N-CA-C	5.89	119.23	111.52
1	A	191	ARG	CA-C-N	5.87	127.18	119.84
1	A	191	ARG	C-N-CA	5.87	127.18	119.84
1	A	60	GLU	CA-C-N	5.75	126.30	120.38
1	A	60	GLU	C-N-CA	5.75	126.30	120.38
1	A	378	VAL	CB-CA-C	5.74	116.28	110.94
1	B	378	VAL	CA-C-N	-5.70	114.06	119.76
1	B	378	VAL	C-N-CA	-5.70	114.06	119.76
1	A	212	ILE	CB-CA-C	-5.69	105.09	111.80
1	A	208	TYR	N-CA-C	5.61	117.78	108.20
1	C	296	VAL	N-CA-C	5.58	113.40	107.76
1	A	383	ILE	N-CA-C	5.57	116.20	110.36
1	B	296	VAL	CA-C-N	5.54	126.77	119.84
1	B	296	VAL	C-N-CA	5.54	126.77	119.84
1	D	38	ASP	N-CA-C	-5.45	102.21	110.28
1	B	227	VAL	N-CA-C	5.45	113.54	108.15
1	D	444	SER	N-CA-C	5.43	119.90	113.12
1	B	59	ILE	N-CA-C	5.42	115.12	106.88
1	B	496	LEU	N-CA-C	-5.42	105.45	111.36
1	B	61	PRO	CA-C-N	5.37	125.79	119.99
1	B	61	PRO	C-N-CA	5.37	125.79	119.99
1	A	378	VAL	N-CA-C	-5.36	104.02	108.63
1	B	268	LYS	N-CA-C	5.36	116.81	111.07
1	A	374	TYR	N-CA-C	-5.36	103.29	109.93
1	A	156	VAL	N-CA-C	5.31	115.97	110.82
1	B	150	VAL	CB-CA-C	-5.30	103.83	111.19
1	B	171	GLU	CA-C-N	5.29	127.83	120.63
1	B	171	GLU	C-N-CA	5.29	127.83	120.63
1	C	38	ASP	N-CA-C	-5.27	102.59	110.23
1	D	445	SER	N-CA-C	5.26	116.88	108.41
1	C	191	ARG	CA-C-N	5.23	124.93	119.64
1	C	191	ARG	C-N-CA	5.23	124.93	119.64
1	D	127	THR	CB-CA-C	-5.23	104.79	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	PRO	CB-CA-C	-5.23	104.54	110.92
1	B	214	ARG	N-CA-C	5.21	121.91	110.80
1	D	164	ILE	N-CA-C	5.20	115.94	108.93
1	B	227	VAL	CB-CA-C	-5.18	106.16	111.08
1	B	38	ASP	N-CA-C	-5.17	102.63	110.28
1	C	441	GLY	N-CA-C	5.09	119.50	112.52
1	D	266	SER	N-CA-C	-5.08	106.34	112.54
1	C	347	GLN	N-CA-C	-5.06	105.21	111.33
1	A	341	GLU	N-CA-C	-5.02	106.42	112.54

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	4064	0	4105	139	0
1	B	4042	0	4106	207	1
1	C	4116	0	4168	132	1
1	D	4017	0	4067	101	0
All	All	16239	0	16446	572	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 18.

All (572) 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:258:LEU:HD23	1:B:388:ILE:CB	1.43	1.45
1:C:75:LYS:NZ	1:C:107:MET:HE2	1.29	1.40
1:C:75:LYS:HZ3	1:C:107:MET:CE	1.37	1.35
1:C:75:LYS:NZ	1:C:107:MET:CE	1.91	1.32
1:C:75:LYS:CD	1:C:107:MET:CE	2.12	1.28
1:C:75:LYS:CE	1:C:107:MET:CE	2.11	1.27
1:D:258:LEU:HD13	1:D:388:ILE:CB	1.65	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:LEU:CD2	1:B:388:ILE:CG2	2.12	1.25
1:A:258:LEU:HD13	1:A:388:ILE:CB	1.66	1.24
1:B:258:LEU:HD23	1:B:388:ILE:CG2	1.65	1.24
1:C:75:LYS:HD3	1:C:107:MET:CE	1.67	1.23
1:B:258:LEU:CD2	1:B:388:ILE:HB	1.72	1.18
1:A:258:LEU:HD13	1:A:388:ILE:HB	1.17	1.17
1:B:258:LEU:CD2	1:B:388:ILE:HG22	1.74	1.16
1:B:258:LEU:CD2	1:B:388:ILE:CB	2.23	1.12
1:A:258:LEU:HD13	1:A:388:ILE:CG2	1.79	1.11
1:B:72:ILE:CG1	1:B:107:MET:HE1	1.82	1.09
1:D:61:PRO:HB3	1:D:115:TYR:HD2	1.15	1.09
1:B:109:LEU:CD1	1:B:116:VAL:HG21	1.82	1.08
1:D:258:LEU:HD13	1:D:388:ILE:HB	1.18	1.08
1:B:260:VAL:HA	1:B:390:LEU:HD11	1.35	1.08
1:C:75:LYS:CD	1:C:107:MET:HE2	1.81	1.08
1:A:144:ILE:HD12	1:A:219:LEU:HD11	1.32	1.07
1:B:260:VAL:HA	1:B:390:LEU:CD1	1.84	1.06
1:B:258:LEU:HD21	1:B:388:ILE:HG22	1.35	1.05
1:B:109:LEU:HD12	1:B:116:VAL:HG21	1.05	1.04
1:D:258:LEU:HD13	1:D:388:ILE:CG2	1.85	1.04
1:D:61:PRO:CB	1:D:115:TYR:HD2	1.69	1.04
1:B:260:VAL:HG22	1:B:390:LEU:HD21	1.36	1.02
1:C:75:LYS:CE	1:C:107:MET:HE2	1.81	1.02
1:B:260:VAL:CA	1:B:390:LEU:HD11	1.89	1.02
1:B:72:ILE:HG13	1:B:107:MET:HE1	1.41	1.01
1:C:75:LYS:CE	1:C:107:MET:HE3	1.86	1.00
1:D:258:LEU:CD1	1:D:388:ILE:HG22	1.90	1.00
1:C:75:LYS:HD3	1:C:107:MET:HE1	1.01	0.99
1:A:258:LEU:CD1	1:A:388:ILE:HG22	1.92	0.98
1:D:61:PRO:HB3	1:D:115:TYR:CD2	1.97	0.98
1:B:107:MET:O	1:B:113:LYS:NZ	1.96	0.98
1:B:109:LEU:HD12	1:B:116:VAL:CG2	1.92	0.98
1:A:219:LEU:HD22	1:A:219:LEU:O	1.64	0.96
1:B:260:VAL:HG13	1:B:390:LEU:HD11	1.43	0.96
1:C:61:PRO:HB3	1:C:115:TYR:HD2	1.31	0.95
1:B:258:LEU:HD23	1:B:388:ILE:HB	0.95	0.95
1:A:258:LEU:CD1	1:A:388:ILE:CG2	2.46	0.93
1:B:260:VAL:CG1	1:B:390:LEU:HD11	1.99	0.91
1:B:109:LEU:CD1	1:B:116:VAL:HG11	2.00	0.91
1:D:258:LEU:HD11	1:D:388:ILE:HG22	1.52	0.91
1:A:61:PRO:HB3	1:A:115:TYR:HD2	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:LEU:CD1	1:D:388:ILE:CG2	2.49	0.89
1:C:75:LYS:HE2	1:C:107:MET:HE3	1.54	0.87
1:C:105:LEU:HD23	1:C:105:LEU:C	1.99	0.87
1:B:390:LEU:HD12	1:B:390:LEU:O	1.74	0.86
1:B:109:LEU:HD11	1:B:116:VAL:HG11	1.56	0.86
1:C:75:LYS:CD	1:C:107:MET:HE1	1.83	0.86
1:B:61:PRO:HB3	1:B:115:TYR:HD2	1.42	0.85
1:C:105:LEU:HD23	1:C:105:LEU:O	1.77	0.85
1:A:258:LEU:HD11	1:A:388:ILE:HG22	1.56	0.84
1:A:23:ILE:HG23	1:A:24:LEU:HD22	1.59	0.83
1:A:80:ILE:HG22	1:A:83:LYS:NZ	1.94	0.83
1:A:258:LEU:HD12	1:A:388:ILE:O	1.78	0.83
1:C:61:PRO:HB3	1:C:115:TYR:CD2	2.14	0.82
1:B:322:LYS:NZ	1:B:326:ARG:HH12	1.76	0.82
1:B:109:LEU:CD1	1:B:116:VAL:CG2	2.55	0.82
1:C:75:LYS:NZ	1:C:107:MET:HE3	1.87	0.82
1:D:64:PRO:HG3	1:D:116:VAL:HG22	1.61	0.82
1:B:258:LEU:HD21	1:B:388:ILE:CG2	1.95	0.81
1:A:80:ILE:HG22	1:A:83:LYS:HZ1	1.45	0.81
1:C:100:LEU:O	1:C:104:LEU:HG	1.81	0.80
1:B:258:LEU:HD13	1:B:258:LEU:C	2.06	0.80
1:A:213:SER:OG	1:A:216:GLY:O	1.99	0.79
1:C:150:VAL:O	1:C:162:THR:OG1	2.00	0.79
1:A:258:LEU:CD1	1:A:388:ILE:HB	2.07	0.77
1:C:61:PRO:CB	1:C:115:TYR:HD2	1.97	0.77
1:B:136:ASP:O	1:B:223:LYS:NZ	2.17	0.77
1:B:105:LEU:O	1:B:105:LEU:HD23	1.84	0.76
1:D:258:LEU:HD12	1:D:388:ILE:O	1.86	0.76
1:B:105:LEU:HD23	1:B:105:LEU:C	2.11	0.76
1:B:322:LYS:HZ1	1:B:326:ARG:HH12	1.32	0.76
1:C:106:ARG:O	1:C:107:MET:HG3	1.86	0.75
1:B:72:ILE:CD1	1:B:107:MET:HE1	2.17	0.75
1:A:251:MET:HG3	1:A:388:ILE:HD11	1.67	0.74
1:B:129:SER:O	1:B:132:PRO:HD2	1.86	0.74
1:A:61:PRO:HB3	1:A:115:TYR:CD2	2.21	0.74
1:A:144:ILE:CD1	1:A:219:LEU:HD11	2.14	0.74
1:B:64:PRO:HG3	1:B:116:VAL:HG22	1.70	0.74
1:B:261:CYS:H	1:B:390:LEU:HD12	1.52	0.74
1:B:260:VAL:HG13	1:B:390:LEU:CD1	2.15	0.74
1:B:390:LEU:HD12	1:B:390:LEU:C	2.12	0.74
1:C:258:LEU:HD13	1:C:388:ILE:HB	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LYS:HZ3	1:C:107:MET:HE2	0.68	0.73
1:A:94:LYS:HD2	1:A:97:ARG:HG3	1.70	0.73
1:B:80:ILE:HG22	1:B:83:LYS:NZ	2.04	0.72
1:A:94:LYS:HA	1:A:97:ARG:HG3	1.71	0.72
1:B:219:LEU:O	1:B:219:LEU:HD22	1.90	0.72
1:C:100:LEU:HD22	1:C:104:LEU:HD11	1.72	0.71
1:B:228:PRO:HB2	1:B:488:TYR:CD2	2.25	0.71
1:C:308:GLU:OE1	1:D:322:LYS:NZ	2.22	0.71
1:D:61:PRO:CB	1:D:115:TYR:CD2	2.62	0.71
1:B:109:LEU:CD1	1:B:116:VAL:CG1	2.69	0.70
1:C:191:ARG:HH11	1:C:191:ARG:HG3	1.56	0.70
1:D:144:ILE:HG12	1:D:150:VAL:HG22	1.73	0.70
1:B:144:ILE:HD12	1:B:219:LEU:HD11	1.71	0.70
1:D:431:ASP:OD2	1:D:434:GLN:HB2	1.90	0.70
1:B:144:ILE:HB	1:B:219:LEU:CD1	2.21	0.70
1:B:219:LEU:HD22	1:B:219:LEU:C	2.16	0.70
1:D:261:CYS:HB2	1:D:391:PHE:CD1	2.27	0.70
1:A:219:LEU:HD22	1:A:219:LEU:C	2.15	0.70
1:D:61:PRO:HB2	1:D:115:TYR:HD2	1.57	0.70
1:B:72:ILE:CG1	1:B:107:MET:CE	2.68	0.70
1:A:258:LEU:CD1	1:A:388:ILE:CB	2.59	0.70
1:B:364:ILE:O	1:B:368:ILE:HG12	1.92	0.69
1:D:130:LEU:HD21	1:D:144:ILE:HD11	1.74	0.69
1:D:258:LEU:CD1	1:D:388:ILE:HB	2.11	0.69
1:A:335:GLY:O	1:A:358:THR:OG1	2.10	0.69
1:C:322:LYS:HE2	1:C:326:ARG:HH12	1.57	0.69
1:C:60:GLU:HB3	1:C:61:PRO:HD2	1.75	0.69
1:D:23:ILE:HG23	1:D:24:LEU:HD22	1.72	0.69
1:A:65:THR:N	1:A:68:GLU:OE1	2.26	0.68
1:A:144:ILE:HB	1:A:219:LEU:HD13	1.74	0.68
1:C:106:ARG:O	1:C:107:MET:CG	2.41	0.68
1:B:40:VAL:HG11	1:B:132:PRO:HB3	1.76	0.67
1:C:271:THR:O	1:C:275:ILE:HG12	1.94	0.67
1:C:64:PRO:HG3	1:C:116:VAL:HG22	1.77	0.67
1:B:191:ARG:HG3	1:B:191:ARG:HH11	1.60	0.67
1:B:260:VAL:HA	1:B:390:LEU:CG	2.24	0.67
1:A:144:ILE:HB	1:A:219:LEU:CD1	2.25	0.67
1:D:136:ASP:O	1:D:223:LYS:NZ	2.28	0.66
1:B:114:GLU:CD	1:B:114:GLU:H	2.03	0.66
1:B:61:PRO:HB3	1:B:115:TYR:CD2	2.27	0.66
1:B:347:GLN:O	1:B:347:GLN:NE2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:LEU:C	1:C:105:LEU:CD2	2.68	0.66
1:B:301:TRP:NE1	1:B:303:ALA:HB2	2.11	0.66
1:D:60:GLU:HB3	1:D:61:PRO:HD2	1.77	0.66
1:B:65:THR:N	1:B:68:GLU:OE1	2.20	0.66
1:B:257:ASN:HD21	1:B:349:MET:HB3	1.60	0.65
1:D:335:GLY:O	1:D:358:THR:OG1	2.11	0.65
1:B:144:ILE:HB	1:B:219:LEU:HD13	1.79	0.65
1:D:413:ILE:HG12	1:D:446:TYR:CD2	2.32	0.65
1:B:258:LEU:HD22	1:B:388:ILE:C	2.22	0.65
1:B:260:VAL:CB	1:B:390:LEU:HD11	2.27	0.65
1:C:100:LEU:HD22	1:C:104:LEU:HD21	1.78	0.65
1:D:258:LEU:CD1	1:D:388:ILE:CB	2.59	0.65
1:D:203:ARG:NH1	1:D:203:ARG:HG3	2.10	0.65
1:B:23:ILE:HG23	1:B:24:LEU:HD22	1.79	0.65
1:A:191:ARG:HG3	1:A:191:ARG:HH11	1.62	0.64
1:C:459:ASP:OD2	1:C:461:ARG:NH1	2.31	0.64
1:A:95:LEU:O	1:A:99:ILE:HG13	1.97	0.64
1:C:207:VAL:HB	1:C:218:ASN:ND2	2.13	0.64
1:D:80:ILE:HG22	1:D:83:LYS:NZ	2.13	0.64
1:B:68:GLU:HB3	1:B:109:LEU:CD2	2.27	0.64
1:D:150:VAL:O	1:D:162:THR:OG1	2.06	0.64
1:A:235:ILE:HD13	1:A:242:SER:HA	1.79	0.63
1:B:260:VAL:O	1:B:358:THR:HA	1.97	0.63
1:B:219:LEU:HD13	1:B:219:LEU:N	2.14	0.63
1:A:219:LEU:HD13	1:A:219:LEU:N	2.13	0.62
1:C:64:PRO:HG2	1:C:116:VAL:HG13	1.81	0.62
1:D:258:LEU:CD1	1:D:388:ILE:C	2.72	0.62
1:C:380:LYS:NZ	1:C:420:ASN:OD1	2.31	0.62
1:B:258:LEU:HD22	1:B:388:ILE:O	2.00	0.62
1:D:141:ASP:HB2	1:D:153:VAL:HB	1.81	0.62
1:A:114:GLU:CD	1:A:114:GLU:H	2.08	0.62
1:B:72:ILE:HD11	1:B:107:MET:HE1	1.81	0.62
1:D:5:GLU:O	1:D:9:THR:OG1	2.17	0.62
1:B:258:LEU:HD23	1:B:388:ILE:HG21	1.74	0.61
1:D:258:LEU:HD12	1:D:388:ILE:C	2.24	0.61
1:A:416:ASP:OD2	1:A:418:VAL:HB	2.00	0.61
1:B:301:TRP:CE2	1:B:303:ALA:HB2	2.34	0.61
1:A:5:GLU:O	1:A:9:THR:OG1	2.18	0.61
1:C:75:LYS:HD2	1:C:107:MET:HE2	1.74	0.61
1:B:286:VAL:HG22	1:B:302:VAL:HB	1.81	0.61
1:D:380:LYS:NZ	1:D:420:ASN:OD1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:VAL:O	1:C:347:GLN:HB3	2.01	0.61
1:B:64:PRO:HG2	1:B:116:VAL:HG13	1.82	0.61
1:B:379:PRO:HG2	1:B:382:TYR:CD1	2.36	0.61
1:B:390:LEU:CD1	1:B:390:LEU:C	2.74	0.61
1:B:219:LEU:HD13	1:B:219:LEU:H	1.65	0.60
1:D:287:THR:HG22	1:D:333:LEU:HB2	1.83	0.60
1:B:184:TYR:O	1:B:185:ARG:NH1	2.35	0.60
1:A:112:PRO:O	1:A:116:VAL:HG23	2.01	0.60
1:A:247:TYR:HA	1:A:470:LEU:HD11	1.84	0.60
1:D:434:GLN:HB3	1:D:436:LYS:HE2	1.83	0.60
1:B:258:LEU:C	1:B:258:LEU:CD1	2.75	0.60
1:B:126:TYR:HB3	1:B:131:GLU:OE1	2.01	0.60
1:B:130:LEU:HD21	1:B:144:ILE:HD11	1.83	0.60
1:B:323:ALA:O	1:B:327:GLN:HG3	2.01	0.60
1:B:180:SER:OG	1:B:187:VAL:HG13	2.01	0.60
1:B:258:LEU:CD2	1:B:388:ILE:HG21	2.24	0.60
1:B:415:ILE:HD13	1:B:422:VAL:HA	1.83	0.60
1:B:273:ASN:O	1:B:273:ASN:ND2	2.26	0.59
1:A:3:PHE:CE1	1:A:61:PRO:HD3	2.36	0.59
1:B:50:GLU:H	1:B:50:GLU:CD	2.09	0.59
1:C:296:VAL:HB	1:C:301:TRP:CD2	2.37	0.59
1:B:3:PHE:CE1	1:B:61:PRO:HD3	2.38	0.58
1:B:185:ARG:NH2	1:B:305:VAL:HG21	2.18	0.58
1:A:141:ASP:HB2	1:A:153:VAL:HB	1.86	0.58
1:A:249:TRP:HE1	1:A:499:ARG:NH2	2.01	0.58
1:B:261:CYS:H	1:B:390:LEU:CD1	2.16	0.58
1:A:258:LEU:CD1	1:A:388:ILE:C	2.77	0.58
1:B:331:TYR:CE2	1:B:354:SER:HB3	2.38	0.58
1:C:130:LEU:HD21	1:C:144:ILE:HD11	1.84	0.58
1:D:203:ARG:HH22	1:D:291:THR:HG22	1.69	0.58
1:A:20:ASN:O	1:A:23:ILE:HG22	2.03	0.58
1:B:105:LEU:C	1:B:105:LEU:CD2	2.76	0.58
1:C:23:ILE:HG23	1:C:24:LEU:HD22	1.86	0.58
1:A:64:PRO:HG3	1:A:116:VAL:HG22	1.86	0.58
1:A:442:LYS:O	1:A:467:TYR:CZ	2.56	0.58
1:C:144:ILE:HG12	1:C:150:VAL:HG22	1.86	0.58
1:D:149:HIS:NE2	1:D:165:LYS:HE2	2.19	0.58
1:D:430:TYR:OH	1:D:435:ASP:OD1	2.13	0.57
1:B:296:VAL:HB	1:B:301:TRP:CD2	2.40	0.57
1:A:219:LEU:HD13	1:A:219:LEU:H	1.69	0.57
1:C:106:ARG:C	1:C:107:MET:HG3	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:MET:O	1:A:246:ALA:HB3	2.04	0.57
1:A:322:LYS:O	1:A:326:ARG:NH1	2.37	0.57
1:B:142:ILE:HB	1:B:221:VAL:HB	1.86	0.57
1:B:231:ILE:O	1:B:235:ILE:HG13	2.04	0.57
1:D:42:ILE:HG21	1:D:56:TYR:CE1	2.39	0.56
1:C:94:LYS:HD2	1:C:97:ARG:HG3	1.87	0.56
1:C:114:GLU:H	1:C:114:GLU:CD	2.13	0.56
1:D:204:VAL:HG23	1:D:221:VAL:HG22	1.86	0.56
1:A:258:LEU:HD12	1:A:388:ILE:C	2.29	0.56
1:A:415:ILE:HD13	1:A:422:VAL:HA	1.86	0.56
1:B:141:ASP:HB2	1:B:153:VAL:HB	1.85	0.56
1:D:203:ARG:HG3	1:D:203:ARG:HH11	1.70	0.56
1:B:228:PRO:HG3	1:B:295:THR:HB	1.87	0.56
1:B:30:PHE:CE2	1:B:46:SER:HB3	2.41	0.56
1:A:7:TYR:O	1:A:10:LYS:HG2	2.06	0.56
1:C:364:ILE:O	1:C:368:ILE:HG12	2.05	0.56
1:A:144:ILE:HD12	1:A:219:LEU:CD1	2.21	0.55
1:C:286:VAL:HG22	1:C:302:VAL:HB	1.89	0.55
1:B:213:SER:O	1:B:216:GLY:N	2.38	0.55
1:C:7:TYR:O	1:C:10:LYS:HG2	2.07	0.55
1:D:296:VAL:HG12	1:D:298:HIS:H	1.71	0.55
1:A:219:LEU:C	1:A:219:LEU:CD2	2.79	0.55
1:C:258:LEU:HD12	1:C:388:ILE:O	2.07	0.55
1:D:251:MET:HG3	1:D:388:ILE:HD11	1.89	0.55
1:B:136:ASP:HB3	1:B:139:ILE:HD12	1.88	0.55
1:B:244:MET:HA	1:B:428:PHE:CZ	2.41	0.55
1:A:382:TYR:O	1:A:385:ASN:HB2	2.07	0.55
1:A:471:GLN:O	1:A:474:SER:HB3	2.07	0.55
1:B:322:LYS:NZ	1:B:326:ARG:NH1	2.50	0.55
1:B:72:ILE:HG12	1:B:107:MET:SD	2.47	0.54
1:C:94:LYS:HA	1:C:97:ARG:HG3	1.88	0.54
1:D:291:THR:HG22	1:D:293:GLU:HG3	1.89	0.54
1:A:64:PRO:HG2	1:A:116:VAL:HG13	1.89	0.54
1:A:243:MET:HE1	1:A:471:GLN:NE2	2.22	0.54
1:B:56:TYR:CD2	1:B:162:THR:HG22	2.43	0.54
1:B:72:ILE:HG13	1:B:107:MET:CE	2.28	0.54
1:B:144:ILE:HB	1:B:219:LEU:HD11	1.88	0.54
1:C:231:ILE:O	1:C:235:ILE:HG13	2.07	0.54
1:B:211:ASP:OD1	1:B:212:ILE:HG12	2.08	0.54
1:D:173:ASP:OD1	1:D:217:SER:OG	2.21	0.54
1:C:431:ASP:OD2	1:C:434:GLN:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:GLU:CD	1:D:114:GLU:H	2.16	0.54
1:A:16:THR:OG1	1:A:17:ILE:N	2.40	0.53
1:B:219:LEU:C	1:B:219:LEU:CD2	2.80	0.53
1:D:50:GLU:H	1:D:50:GLU:CD	2.16	0.53
1:B:14:ARG:HG2	1:B:14:ARG:HH11	1.73	0.53
1:C:61:PRO:CB	1:C:115:TYR:CD2	2.83	0.53
1:D:7:TYR:O	1:D:10:LYS:HG2	2.09	0.53
1:B:228:PRO:HB2	1:B:488:TYR:CE2	2.43	0.53
1:C:333:LEU:HD22	1:C:356:MET:HB2	1.90	0.53
1:B:333:LEU:HD22	1:B:356:MET:HB2	1.89	0.53
1:D:126:TYR:HB3	1:D:131:GLU:OE1	2.08	0.53
1:C:258:LEU:O	1:C:356:MET:HA	2.08	0.53
1:A:251:MET:SD	1:A:256:MET:HG3	2.48	0.53
1:B:191:ARG:HG3	1:B:191:ARG:NH1	2.23	0.53
1:B:250:THR:OG1	1:B:473:ARG:NH1	2.41	0.53
1:B:260:VAL:CA	1:B:390:LEU:CD1	2.62	0.52
1:A:244:MET:HA	1:A:428:PHE:CZ	2.44	0.52
1:B:325:LEU:HD21	1:B:348:ALA:HB2	1.90	0.52
1:C:408:GLU:HA	1:C:428:PHE:O	2.09	0.52
1:D:459:ASP:OD2	1:D:461:ARG:NH1	2.42	0.52
1:D:104:LEU:HB3	1:D:113:LYS:HE3	1.91	0.52
1:B:192:PRO:HG2	1:B:193:VAL:HG23	1.91	0.52
1:A:61:PRO:CB	1:A:115:TYR:HD2	2.16	0.52
1:A:147:LEU:HD22	1:A:167:GLU:O	2.10	0.52
1:A:510:VAL:C	1:A:512:ASN:H	2.18	0.52
1:B:40:VAL:CG1	1:B:132:PRO:HB3	2.38	0.52
1:B:257:ASN:ND2	1:B:349:MET:HB3	2.25	0.52
1:C:100:LEU:HD11	1:C:120:PHE:CD2	2.45	0.52
1:C:492:TRP:O	1:C:496:LEU:HG	2.10	0.52
1:B:80:ILE:HG22	1:B:83:LYS:HZ1	1.75	0.51
1:B:109:LEU:HD13	1:B:116:VAL:CG2	2.39	0.51
1:B:68:GLU:HB3	1:B:109:LEU:HD22	1.92	0.51
1:B:104:LEU:HD23	1:B:107:MET:SD	2.51	0.51
1:B:213:SER:OG	1:B:216:GLY:O	2.21	0.51
1:B:260:VAL:HA	1:B:390:LEU:HG	1.92	0.51
1:B:374:TYR:CG	1:B:375:PRO:HA	2.45	0.51
1:D:281:PRO:HA	1:D:298:HIS:CD2	2.45	0.51
1:D:368:ILE:HD12	1:D:383:ILE:HG21	1.92	0.51
1:A:129:SER:O	1:A:132:PRO:HD2	2.09	0.51
1:A:322:LYS:HG2	1:A:344:VAL:HG11	1.92	0.51
1:B:273:ASN:HD22	1:B:273:ASN:C	2.16	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:PRO:CG	1:B:295:THR:HB	2.41	0.51
1:C:251:MET:SD	1:C:256:MET:HG3	2.50	0.51
1:B:416:ASP:OD2	1:B:418:VAL:HB	2.10	0.51
1:C:269:THR:HG21	1:C:293:GLU:OE1	2.10	0.51
1:A:125:LEU:HB3	1:A:126:TYR:CD1	2.45	0.51
1:A:398:LYS:HD2	1:A:398:LYS:N	2.26	0.51
1:B:439:PHE:CD1	1:B:440:ALA:N	2.79	0.50
1:B:3:PHE:HB3	1:B:115:TYR:HE2	1.76	0.50
1:D:415:ILE:HD13	1:D:422:VAL:HA	1.94	0.50
1:D:497:ARG:O	1:D:501:MET:HG2	2.10	0.50
1:A:176:ILE:HD11	1:A:219:LEU:HD12	1.93	0.50
1:A:497:ARG:HG3	1:A:501:MET:HE3	1.92	0.50
1:B:19:GLU:HA	1:B:34:TYR:HB2	1.92	0.50
1:B:288:ILE:HG22	1:B:317:LEU:HD22	1.94	0.50
1:A:63:ARG:HH11	1:A:119:HIS:HB3	1.76	0.50
1:A:88:ASP:O	1:A:92:LYS:HB2	2.12	0.50
1:B:279:ILE:HD13	1:B:331:TYR:CD1	2.47	0.50
1:C:20:ASN:OD1	1:C:22:ASN:HB2	2.11	0.50
1:B:118:TYR:O	1:B:122:ARG:HB2	2.12	0.50
1:A:43:HIS:HB3	1:A:57:ASN:HB2	1.94	0.49
1:C:117:ILE:O	1:C:121:ILE:HG12	2.12	0.49
1:D:61:PRO:HB2	1:D:115:TYR:CD2	2.42	0.49
1:C:72:ILE:HG23	1:C:103:ILE:HD11	1.94	0.49
1:D:30:PHE:CE2	1:D:46:SER:HB3	2.46	0.49
1:B:68:GLU:OE2	1:B:109:LEU:HD22	2.12	0.49
1:B:139:ILE:O	1:B:223:LYS:HD3	2.12	0.49
1:A:99:ILE:O	1:A:103:ILE:HG23	2.13	0.49
1:D:333:LEU:HD22	1:D:356:MET:HB2	1.94	0.49
1:A:325:LEU:HD21	1:A:348:ALA:HB2	1.95	0.49
1:B:65:THR:HG22	1:B:68:GLU:HG3	1.94	0.49
1:D:376:ILE:HG22	1:D:378:VAL:HG23	1.93	0.49
1:A:44:ILE:HD12	1:A:157:PHE:CZ	2.47	0.49
1:B:201:GLY:HA3	1:B:226:ARG:HB3	1.93	0.49
1:B:247:TYR:C	1:B:247:TYR:CD2	2.90	0.49
1:B:347:GLN:NE2	1:B:347:GLN:HA	2.27	0.49
1:A:125:LEU:HB3	1:A:126:TYR:CE1	2.48	0.48
1:B:3:PHE:HB3	1:B:115:TYR:CE2	2.48	0.48
1:B:461:ARG:HD3	1:C:440:ALA:O	2.13	0.48
1:D:166:PHE:CZ	1:D:175:LEU:HD22	2.48	0.48
1:C:86:PRO:HB2	1:C:92:LYS:CD	2.44	0.48
1:C:445:SER:HB3	1:C:448:ILE:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:O	1:A:121:ILE:HG12	2.14	0.48
1:C:100:LEU:O	1:C:104:LEU:CG	2.58	0.48
1:C:88:ASP:O	1:C:92:LYS:HB2	2.13	0.48
1:D:243:MET:O	1:D:243:MET:HG3	2.13	0.48
1:C:142:ILE:HB	1:C:221:VAL:HB	1.94	0.48
1:A:291:THR:O	1:A:293:GLU:HG3	2.14	0.48
1:B:72:ILE:HG12	1:B:107:MET:HE1	1.88	0.48
1:C:99:ILE:O	1:C:103:ILE:HG23	2.13	0.48
1:C:473:ARG:HG3	1:C:503:LEU:HD21	1.96	0.48
1:D:262:GLY:O	1:D:268:LYS:HD3	2.14	0.48
1:B:80:ILE:HG22	1:B:83:LYS:HZ2	1.77	0.48
1:A:301:TRP:CE2	1:A:303:ALA:HB2	2.48	0.47
1:B:321:LEU:O	1:B:324:ALA:HB3	2.14	0.47
1:B:382:TYR:O	1:B:385:ASN:HB2	2.14	0.47
1:B:346:PHE:HA	1:B:349:MET:HE3	1.95	0.47
1:A:275:ILE:O	1:A:278:PHE:HB2	2.14	0.47
1:A:176:ILE:HG12	1:A:217:SER:HB3	1.96	0.47
1:B:42:ILE:HG21	1:B:56:TYR:CE1	2.49	0.47
1:B:94:LYS:HA	1:B:97:ARG:HG3	1.95	0.47
1:C:88:ASP:HB3	1:C:92:LYS:HD2	1.96	0.47
1:D:60:GLU:CB	1:D:61:PRO:HD2	2.45	0.47
1:D:144:ILE:O	1:D:218:ASN:HB2	2.15	0.47
1:B:21:PRO:HD2	1:B:138:TYR:CE1	2.50	0.47
1:B:180:SER:CB	1:B:187:VAL:HG13	2.44	0.47
1:B:203:ARG:HA	1:B:203:ARG:HD3	1.53	0.47
1:B:405:ARG:O	1:B:407:VAL:HG13	2.15	0.47
1:C:60:GLU:OE2	1:C:122:ARG:NH1	2.41	0.47
1:C:151:TYR:HE1	1:C:161:ARG:HB2	1.80	0.47
1:C:413:ILE:HD11	1:C:425:ILE:HG13	1.97	0.47
1:A:193:VAL:HG22	1:A:207:VAL:HG22	1.97	0.47
1:A:487:ASN:O	1:A:491:VAL:HG23	2.14	0.47
1:A:179:LEU:HD23	1:A:179:LEU:HA	1.67	0.46
1:A:318:PHE:N	1:A:341:GLU:HB3	2.30	0.46
1:B:94:LYS:HD2	1:B:97:ARG:HG3	1.98	0.46
1:B:200:ASP:O	1:B:226:ARG:HD3	2.15	0.46
1:B:72:ILE:HD11	1:B:107:MET:CE	2.44	0.46
1:A:290:ASP:HA	1:A:306:THR:OG1	2.14	0.46
1:B:50:GLU:CD	1:B:50:GLU:N	2.73	0.46
1:B:125:LEU:HB3	1:B:126:TYR:CD1	2.49	0.46
1:C:30:PHE:CE2	1:C:46:SER:HB3	2.51	0.46
1:D:374:TYR:CG	1:D:375:PRO:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ARG:HG3	1:A:503:LEU:HD21	1.96	0.46
1:A:503:LEU:HD12	1:A:503:LEU:HA	1.75	0.46
1:B:166:PHE:CZ	1:B:175:LEU:HD22	2.50	0.46
1:C:249:TRP:CG	1:C:278:PHE:CD1	3.03	0.46
1:C:141:ASP:HB2	1:C:153:VAL:HB	1.97	0.46
1:A:350:GLN:HG2	1:A:382:TYR:CE2	2.50	0.46
1:B:7:TYR:O	1:B:10:LYS:HG2	2.16	0.46
1:B:261:CYS:N	1:B:390:LEU:CD1	2.79	0.46
1:C:17:ILE:HD13	1:C:33:ILE:HG23	1.98	0.46
1:D:24:LEU:O	1:D:27:SER:N	2.38	0.46
1:A:138:TYR:HB3	1:A:154:HIS:CE1	2.51	0.46
1:B:268:LYS:HD2	1:B:358:THR:HB	1.96	0.46
1:A:364:ILE:O	1:A:368:ILE:HG12	2.16	0.46
1:B:379:PRO:HD2	1:B:382:TYR:HB2	1.97	0.46
1:C:253:ASP:OD1	1:C:499:ARG:NH2	2.44	0.46
1:D:65:THR:HG22	1:D:68:GLU:HG3	1.98	0.46
1:B:20:ASN:O	1:B:23:ILE:HG22	2.17	0.45
1:B:137:PRO:HG2	1:B:138:TYR:CD2	2.51	0.45
1:B:403:ILE:HD12	1:B:405:ARG:NE	2.31	0.45
1:C:144:ILE:O	1:C:218:ASN:HB2	2.16	0.45
1:C:166:PHE:CZ	1:C:175:LEU:HD22	2.50	0.45
1:C:223:LYS:HB3	1:C:223:LYS:HE2	1.84	0.45
1:A:235:ILE:CD1	1:A:242:SER:HA	2.47	0.45
1:A:380:LYS:C	1:A:382:TYR:H	2.23	0.45
1:B:14:ARG:HG2	1:B:14:ARG:NH1	2.31	0.45
1:B:219:LEU:CD1	1:B:219:LEU:N	2.80	0.45
1:C:50:GLU:CD	1:C:50:GLU:H	2.25	0.45
1:C:191:ARG:HG3	1:C:191:ARG:NH1	2.28	0.45
1:C:212:ILE:HD11	1:D:307:ARG:NH1	2.32	0.45
1:C:261:CYS:HB2	1:C:391:PHE:CD1	2.50	0.45
1:C:368:ILE:HD12	1:C:383:ILE:HG21	1.98	0.45
1:D:452:ILE:O	1:D:456:ARG:HB2	2.16	0.45
1:A:219:LEU:CD1	1:A:219:LEU:N	2.80	0.45
1:B:44:ILE:HD12	1:B:157:PHE:CZ	2.52	0.45
1:B:144:ILE:HG12	1:B:150:VAL:HG22	1.97	0.45
1:B:402:LEU:HD23	1:B:404:ARG:NH1	2.32	0.45
1:C:226:ARG:HG3	1:C:227:VAL:HG23	1.96	0.45
1:D:342:GLY:O	1:D:345:ALA:HB3	2.17	0.45
1:C:126:TYR:HB3	1:C:131:GLU:OE1	2.16	0.45
1:B:439:PHE:HD1	1:B:440:ALA:N	2.15	0.45
1:C:96:ILE:H	1:C:96:ILE:HG12	1.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LEU:CD2	1:C:104:LEU:HD21	2.45	0.45
1:B:150:VAL:O	1:B:162:THR:OG1	2.19	0.45
1:C:80:ILE:HG22	1:C:83:LYS:NZ	2.32	0.45
1:C:133:LEU:HD11	1:C:164:ILE:HD12	1.99	0.45
1:D:44:ILE:H	1:D:44:ILE:HG12	1.62	0.45
1:D:272:LEU:HD22	1:D:358:THR:HG23	1.97	0.45
1:B:176:ILE:HD11	1:B:219:LEU:HD12	1.99	0.45
1:C:409:VAL:O	1:C:427:ALA:N	2.49	0.45
1:A:142:ILE:HB	1:A:221:VAL:HB	1.98	0.45
1:A:503:LEU:O	1:A:507:ILE:HG13	2.17	0.45
1:D:74:GLU:O	1:D:78:LEU:HG	2.17	0.45
1:A:44:ILE:HD12	1:A:157:PHE:CE2	2.52	0.44
1:B:104:LEU:HD13	1:B:113:LYS:HG3	1.98	0.44
1:C:60:GLU:CB	1:C:61:PRO:HD2	2.45	0.44
1:A:185:ARG:HG3	1:A:196:ALA:HB2	2.00	0.44
1:D:139:ILE:O	1:D:223:LYS:HD3	2.16	0.44
1:A:212:ILE:O	1:B:304:GLU:HA	2.18	0.44
1:A:501:MET:HE2	1:A:501:MET:HB3	1.79	0.44
1:B:104:LEU:HB3	1:B:113:LYS:HE3	2.00	0.44
1:A:463:ILE:HD12	1:A:463:ILE:HA	1.72	0.44
1:B:343:ASN:HB2	1:B:376:ILE:O	2.18	0.44
1:B:68:GLU:HB3	1:B:109:LEU:HD21	1.98	0.44
1:C:43:HIS:HB3	1:C:57:ASN:HB2	1.98	0.44
1:C:95:LEU:O	1:C:99:ILE:HG13	2.17	0.44
1:D:477:LEU:HD23	1:D:477:LEU:HA	1.82	0.44
1:A:173:ASP:O	1:A:177:VAL:HG23	2.18	0.44
1:C:33:ILE:HA	1:C:42:ILE:O	2.18	0.44
1:A:431:ASP:OD2	1:A:434:GLN:HB2	2.17	0.44
1:B:495:ILE:O	1:B:499:ARG:HG3	2.17	0.44
1:C:207:VAL:HB	1:C:218:ASN:HD21	1.82	0.44
1:A:41:TYR:O	1:A:59:ILE:HB	2.18	0.44
1:B:180:SER:HB2	1:B:185:ARG:O	2.18	0.44
1:B:434:GLN:HG3	1:B:436:LYS:HZ1	1.83	0.43
1:A:64:PRO:CG	1:A:116:VAL:HG13	2.48	0.43
1:A:114:GLU:CD	1:A:114:GLU:N	2.75	0.43
1:C:331:TYR:CE2	1:C:354:SER:HB3	2.53	0.43
1:A:21:PRO:HB2	1:A:156:VAL:HG21	2.00	0.43
1:A:376:ILE:HG22	1:A:378:VAL:HG23	1.99	0.43
1:C:88:ASP:HB3	1:C:91:GLU:OE2	2.18	0.43
1:D:247:TYR:HA	1:D:470:LEU:HD11	1.99	0.43
1:A:20:ASN:OD1	1:A:22:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PRO:HB2	1:A:488:TYR:CD2	2.53	0.43
1:B:58:VAL:HG21	1:B:164:ILE:HD11	2.01	0.43
1:B:76:PHE:CE2	1:B:124:LYS:HE2	2.53	0.43
1:C:151:TYR:CE1	1:C:161:ARG:HB2	2.53	0.43
1:A:195:ASP:OD2	1:B:326:ARG:HG2	2.19	0.43
1:B:301:TRP:CD1	1:B:301:TRP:C	2.96	0.43
1:A:297:PRO:HG3	1:A:488:TYR:HE1	1.84	0.43
1:B:117:ILE:O	1:B:121:ILE:HG12	2.18	0.43
1:A:76:PHE:CE2	1:A:124:LYS:HE2	2.54	0.43
1:A:322:LYS:HB3	1:A:322:LYS:HE2	1.76	0.43
1:A:350:GLN:HG2	1:A:382:TYR:HE2	1.82	0.43
1:B:144:ILE:CD1	1:B:219:LEU:HD11	2.45	0.43
1:B:431:ASP:OD2	1:B:434:GLN:HB2	2.19	0.43
1:D:330:ASN:O	1:D:354:SER:HB2	2.18	0.43
1:D:494:TYR:O	1:D:497:ARG:HB3	2.19	0.43
1:C:100:LEU:HD22	1:C:104:LEU:CD1	2.46	0.43
1:C:280:PRO:HD2	1:C:283:LEU:HD12	2.01	0.43
1:D:261:CYS:O	1:D:391:PHE:HA	2.19	0.43
1:D:445:SER:OG	1:D:448:ILE:HG13	2.19	0.43
1:A:104:LEU:HB3	1:A:113:LYS:HE3	2.01	0.42
1:A:261:CYS:HB2	1:A:391:PHE:CD1	2.54	0.42
1:A:459:ASP:OD2	1:A:461:ARG:NH1	2.52	0.42
1:B:345:ALA:O	1:B:349:MET:HG3	2.19	0.42
1:C:7:TYR:CD1	1:C:10:LYS:HE3	2.54	0.42
1:C:291:THR:O	1:C:293:GLU:N	2.49	0.42
1:B:409:VAL:O	1:B:427:ALA:N	2.47	0.42
1:D:430:TYR:CE2	1:D:432:SER:HA	2.54	0.42
1:A:227:VAL:HA	1:A:228:PRO:HD3	1.77	0.42
1:B:72:ILE:HG12	1:B:107:MET:CE	2.47	0.42
1:B:247:TYR:HA	1:B:470:LEU:HD11	2.01	0.42
1:B:258:LEU:HA	1:B:388:ILE:O	2.19	0.42
1:B:439:PHE:HD1	1:B:440:ALA:H	1.67	0.42
1:C:30:PHE:CD2	1:C:46:SER:HB3	2.54	0.42
1:C:61:PRO:HB2	1:C:115:TYR:HB3	2.01	0.42
1:C:244:MET:O	1:C:247:TYR:HB3	2.19	0.42
1:D:80:ILE:HG22	1:D:83:LYS:HZ2	1.82	0.42
1:B:413:ILE:HG12	1:B:446:TYR:CD2	2.55	0.42
1:C:58:VAL:HG21	1:C:164:ILE:HD11	2.01	0.42
1:C:244:MET:HA	1:C:428:PHE:CZ	2.54	0.42
1:D:191:ARG:NE	1:D:308:GLU:O	2.51	0.42
1:A:57:ASN:HA	1:A:163:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LEU:HD22	1:C:125:LEU:HA	1.84	0.42
1:D:203:ARG:HH12	1:D:291:THR:HG23	1.84	0.42
1:A:85:PRO:HA	1:A:86:PRO:HD3	1.89	0.42
1:C:129:SER:O	1:C:132:PRO:HD2	2.20	0.42
1:A:144:ILE:HB	1:A:219:LEU:HD11	2.00	0.42
1:A:333:LEU:HD22	1:A:356:MET:HB2	2.02	0.42
1:A:475:ARG:O	1:A:479:LEU:HD13	2.20	0.42
1:C:74:GLU:O	1:C:78:LEU:HG	2.19	0.42
1:A:501:MET:O	1:A:505:GLU:HB2	2.20	0.42
1:C:76:PHE:CE2	1:C:124:LYS:HE2	2.55	0.42
1:C:220:THR:HG21	1:D:327:GLN:C	2.45	0.42
1:A:86:PRO:HB2	1:A:92:LYS:CD	2.50	0.41
1:A:183:SER:OG	1:A:198:LEU:HD23	2.19	0.41
1:A:296:VAL:HB	1:A:301:TRP:CD2	2.55	0.41
1:B:242:SER:OG	1:B:474:SER:O	2.37	0.41
1:B:283:LEU:HB3	1:B:330:ASN:CB	2.50	0.41
1:B:342:GLY:O	1:B:345:ALA:N	2.49	0.41
1:D:20:ASN:OD1	1:D:22:ASN:HB2	2.20	0.41
1:C:387:ASN:C	1:C:388:ILE:HG13	2.45	0.41
1:D:364:ILE:O	1:D:368:ILE:HG12	2.21	0.41
1:A:383:ILE:O	1:A:385:ASN:N	2.54	0.41
1:C:365:THR:O	1:C:369:GLN:HG3	2.20	0.41
1:A:63:ARG:HD2	1:A:119:HIS:CG	2.56	0.41
1:B:68:GLU:OE2	1:B:109:LEU:CD2	2.67	0.41
1:C:281:PRO:HG3	1:C:496:LEU:HD22	2.02	0.41
1:D:20:ASN:O	1:D:23:ILE:HG22	2.20	0.41
1:D:180:SER:HB2	1:D:185:ARG:O	2.20	0.41
1:D:495:ILE:O	1:D:499:ARG:HG3	2.19	0.41
1:B:126:TYR:HB3	1:B:131:GLU:CD	2.45	0.41
1:C:8:LEU:HA	1:C:8:LEU:HD12	1.87	0.41
1:C:276:THR:HG23	1:C:279:ILE:HD12	2.01	0.41
1:B:47:ILE:HD11	1:B:49:SER:HB2	2.03	0.41
1:B:371:LEU:HD23	1:B:371:LEU:HA	1.87	0.41
1:C:391:PHE:O	1:C:407:VAL:HG22	2.21	0.41
1:D:76:PHE:CE2	1:D:124:LYS:HE2	2.55	0.41
1:A:88:ASP:HB3	1:A:91:GLU:OE2	2.21	0.41
1:A:245:ALA:HB3	1:A:477:LEU:HD13	2.01	0.41
1:C:258:LEU:HD13	1:C:388:ILE:CB	2.43	0.41
1:A:383:ILE:C	1:A:385:ASN:N	2.77	0.41
1:A:494:TYR:HA	1:A:497:ARG:HB3	2.03	0.41
1:B:440:ALA:O	1:D:460:ARG:NH2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:GLN:O	1:B:475:ARG:HG3	2.20	0.41
1:C:183:SER:OG	1:C:198:LEU:HD23	2.20	0.41
1:C:283:LEU:HB3	1:C:330:ASN:CB	2.50	0.41
1:B:43:HIS:CD2	1:B:43:HIS:C	2.99	0.41
1:D:3:PHE:CD2	1:D:115:TYR:HE2	2.39	0.41
1:D:112:PRO:HB2	1:D:115:TYR:HD1	1.86	0.41
1:A:53:TYR:HB2	1:A:161:ARG:NH1	2.36	0.40
1:A:349:MET:HA	1:A:353:HIS:O	2.20	0.40
1:C:106:ARG:C	1:C:107:MET:CG	2.93	0.40
1:D:125:LEU:HA	1:D:125:LEU:HD22	1.86	0.40
1:A:30:PHE:CE2	1:A:46:SER:HB3	2.57	0.40
1:A:380:LYS:NZ	1:A:420:ASN:OD1	2.52	0.40
1:B:104:LEU:O	1:B:105:LEU:C	2.64	0.40
1:B:112:PRO:O	1:B:116:VAL:HG23	2.20	0.40
1:B:402:LEU:HD12	1:B:402:LEU:HA	1.77	0.40
1:D:285:ILE:HD13	1:D:298:HIS:CG	2.55	0.40
1:D:380:LYS:HB2	1:D:380:LYS:HE3	1.86	0.40
1:A:88:ASP:HB3	1:A:92:LYS:HD2	2.03	0.40
1:A:285:ILE:HD12	1:A:285:ILE:N	2.37	0.40
1:A:370:ARG:O	1:A:376:ILE:HD12	2.21	0.40
1:B:30:PHE:CZ	1:B:46:SER:HB3	2.57	0.40
1:C:380:LYS:HB2	1:C:380:LYS:HE3	1.85	0.40
1:D:112:PRO:HB2	1:D:115:TYR:CD1	2.56	0.40
1:A:247:TYR:O	1:A:251:MET:HG2	2.22	0.40
1:B:251:MET:SD	1:B:256:MET:HG3	2.62	0.40
1:C:173:ASP:O	1:C:177:VAL:HG23	2.22	0.40
1:D:8:LEU:HD12	1:D:8:LEU:HA	1.78	0.40
1:D:441:GLY:O	1:D:444:SER:OG	2.34	0.40
1:B:8:LEU:HD12	1:B:8:LEU:HA	1.83	0.40
1:C:63:ARG:HD2	1:C:119:HIS:CG	2.56	0.40
1:C:75:LYS:HE2	1:C:107:MET:CE	2.16	0.40
1:D:243:MET:HE2	1:D:243:MET:HB2	1.90	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ARG:O	1:C:107:MET:CA[4_544]	1.94	0.26

5.3 Torsion angles

5.3.1 Protein backbone

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	498/513 (97%)	464 (93%)	26 (5%)	8 (2%)	7	36
1	B	492/513 (96%)	457 (93%)	30 (6%)	5 (1%)	12	45
1	C	506/513 (99%)	476 (94%)	27 (5%)	3 (1%)	21	54
1	D	490/513 (96%)	464 (95%)	23 (5%)	3 (1%)	21	54
All	All	1986/2052 (97%)	1861 (94%)	106 (5%)	19 (1%)	12	45

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	PRO
1	A	88	ASP
1	A	95	LEU
1	A	384	ASN
1	B	214	ARG
1	C	95	LEU
1	C	338	ARG
1	A	87	GLU
1	D	95	LEU
1	D	263	GLU
1	A	94	LYS
1	A	511	SER
1	B	18	ILE
1	B	61	PRO
1	B	95	LEU
1	A	311	GLY
1	B	311	GLY
1	C	311	GLY
1	D	311	GLY

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	454/463 (98%)	430 (95%)	24 (5%)	20	48
1	B	451/463 (97%)	429 (95%)	22 (5%)	22	49
1	C	460/463 (99%)	439 (95%)	21 (5%)	24	51
1	D	448/463 (97%)	427 (95%)	21 (5%)	23	50
All	All	1813/1852 (98%)	1725 (95%)	88 (5%)	22	49

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	9	THR
1	A	11	LEU
1	A	17	ILE
1	A	24	LEU
1	A	29	ILE
1	A	33	ILE
1	A	44	ILE
1	A	91	GLU
1	A	96	ILE
1	A	117	ILE
1	A	125	LEU
1	A	129	SER
1	A	172	LEU
1	A	191	ARG
1	A	219	LEU
1	A	273	ASN
1	A	321	LEU
1	A	322	LYS
1	A	376	ILE
1	A	384	ASN
1	A	463	ILE
1	A	480	LEU
1	A	503	LEU

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Mol	Chain	Res	Type
1	B	11	LEU
1	B	29	ILE
1	B	69	MET
1	B	91	GLU
1	B	105	LEU
1	B	113	LYS
1	B	117	ILE
1	B	125	LEU
1	B	172	LEU
1	B	203	ARG
1	B	204	VAL
1	B	211	ASP
1	B	219	LEU
1	B	236	MET
1	B	273	ASN
1	B	285	ILE
1	B	321	LEU
1	B	322	LYS
1	B	340	LYS
1	B	347	GLN
1	B	390	LEU
1	B	480	LEU
1	C	6	ASP
1	C	11	LEU
1	C	24	LEU
1	C	29	ILE
1	C	44	ILE
1	C	91	GLU
1	C	96	ILE
1	C	105	LEU
1	C	109	LEU
1	C	117	ILE
1	C	125	LEU
1	C	172	LEU
1	C	191	ARG
1	C	219	LEU
1	C	236	MET
1	C	273	ASN
1	C	321	LEU
1	C	322	LYS
1	C	340	LYS
1	C	351	THR

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Mol	Chain	Res	Type
1	C	480	LEU
1	D	9	THR
1	D	11	LEU
1	D	29	ILE
1	D	33	ILE
1	D	44	ILE
1	D	91	GLU
1	D	96	ILE
1	D	117	ILE
1	D	125	LEU
1	D	129	SER
1	D	163	SER
1	D	172	LEU
1	D	219	LEU
1	D	236	MET
1	D	264	THR
1	D	273	ASN
1	D	321	LEU
1	D	322	LYS
1	D	347	GLN
1	D	480	LEU
1	D	504	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	HIS
1	A	360	HIS
1	A	385	ASN
1	A	471	GLN
1	B	257	ASN
1	B	347	GLN
1	B	385	ASN
1	B	401	ASN
1	B	434	GLN
1	C	205	ASN
1	C	218	ASN
1	C	347	GLN
1	C	434	GLN
1	C	450	ASN
1	D	189	HIS
1	D	347	GLN

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Mol	Chain	Res	Type
1	D	401	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	504/513 (98%)	-0.61	1 (0%) 91 80	1, 11, 79, 112	0
1	B	500/513 (97%)	-0.61	2 (0%) 88 70	1, 19, 81, 138	0
1	C	510/513 (99%)	-0.63	2 (0%) 88 70	3, 49, 85, 133	1 (0%)
1	D	498/513 (97%)	-0.58	2 (0%) 88 70	7, 47, 88, 108	1 (0%)
All	All	2012/2052 (98%)	-0.61	7 (0%) 90 75	1, 35, 83, 138	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	104	LEU	2.7
1	B	267	GLY	2.5
1	C	141	ASP	2.3
1	D	100	LEU	2.2
1	C	134	ILE	2.2
1	A	308	GLU	2.1
1	B	109	LEU	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.