



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:58 PM UTC

PDB ID : 4K1N / pdb_00004k1n
Title : Crystal structure of full-length mouse alphaE-catenin
Authors : Ishiyama, N.; Ikura, M.
Deposited on : 2013-04-05
Resolution : 6.50 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

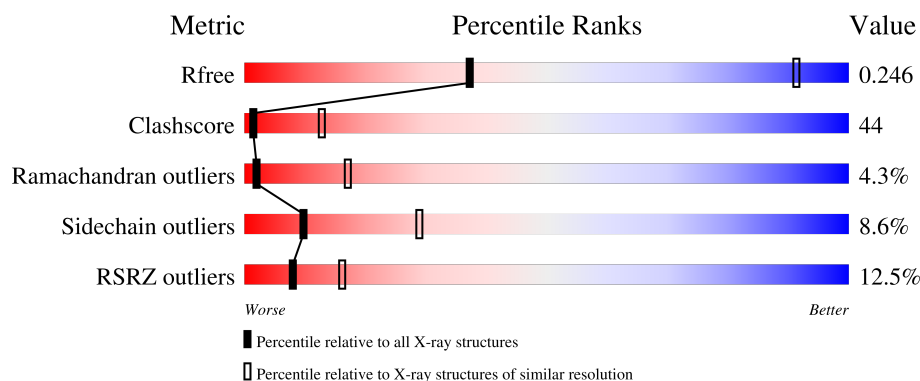
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.50 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	1162 (9.00-4.00)
Clashscore	190562	1020 (8.98-4.02)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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	912	6% 24% 28% • 43%
1	B	912	8% 24% 29% • 43%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8020 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 Catenin alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			4010	2486	713	789	22			
1	B	520	Total	C	N	O	S	0	0	0
			4010	2486	713	789	22			

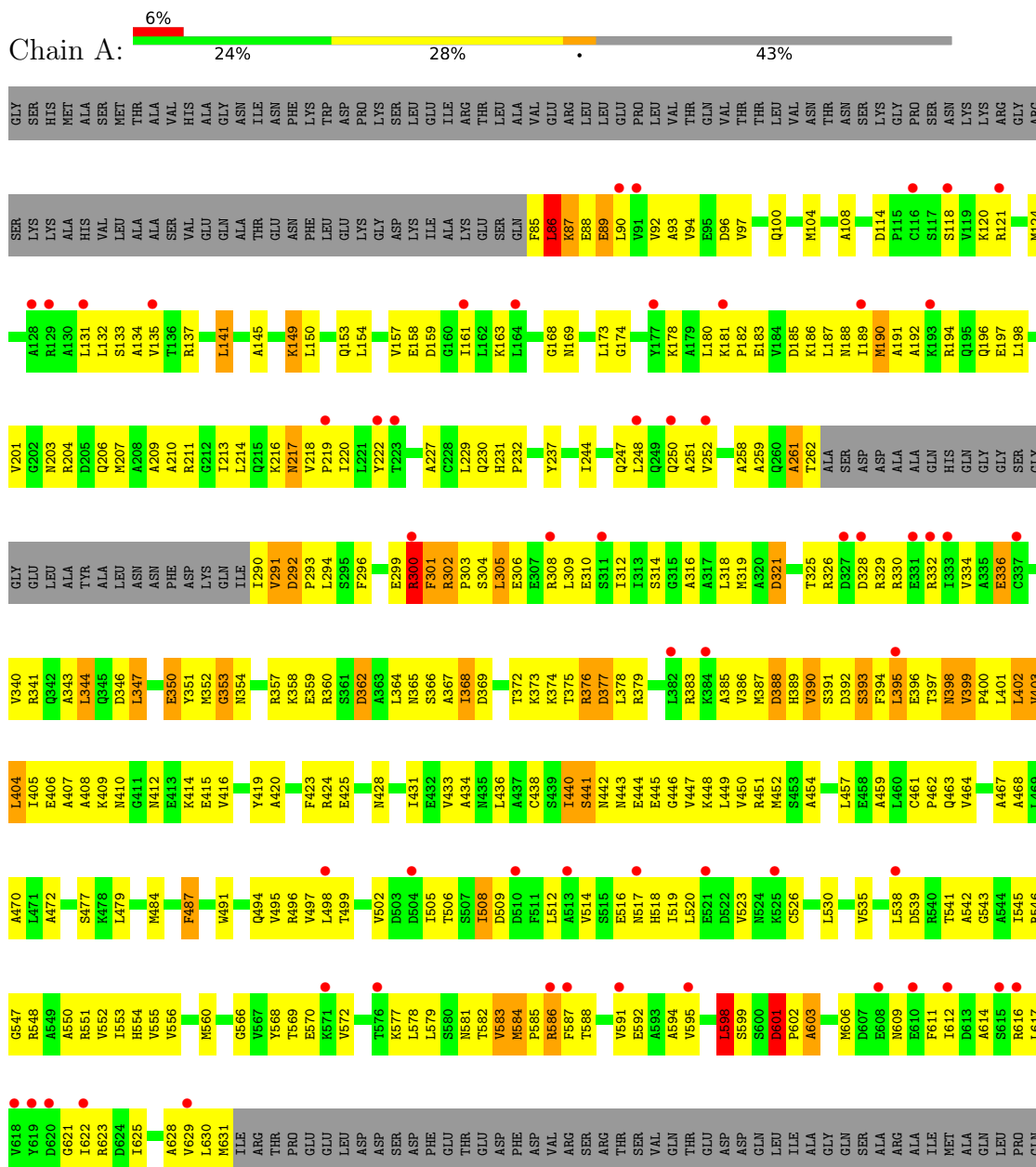
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP P26231
A	-4	SER	-	expression tag	UNP P26231
A	-3	HIS	-	expression tag	UNP P26231
A	-2	MET	-	expression tag	UNP P26231
A	-1	ALA	-	expression tag	UNP P26231
A	0	SER	-	expression tag	UNP P26231
B	-5	GLY	-	expression tag	UNP P26231
B	-4	SER	-	expression tag	UNP P26231
B	-3	HIS	-	expression tag	UNP P26231
B	-2	MET	-	expression tag	UNP P26231
B	-1	ALA	-	expression tag	UNP P26231
B	0	SER	-	expression tag	UNP P26231

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: Catenin alpha-1



MET	ILE	TYR	MET
MET	ALA	GLN	ASP
LEU	LEU	LYS	SER
MET	TYR	SER	ILE
THR	CYS	GLN	GLY
ASP	HIS	GLY	MET
PHE	GLN	MET	ALA
THR	LEU	SER	SER
ARG	ASN	LEU	LEU
GLY	ILE	ASN	ASN
LYS	CYS	LEU	PRO
GLY	SER	LEU	ALA
PRO	LYS	PRO	VAL
LEU	VAL	VAL	VAL
LYS	LYS	SER	SER
ASN	ALA	THR	THR
THR	GLU	TRP	LYS
SER	VAL	LYS	MET
ASP	GLN	MET	LYS
VAL	ASN	LYS	ALA
ILE	LEU	ALA	PRO
ALA	GLY	SER	GLY
GLY	GLY	GLU	LYS
ALA	ALA	LYS	PRO
LYS	LEU	LYS	LEU
LYS	VAL	PRO	VAL
ILE	VAL	LEU	VAL
ALA	SER	VAL	LYS
GLY	GLY	ARG	ARG
VAL	VAL	GLY	LYS
ASP	ASP	SER	GLN
SER	SER	GLN	THR
ARG	ALA	ASN	LYS
MET	LEU	ALA	ILE
ASP	LYS	ARG	LYS
THR	ILE	ALA	THR
LEU	GLY	LYS	ILE
GLY	ARG	LYS	ARG
ASP	ALA	ALA	SER
HIS	ASP	SER	GLN
CYS	HIS	GLN	LYS
PRO	CYS	ASN	LYS
ASP	PRO	VAL	HIS
THR	VAL	THR	ASN
ALA	THR	VAL	PRO
LYS	LYS	VAL	VAL
GLN	GLN	ALA	GLN
ASP	ASP	ALA	ALA
LEU	LEU	TYR	LEU
ALA	VAL	VAL	SER
TYR	ALA	ALA	GLU
LEU	SER	THR	PHE
GLN	THR	LYS	LYS
ARG	ARG	LYS	ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	144.68Å 144.68Å 136.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 6.50 50.00 – 6.50	Depositor EDS
% Data completeness (in resolution range)	94.6 (50.00-6.50) 94.4 (50.00-6.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.84 (at 6.67Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.247 0.224 , 0.246	Depositor DCC
R_{free} test set	716 reflections (10.90%)	wwPDB-VP
Wilson B-factor (Å ²)	439.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 459.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l 0.051 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8020	wwPDB-VP
Average B, all atoms (Å ²)	354.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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](#)

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	0.29	0/4048	0.80	5/5464 (0.1%)
1	B	0.29	0/4048	0.80	4/5464 (0.1%)
All	All	0.29	0/8096	0.80	9/10928 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	ILE	N-CA-C	-6.01	106.64	111.81
1	B	368	ILE	N-CA-C	-5.95	106.69	111.81
1	B	302	ARG	CA-C-N	5.42	126.62	119.84
1	B	302	ARG	C-N-CA	5.42	126.62	119.84
1	A	302	ARG	CA-C-N	5.38	126.56	119.84
1	A	302	ARG	C-N-CA	5.38	126.56	119.84
1	A	217	ASN	N-CA-C	5.32	117.16	111.36
1	A	341	ARG	N-CA-C	-5.24	105.65	111.36
1	B	341	ARG	N-CA-C	-5.18	105.72	111.36

There are no chirality outliers.

There are no planarity outliers.

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	4010	0	4051	357	0
1	B	4010	0	4051	366	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8020	0	8102	706	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

All (706) 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:369:ASP:O	1:A:373:LYS:HB3	1.65	0.97
1:A:104:MET:HG2	1:A:131:LEU:HD22	1.48	0.96
1:A:209:ALA:HB1	1:A:452:MET:HE2	1.44	0.96
1:B:86:LEU:HD22	1:B:87:LYS:H	1.31	0.95
1:B:104:MET:HG2	1:B:131:LEU:HD22	1.48	0.93
1:A:451:ARG:HH12	1:B:308:ARG:HG3	1.35	0.92
1:B:208:ALA:HB3	1:B:448:LYS:NZ	1.84	0.91
1:A:86:LEU:HD22	1:A:87:LYS:H	1.34	0.90
1:A:519:ILE:HG12	1:A:548:ARG:HD2	1.55	0.86
1:B:519:ILE:HG12	1:B:548:ARG:HD2	1.57	0.85
1:A:399:VAL:HG12	1:A:400:PRO:HD3	1.59	0.85
1:A:291:VAL:HG22	1:A:292:ASP:H	1.41	0.85
1:B:243:LEU:HD12	1:B:466:ASN:HD21	1.40	0.84
1:B:174:GLY:O	1:B:178:LYS:HG3	1.78	0.83
1:B:546:ARG:HA	1:B:584:MET:HE2	1.58	0.83
1:A:395:LEU:HD22	1:A:547:GLY:HA2	1.61	0.83
1:B:399:VAL:HG12	1:B:400:PRO:HD3	1.59	0.83
1:A:347:LEU:HB2	1:A:372:THR:OG1	1.80	0.81
1:A:546:ARG:HA	1:A:584:MET:HE2	1.60	0.81
1:B:347:LEU:HB2	1:B:372:THR:OG1	1.80	0.81
1:B:369:ASP:O	1:B:373:LYS:HB3	1.80	0.81
1:B:231:HIS:NE2	1:B:479:LEU:HD13	1.96	0.81
1:A:444:GLU:O	1:A:447:VAL:HG12	1.80	0.81
1:B:291:VAL:HG22	1:B:292:ASP:H	1.43	0.81
1:A:174:GLY:O	1:A:178:LYS:HG3	1.81	0.80
1:A:502:VAL:O	1:A:505:ILE:HG22	1.81	0.80
1:B:329:ARG:NH2	1:B:389:HIS:HB2	1.97	0.80
1:B:502:VAL:O	1:B:505:ILE:HG22	1.81	0.80
1:A:387:MET:HE2	1:A:506:THR:HB	1.62	0.80
1:B:89:GLU:C	1:B:141:LEU:HD11	2.07	0.79
1:A:89:GLU:C	1:A:141:LEU:HD11	2.08	0.79
1:A:149:LYS:HG2	1:A:190:MET:HE1	1.66	0.78
1:B:444:GLU:O	1:B:447:VAL:HG12	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HD12	1:A:187:LEU:HD21	1.65	0.78
1:B:154:LEU:HD12	1:B:187:LEU:HD21	1.65	0.78
1:A:354:ASN:HA	1:A:358:LYS:HD2	1.66	0.78
1:A:601:ASP:HB3	1:A:602:PRO:HD2	1.65	0.78
1:A:149:LYS:HZ3	1:A:190:MET:HE2	1.47	0.77
1:B:208:ALA:HB3	1:B:448:LYS:HZ3	1.50	0.77
1:B:302:ARG:HE	1:B:309:LEU:HD11	1.48	0.77
1:A:290:ILE:HG13	1:B:308:ARG:NH2	1.99	0.77
1:A:550:ALA:O	1:A:553:ILE:HG13	1.85	0.77
1:B:149:LYS:HG2	1:B:190:MET:HE1	1.67	0.77
1:A:201:VAL:HA	1:A:204:ARG:HD3	1.68	0.76
1:B:601:ASP:HB3	1:B:602:PRO:HD2	1.65	0.76
1:A:329:ARG:NH2	1:A:389:HIS:HB2	2.00	0.76
1:B:542:ALA:HA	1:B:545:ILE:HD12	1.68	0.76
1:B:354:ASN:HA	1:B:358:LYS:HD2	1.68	0.75
1:B:550:ALA:O	1:B:553:ILE:HG13	1.87	0.75
1:A:90:LEU:HD11	1:B:124:MET:HE1	1.68	0.74
1:B:149:LYS:HZ3	1:B:190:MET:HE2	1.51	0.74
1:A:161:ILE:HD13	1:A:180:LEU:HD21	1.70	0.73
1:B:168:GLY:O	1:B:229:LEU:HD22	1.88	0.73
1:A:614:ALA:HA	1:A:617:LEU:HD12	1.69	0.73
1:A:302:ARG:HE	1:A:309:LEU:HD11	1.53	0.73
1:A:542:ALA:HA	1:A:545:ILE:HD12	1.71	0.72
1:B:292:ASP:CG	1:B:293:PRO:HD3	2.15	0.72
1:B:161:ILE:HD13	1:B:180:LEU:HD21	1.72	0.72
1:B:614:ALA:HA	1:B:617:LEU:HD12	1.71	0.72
1:A:292:ASP:CG	1:A:293:PRO:HD3	2.15	0.72
1:B:387:MET:HE2	1:B:506:THR:HB	1.71	0.72
1:B:391:SER:HB3	1:B:548:ARG:HG3	1.71	0.72
1:A:347:LEU:HD22	1:A:372:THR:HG23	1.72	0.72
1:B:234:VAL:HG22	1:B:474:LYS:HZ1	1.55	0.71
1:A:89:GLU:HB3	1:A:141:LEU:HG	1.72	0.71
1:A:291:VAL:HB	1:A:442:ASN:HA	1.72	0.71
1:A:350:GLU:C	1:A:368:ILE:HD11	2.16	0.70
1:B:86:LEU:CD2	1:B:87:LYS:H	2.05	0.69
1:B:291:VAL:HB	1:B:442:ASN:HA	1.72	0.69
1:B:351:TYR:HB2	1:B:368:ILE:HG12	1.74	0.69
1:A:508:ILE:HD13	1:A:555:VAL:HG12	1.75	0.69
1:B:519:ILE:HD11	1:B:548:ARG:HB3	1.75	0.69
1:A:218:VAL:HB	1:A:219:PRO:HD3	1.75	0.69
1:B:350:GLU:C	1:B:368:ILE:HD11	2.17	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:LEU:HD22	1:B:547:GLY:HA2	1.74	0.69
1:B:89:GLU:HB3	1:B:141:LEU:HG	1.74	0.69
1:B:198:LEU:HD22	1:B:261:ALA:HB3	1.75	0.69
1:A:395:LEU:HD13	1:A:547:GLY:O	1.92	0.68
1:A:451:ARG:HH12	1:B:308:ARG:CG	2.07	0.68
1:B:508:ILE:HD13	1:B:555:VAL:HG12	1.74	0.68
1:A:86:LEU:CD2	1:A:87:LYS:H	2.07	0.68
1:B:467:ALA:C	1:B:484:MET:HE1	2.19	0.68
1:A:440:ILE:O	1:A:441:SER:HB2	1.94	0.68
1:B:329:ARG:NH1	1:B:389:HIS:N	2.42	0.68
1:B:218:VAL:HB	1:B:219:PRO:HD3	1.74	0.67
1:A:220:ILE:HG22	1:A:244:ILE:HD13	1.76	0.67
1:B:194:ARG:O	1:B:198:LEU:HG	1.93	0.67
1:B:205:ASP:HA	1:B:448:LYS:HZ2	1.60	0.67
1:A:291:VAL:HG22	1:A:293:PRO:HD2	1.76	0.67
1:A:375:THR:C	1:A:377:ASP:H	2.03	0.67
1:B:201:VAL:HA	1:B:204:ARG:HD3	1.77	0.66
1:B:347:LEU:HD22	1:B:372:THR:HG23	1.77	0.66
1:A:412:ASN:OD1	1:A:414:LYS:HG3	1.96	0.66
1:A:85:PHE:N	1:A:88:GLU:HG3	2.11	0.66
1:A:351:TYR:HB2	1:A:368:ILE:HG12	1.77	0.66
1:A:391:SER:HB3	1:A:548:ARG:HG3	1.77	0.66
1:B:205:ASP:HA	1:B:448:LYS:NZ	2.10	0.66
1:B:340:VAL:HG21	1:B:378:LEU:CB	2.26	0.66
1:A:468:ALA:N	1:A:484:MET:HE1	2.12	0.65
1:B:114:ASP:HB3	1:B:120:LYS:HD2	1.78	0.65
1:B:93:ALA:HB2	1:B:141:LEU:HD12	1.77	0.65
1:A:194:ARG:O	1:A:198:LEU:HG	1.96	0.65
1:A:390:VAL:HA	1:A:394:PHE:CD2	2.31	0.65
1:A:379:ARG:O	1:A:383:ARG:HG3	1.96	0.65
1:B:440:ILE:O	1:B:441:SER:HB2	1.94	0.65
1:B:291:VAL:HG22	1:B:293:PRO:HD2	1.77	0.65
1:B:86:LEU:HD12	1:B:86:LEU:H	1.60	0.65
1:B:343:ALA:HB1	1:B:375:THR:HG21	1.79	0.65
1:B:468:ALA:N	1:B:484:MET:HE1	2.11	0.65
1:B:375:THR:C	1:B:377:ASP:H	2.03	0.64
1:A:168:GLY:O	1:A:229:LEU:HD22	1.97	0.64
1:B:566:GLY:O	1:B:570:GLU:HG2	1.98	0.64
1:A:340:VAL:HG21	1:A:378:LEU:CB	2.28	0.64
1:B:302:ARG:CZ	1:B:305:LEU:HD11	2.27	0.64
1:B:412:ASN:OD1	1:B:414:LYS:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ALA:HB2	1:A:141:LEU:HD12	1.80	0.64
1:A:93:ALA:HB2	1:A:137:ARG:NH1	2.13	0.64
1:A:198:LEU:HD22	1:A:261:ALA:HB3	1.79	0.63
1:B:93:ALA:HB2	1:B:137:ARG:NH1	2.13	0.63
1:B:351:TYR:N	1:B:368:ILE:HD11	2.13	0.63
1:B:220:ILE:HG22	1:B:244:ILE:HD13	1.78	0.63
1:A:86:LEU:HD12	1:A:86:LEU:H	1.62	0.63
1:A:290:ILE:HG13	1:B:308:ARG:HH21	1.63	0.63
1:A:625:ILE:O	1:A:629:VAL:HG23	1.99	0.63
1:B:291:VAL:HG11	1:B:294:LEU:HB3	1.81	0.63
1:A:97:VAL:HA	1:A:134:ALA:HB1	1.79	0.63
1:A:114:ASP:HB3	1:A:120:LYS:HD2	1.80	0.63
1:A:227:ALA:HB2	1:A:479:LEU:HD21	1.80	0.63
1:A:463:GLN:HB3	1:A:487:PHE:CZ	2.33	0.63
1:A:90:LEU:O	1:A:94:VAL:HG23	1.99	0.63
1:A:198:LEU:HA	1:A:262:THR:HG22	1.81	0.63
1:A:519:ILE:HD11	1:A:548:ARG:HB3	1.79	0.63
1:B:463:GLN:HB3	1:B:487:PHE:CZ	2.34	0.62
1:A:351:TYR:N	1:A:368:ILE:HD11	2.14	0.62
1:A:457:LEU:HD13	1:A:494:GLN:HB3	1.81	0.62
1:B:625:ILE:O	1:B:629:VAL:HG23	1.98	0.62
1:A:90:LEU:N	1:A:141:LEU:HD11	2.13	0.62
1:A:247:GLN:HE22	1:A:463:GLN:NE2	1.96	0.62
1:A:601:ASP:CB	1:A:602:PRO:HD2	2.29	0.62
1:A:467:ALA:C	1:A:484:MET:HE1	2.24	0.62
1:B:97:VAL:HA	1:B:134:ALA:HB1	1.81	0.62
1:B:362:ASP:O	1:B:366:SER:HB2	1.99	0.62
1:B:587:PHE:O	1:B:591:VAL:HG23	1.99	0.62
1:A:389:HIS:HD1	1:A:394:PHE:HE1	1.46	0.62
1:A:291:VAL:HG11	1:A:294:LEU:HB3	1.82	0.62
1:A:329:ARG:NH1	1:A:389:HIS:N	2.48	0.62
1:B:90:LEU:N	1:B:141:LEU:HD11	2.14	0.62
1:B:440:ILE:O	1:B:440:ILE:HD13	1.99	0.62
1:A:214:LEU:O	1:A:218:VAL:HG23	2.00	0.62
1:B:395:LEU:HD13	1:B:547:GLY:O	2.00	0.62
1:A:362:ASP:O	1:A:366:SER:HB2	2.00	0.61
1:B:302:ARG:HH21	1:B:309:LEU:HG	1.64	0.61
1:B:214:LEU:O	1:B:218:VAL:HG23	2.01	0.61
1:A:343:ALA:HB1	1:A:375:THR:HG21	1.82	0.61
1:B:379:ARG:O	1:B:383:ARG:HG3	2.01	0.61
1:A:408:ALA:HB1	1:A:472:ALA:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:SER:HA	1:B:369:ASP:HB3	1.81	0.60
1:A:344:LEU:HD23	1:A:347:LEU:HD23	1.82	0.60
1:B:198:LEU:HA	1:B:262:THR:HG22	1.83	0.60
1:A:149:LYS:NZ	1:A:190:MET:HE2	2.15	0.60
1:A:159:ASP:HB3	1:A:163:LYS:HE3	1.84	0.60
1:A:302:ARG:CZ	1:A:305:LEU:HD11	2.32	0.60
1:B:601:ASP:CB	1:B:602:PRO:HD2	2.30	0.60
1:B:546:ARG:HA	1:B:584:MET:CE	2.30	0.60
1:B:390:VAL:HA	1:B:394:PHE:CD2	2.35	0.60
1:A:302:ARG:HH21	1:A:309:LEU:HG	1.66	0.60
1:A:347:LEU:HD22	1:A:372:THR:CG2	2.32	0.60
1:A:512:LEU:CD1	1:A:629:VAL:HG21	2.32	0.60
1:B:526:CYS:SG	1:B:538:LEU:HD12	2.42	0.60
1:A:366:SER:HA	1:A:369:ASP:HB3	1.82	0.60
1:A:519:ILE:O	1:A:523:VAL:HG23	2.02	0.60
1:A:468:ALA:HA	1:A:484:MET:HE1	1.85	0.59
1:A:498:LEU:O	1:A:502:VAL:HG23	2.02	0.59
1:B:149:LYS:NZ	1:B:190:MET:HE2	2.16	0.59
1:B:207:MET:HG2	1:B:258:ALA:CB	2.32	0.59
1:B:302:ARG:HE	1:B:309:LEU:CD1	2.15	0.59
1:B:207:MET:O	1:B:211:ARG:HG3	2.03	0.59
1:A:405:ILE:HG22	1:A:409:LYS:HE3	1.84	0.58
1:A:314:SER:O	1:A:318:LEU:HD13	2.03	0.58
1:A:325:THR:HB	1:A:329:ARG:HE	1.67	0.58
1:A:207:MET:HG2	1:A:258:ALA:HB3	1.86	0.58
1:A:404:LEU:C	1:A:404:LEU:HD13	2.29	0.58
1:B:344:LEU:HD23	1:B:347:LEU:HD23	1.84	0.58
1:A:207:MET:HG2	1:A:258:ALA:CB	2.33	0.58
1:B:89:GLU:HB3	1:B:141:LEU:CG	2.33	0.58
1:A:159:ASP:O	1:A:163:LYS:HG3	2.03	0.58
1:A:209:ALA:CB	1:A:452:MET:HE2	2.27	0.58
1:B:291:VAL:HG13	1:B:292:ASP:N	2.18	0.58
1:A:153:GLN:HG3	1:A:187:LEU:HB2	1.85	0.58
1:B:329:ARG:HH22	1:B:389:HIS:HB2	1.67	0.58
1:B:325:THR:HB	1:B:329:ARG:HE	1.69	0.58
1:B:208:ALA:HB3	1:B:448:LYS:HZ1	1.67	0.57
1:B:498:LEU:O	1:B:502:VAL:HG23	2.04	0.57
1:B:530:LEU:HD22	1:B:611:PHE:CG	2.38	0.57
1:B:408:ALA:HB1	1:B:472:ALA:N	2.19	0.57
1:A:545:ILE:HG22	1:A:584:MET:HE1	1.86	0.57
1:B:601:ASP:HB3	1:B:602:PRO:CD	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:GLY:O	1:A:570:GLU:HG2	2.04	0.57
1:B:512:LEU:CD1	1:B:629:VAL:HG21	2.34	0.57
1:A:89:GLU:HB3	1:A:141:LEU:CG	2.35	0.57
1:A:412:ASN:HD21	1:A:414:LYS:HE3	1.69	0.57
1:A:587:PHE:O	1:A:591:VAL:HG23	2.04	0.57
1:B:207:MET:HG2	1:B:258:ALA:HB3	1.87	0.57
1:A:207:MET:O	1:A:211:ARG:HG3	2.05	0.57
1:A:601:ASP:HB3	1:A:602:PRO:CD	2.34	0.56
1:B:159:ASP:HB3	1:B:163:LYS:HE3	1.87	0.56
1:B:412:ASN:HD21	1:B:414:LYS:HE3	1.70	0.56
1:A:499:THR:HG23	1:A:551:ARG:NH2	2.19	0.56
1:B:159:ASP:O	1:B:163:LYS:HG3	2.05	0.56
1:A:121:ARG:NH2	1:B:145:ALA:HB1	2.20	0.56
1:A:397:THR:O	1:A:400:PRO:HD2	2.06	0.56
1:B:457:LEU:HD13	1:B:494:GLN:HB3	1.87	0.56
1:A:395:LEU:C	1:A:397:THR:H	2.13	0.56
1:A:457:LEU:HD23	1:A:498:LEU:HD22	1.87	0.56
1:B:391:SER:CB	1:B:548:ARG:HG3	2.36	0.56
1:A:491:TRP:O	1:A:495:VAL:HG23	2.06	0.56
1:B:375:THR:C	1:B:377:ASP:N	2.63	0.56
1:A:173:LEU:HG	1:A:222:TYR:CE1	2.41	0.56
1:A:291:VAL:HG22	1:A:292:ASP:N	2.16	0.56
1:A:291:VAL:HG13	1:A:292:ASP:N	2.20	0.56
1:A:375:THR:HA	1:A:377:ASP:OD1	2.06	0.56
1:B:468:ALA:HA	1:B:484:MET:HE1	1.86	0.56
1:B:90:LEU:O	1:B:94:VAL:HG23	2.06	0.56
1:B:499:THR:HG23	1:B:551:ARG:NH2	2.20	0.56
1:B:519:ILE:O	1:B:523:VAL:HG23	2.06	0.56
1:A:375:THR:C	1:A:377:ASP:N	2.62	0.55
1:A:416:VAL:HG21	1:A:472:ALA:HB2	1.87	0.55
1:B:325:THR:CG2	1:B:329:ARG:HE	2.20	0.55
1:B:329:ARG:HH11	1:B:388:ASP:HB2	1.70	0.55
1:B:191:ALA:HB1	1:B:211:ARG:HD2	1.87	0.55
1:B:302:ARG:NE	1:B:309:LEU:HD11	2.18	0.55
1:A:440:ILE:O	1:A:440:ILE:HD13	2.07	0.55
1:A:526:CYS:SG	1:A:538:LEU:HD12	2.46	0.55
1:A:552:VAL:O	1:A:556:VAL:HG23	2.06	0.55
1:B:291:VAL:HG22	1:B:292:ASP:N	2.18	0.55
1:B:347:LEU:HD22	1:B:372:THR:CG2	2.35	0.55
1:B:387:MET:O	1:B:390:VAL:HG23	2.07	0.55
1:B:395:LEU:C	1:B:397:THR:H	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:VAL:HG21	1:B:472:ALA:HB2	1.88	0.55
1:B:583:VAL:HG13	1:B:617:LEU:CB	2.36	0.55
1:A:329:ARG:HH22	1:A:389:HIS:HB2	1.72	0.55
1:B:397:THR:O	1:B:400:PRO:HD2	2.06	0.55
1:B:404:LEU:HD13	1:B:404:LEU:C	2.32	0.55
1:B:153:GLN:HG3	1:B:187:LEU:HB2	1.88	0.55
1:B:543:GLY:HA2	1:B:546:ARG:NH1	2.22	0.55
1:A:181:LYS:N	1:A:182:PRO:HD2	2.22	0.55
1:A:302:ARG:NE	1:A:309:LEU:HD11	2.22	0.55
1:A:390:VAL:HA	1:A:394:PHE:CE2	2.42	0.55
1:B:403:VAL:HG21	1:B:419:TYR:OH	2.06	0.55
1:B:491:TRP:O	1:B:495:VAL:HG23	2.06	0.55
1:B:85:PHE:N	1:B:88:GLU:HG3	2.22	0.55
1:A:191:ALA:HB1	1:A:211:ARG:HD2	1.88	0.54
1:A:551:ARG:O	1:A:555:VAL:HG23	2.07	0.54
1:B:328:ASP:O	1:B:332:ARG:HG3	2.06	0.54
1:A:325:THR:CG2	1:A:329:ARG:HE	2.20	0.54
1:A:517:ASN:O	1:A:520:LEU:HB3	2.07	0.54
1:B:131:LEU:O	1:B:135:VAL:HG23	2.07	0.54
1:B:181:LYS:N	1:B:182:PRO:HD2	2.22	0.54
1:A:131:LEU:O	1:A:135:VAL:HG23	2.08	0.54
1:B:203:ASN:HA	1:B:206:GLN:NE2	2.23	0.54
1:A:530:LEU:HD22	1:A:611:PHE:CG	2.42	0.54
1:A:203:ASN:HA	1:A:206:GLN:NE2	2.23	0.54
1:A:302:ARG:HE	1:A:309:LEU:CD1	2.20	0.54
1:A:329:ARG:HH11	1:A:388:ASP:HB2	1.73	0.54
1:A:388:ASP:OD2	1:A:388:ASP:N	2.41	0.54
1:B:461:CYS:N	1:B:462:PRO:HD2	2.22	0.54
1:A:461:CYS:N	1:A:462:PRO:HD2	2.22	0.54
1:A:389:HIS:ND1	1:A:394:PHE:HE1	2.06	0.54
1:B:319:MET:SD	1:B:319:MET:N	2.81	0.54
1:A:194:ARG:HD2	1:A:197:GLU:OE1	2.08	0.54
1:A:319:MET:SD	1:A:319:MET:N	2.81	0.54
1:B:468:ALA:CA	1:B:484:MET:HE1	2.38	0.53
1:B:545:ILE:HG22	1:B:584:MET:HE1	1.89	0.53
1:A:209:ALA:HB1	1:A:452:MET:CE	2.30	0.53
1:A:457:LEU:HD23	1:A:498:LEU:CD2	2.38	0.53
1:B:194:ARG:HD2	1:B:197:GLU:OE1	2.08	0.53
1:B:389:HIS:ND1	1:B:394:PHE:HE1	2.06	0.53
1:B:388:ASP:OD2	1:B:388:ASP:N	2.40	0.53
1:B:214:LEU:HA	1:B:248:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:VAL:HG13	1:B:108:ALA:HB1	1.89	0.53
1:B:209:ALA:HA	1:B:452:MET:SD	2.49	0.53
1:B:375:THR:HA	1:B:377:ASP:OD1	2.09	0.53
1:A:191:ALA:HB1	1:A:207:MET:HE1	1.90	0.53
1:A:387:MET:O	1:A:390:VAL:HG23	2.09	0.53
1:A:300:ARG:O	1:A:301:PHE:HB2	2.08	0.53
1:A:368:ILE:HD12	1:A:368:ILE:N	2.24	0.53
1:B:234:VAL:HG13	1:B:474:LYS:HZ1	1.74	0.53
1:A:390:VAL:HA	1:A:394:PHE:CG	2.43	0.53
1:A:468:ALA:CA	1:A:484:MET:HE1	2.38	0.53
1:A:398:ASN:O	1:A:402:LEU:HD22	2.08	0.52
1:B:173:LEU:HG	1:B:222:TYR:CE1	2.44	0.52
1:B:243:LEU:HD13	1:B:462:PRO:HB2	1.90	0.52
1:B:314:SER:O	1:B:318:LEU:HD13	2.09	0.52
1:B:357:ARG:NH1	1:B:358:LYS:HE3	2.23	0.52
1:B:373:LYS:HA	1:B:376:ARG:NE	2.24	0.52
1:B:390:VAL:HA	1:B:394:PHE:CG	2.45	0.52
1:B:457:LEU:HD13	1:B:494:GLN:HG3	1.91	0.52
1:A:87:LYS:NZ	1:B:116:CYS:HA	2.25	0.52
1:A:96:ASP:O	1:A:100:GLN:HG2	2.09	0.52
1:A:350:GLU:HB3	1:A:368:ILE:CD1	2.39	0.52
1:A:149:LYS:HZ3	1:A:190:MET:CE	2.22	0.52
1:A:357:ARG:NH1	1:A:358:LYS:HE3	2.25	0.52
1:A:395:LEU:HD22	1:A:547:GLY:CA	2.38	0.52
1:B:158:GLU:HG2	1:B:252:VAL:HG11	1.91	0.52
1:A:628:ALA:O	1:A:631:MET:HG3	2.10	0.52
1:B:149:LYS:HG2	1:B:190:MET:CE	2.38	0.52
1:B:350:GLU:HB3	1:B:368:ILE:CD1	2.40	0.52
1:A:214:LEU:HA	1:A:248:LEU:HD12	1.91	0.51
1:B:217:ASN:HB2	1:B:248:LEU:HD13	1.92	0.51
1:A:149:LYS:HG2	1:A:190:MET:CE	2.36	0.51
1:B:457:LEU:HD21	1:B:495:VAL:HA	1.93	0.51
1:A:583:VAL:HG13	1:A:617:LEU:CB	2.41	0.51
1:B:88:GLU:O	1:B:92:VAL:HG23	2.11	0.51
1:B:398:ASN:O	1:B:402:LEU:HD22	2.11	0.51
1:A:375:THR:O	1:A:377:ASP:N	2.43	0.51
1:B:300:ARG:O	1:B:301:PHE:HB2	2.11	0.51
1:B:517:ASN:O	1:B:520:LEU:HB3	2.11	0.51
1:A:543:GLY:HA2	1:A:546:ARG:NH1	2.26	0.51
1:B:518:HIS:HB3	1:B:548:ARG:CZ	2.40	0.51
1:A:451:ARG:NH1	1:B:308:ARG:HG3	2.16	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LEU:HD21	1:A:556:VAL:CG2	2.41	0.51
1:B:343:ALA:CB	1:B:375:THR:HG21	2.41	0.51
1:A:433:VAL:HA	1:A:436:LEU:HD12	1.92	0.50
1:B:86:LEU:HD22	1:B:87:LYS:N	2.14	0.50
1:A:594:ALA:HA	1:A:606:MET:SD	2.52	0.50
1:B:383:ARG:C	1:B:385:ALA:H	2.18	0.50
1:B:389:HIS:HE2	1:B:429:LYS:HE2	1.75	0.50
1:B:390:VAL:HA	1:B:394:PHE:CE2	2.45	0.50
1:B:463:GLN:HB3	1:B:487:PHE:CE1	2.47	0.50
1:B:350:GLU:CD	1:B:367:ALA:HB1	2.36	0.50
1:A:343:ALA:CB	1:A:375:THR:HG21	2.40	0.50
1:A:425:GLU:O	1:A:428:ASN:OD1	2.29	0.50
1:A:530:LEU:HD22	1:A:611:PHE:CD1	2.46	0.50
1:B:350:GLU:HB3	1:B:368:ILE:HD11	1.94	0.50
1:A:463:GLN:HB3	1:A:487:PHE:CE1	2.46	0.50
1:B:194:ARG:NH2	1:B:259:ALA:O	2.44	0.50
1:A:457:LEU:HD21	1:A:495:VAL:HA	1.93	0.50
1:A:291:VAL:HB	1:A:442:ASN:CA	2.39	0.50
1:A:374:LYS:O	1:A:377:ASP:OD1	2.29	0.50
1:A:328:ASP:O	1:A:332:ARG:HG3	2.11	0.50
1:A:518:HIS:HB3	1:A:548:ARG:CZ	2.42	0.50
1:B:90:LEU:HA	1:B:141:LEU:CD1	2.42	0.50
1:B:394:PHE:HD2	1:B:551:ARG:HH21	1.59	0.50
1:B:628:ALA:CA	1:B:631:MET:HE2	2.42	0.50
1:B:171:GLN:O	1:B:175:ILE:HG13	2.12	0.49
1:B:400:PRO:HB2	1:B:423:PHE:HA	1.94	0.49
1:B:512:LEU:HD21	1:B:556:VAL:CG2	2.41	0.49
1:A:153:GLN:NE2	1:A:183:GLU:HA	2.28	0.49
1:A:393:SER:C	1:A:394:PHE:HD1	2.19	0.49
1:B:291:VAL:HB	1:B:442:ASN:CA	2.39	0.49
1:B:368:ILE:N	1:B:368:ILE:HD12	2.27	0.49
1:B:375:THR:O	1:B:377:ASP:N	2.45	0.49
1:B:628:ALA:O	1:B:631:MET:HG3	2.12	0.49
1:A:213:ILE:HG23	1:A:217:ASN:ND2	2.27	0.49
1:A:346:ASP:O	1:A:350:GLU:HB2	2.11	0.49
1:A:443:ASN:OD1	1:A:446:GLY:N	2.39	0.49
1:B:191:ALA:HB1	1:B:207:MET:HE1	1.93	0.49
1:B:247:GLN:OE1	1:B:459:ALA:HB1	2.11	0.49
1:A:400:PRO:HB2	1:A:423:PHE:HA	1.94	0.49
1:B:346:ASP:O	1:B:350:GLU:HB2	2.12	0.49
1:A:290:ILE:N	1:B:308:ARG:CZ	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ARG:HH12	1:B:389:HIS:H	1.60	0.49
1:B:457:LEU:HD23	1:B:498:LEU:HD22	1.94	0.49
1:A:90:LEU:HA	1:A:141:LEU:CD1	2.42	0.49
1:A:350:GLU:HB3	1:A:368:ILE:HD11	1.94	0.49
1:A:217:ASN:HB2	1:A:248:LEU:HD13	1.94	0.49
1:A:395:LEU:CD1	1:A:550:ALA:HB3	2.43	0.49
1:B:560:MET:SD	1:B:572:VAL:HG11	2.52	0.49
1:B:457:LEU:CD2	1:B:495:VAL:HA	2.43	0.49
1:A:291:VAL:HG22	1:A:293:PRO:CD	2.43	0.49
1:A:403:VAL:HG21	1:A:419:TYR:OH	2.13	0.49
1:A:90:LEU:HA	1:A:141:LEU:HD11	1.95	0.48
1:B:234:VAL:HG13	1:B:474:LYS:NZ	2.27	0.48
1:B:457:LEU:HD23	1:B:498:LEU:CD2	2.43	0.48
1:B:505:ILE:HG23	1:B:506:THR:HG23	1.94	0.48
1:A:373:LYS:O	1:A:373:LYS:HG3	2.13	0.48
1:B:347:LEU:HD13	1:B:368:ILE:HG23	1.95	0.48
1:B:594:ALA:HA	1:B:606:MET:SD	2.53	0.48
1:A:351:TYR:O	1:A:353:GLY:N	2.44	0.48
1:A:373:LYS:HA	1:A:376:ARG:NE	2.27	0.48
1:A:505:ILE:HG23	1:A:506:THR:HG23	1.96	0.48
1:B:329:ARG:NH1	1:B:389:HIS:H	2.11	0.48
1:B:516:GLU:OE1	1:B:623:ARG:HG2	2.14	0.48
1:A:94:VAL:CG1	1:B:108:ALA:HB1	2.44	0.48
1:A:303:PRO:HD3	1:A:359:GLU:OE2	2.14	0.48
1:A:391:SER:CB	1:A:548:ARG:HG3	2.43	0.48
1:A:457:LEU:CD2	1:A:495:VAL:HA	2.44	0.48
1:B:90:LEU:HA	1:B:141:LEU:HD11	1.95	0.48
1:A:394:PHE:HD2	1:A:551:ARG:HH21	1.61	0.48
1:A:438:CYS:SG	1:A:447:VAL:HG23	2.54	0.48
1:B:96:ASP:O	1:B:100:GLN:HG2	2.13	0.48
1:A:325:THR:HB	1:A:329:ARG:NE	2.29	0.48
1:B:203:ASN:ND2	1:B:261:ALA:HB1	2.29	0.48
1:B:393:SER:C	1:B:394:PHE:HD1	2.21	0.48
1:B:552:VAL:O	1:B:556:VAL:HG23	2.12	0.48
1:A:158:GLU:HG2	1:A:252:VAL:HG11	1.95	0.48
1:A:194:ARG:NH2	1:A:259:ALA:O	2.46	0.48
1:B:234:VAL:CG2	1:B:474:LYS:HZ1	2.25	0.48
1:A:145:ALA:CB	1:B:121:ARG:NH2	2.77	0.48
1:A:330:ARG:O	1:A:334:VAL:HG23	2.13	0.48
1:B:628:ALA:HA	1:B:631:MET:HE2	1.94	0.48
1:A:398:ASN:C	1:A:402:LEU:HD22	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:PRO:O	1:A:603:ALA:HB2	2.14	0.48
1:B:93:ALA:CB	1:B:138:LEU:HD13	2.44	0.48
1:B:443:ASN:OD1	1:B:446:GLY:N	2.41	0.48
1:A:153:GLN:HE22	1:A:183:GLU:HA	1.79	0.47
1:A:325:THR:CB	1:A:329:ARG:HE	2.27	0.47
1:B:519:ILE:CD1	1:B:548:ARG:HB3	2.43	0.47
1:B:583:VAL:HG13	1:B:617:LEU:HB2	1.96	0.47
1:A:161:ILE:HD12	1:A:248:LEU:CD2	2.44	0.47
1:A:467:ALA:HB2	1:A:487:PHE:HD2	1.80	0.47
1:B:240:ASN:HA	1:B:466:ASN:ND2	2.29	0.47
1:B:551:ARG:O	1:B:555:VAL:HG23	2.14	0.47
1:A:173:LEU:HG	1:A:222:TYR:HE1	1.79	0.47
1:B:157:VAL:O	1:B:161:ILE:HG12	2.14	0.47
1:A:185:ASP:O	1:A:188:ASN:HB3	2.14	0.47
1:A:579:LEU:HA	1:A:583:VAL:HB	1.96	0.47
1:B:457:LEU:HD13	1:B:494:GLN:CG	2.45	0.47
1:A:383:ARG:C	1:A:385:ALA:H	2.21	0.47
1:A:431:ILE:O	1:A:434:ALA:HB3	2.14	0.47
1:B:329:ARG:CZ	1:B:385:ALA:O	2.62	0.47
1:B:535:VAL:HA	1:B:538:LEU:HB3	1.96	0.47
1:B:598:LEU:HA	1:B:603:ALA:HA	1.97	0.47
1:A:292:ASP:OD1	1:A:293:PRO:HD3	2.15	0.47
1:B:325:THR:CB	1:B:329:ARG:HE	2.28	0.47
1:B:611:PHE:CD1	1:B:611:PHE:C	2.93	0.47
1:A:383:ARG:HG2	1:A:440:ILE:CD1	2.45	0.47
1:A:518:HIS:HB3	1:A:548:ARG:NH1	2.30	0.47
1:B:303:PRO:HD3	1:B:359:GLU:OE2	2.15	0.47
1:A:157:VAL:O	1:A:161:ILE:HG12	2.16	0.46
1:A:582:THR:O	1:A:586:ARG:HG2	2.14	0.46
1:B:425:GLU:O	1:B:428:ASN:OD1	2.33	0.46
1:B:457:LEU:HD13	1:B:494:GLN:CB	2.45	0.46
1:A:351:TYR:CB	1:A:368:ILE:HG12	2.45	0.46
1:A:457:LEU:HD13	1:A:494:GLN:HG3	1.97	0.46
1:A:145:ALA:HB1	1:B:121:ARG:NH2	2.30	0.46
1:A:353:GLY:O	1:A:364:LEU:HD23	2.14	0.46
1:A:512:LEU:HD11	1:A:629:VAL:HG21	1.97	0.46
1:B:213:ILE:HG23	1:B:217:ASN:ND2	2.30	0.46
1:B:325:THR:HB	1:B:329:ARG:NE	2.31	0.46
1:B:584:MET:HB3	1:B:585:PRO:HD3	1.97	0.46
1:A:203:ASN:ND2	1:A:261:ALA:HB1	2.30	0.46
1:A:568:TYR:O	1:A:572:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ALA:C	1:B:319:MET:HE1	2.39	0.46
1:A:401:LEU:C	1:A:403:VAL:H	2.23	0.46
1:B:329:ARG:HH11	1:B:388:ASP:CB	2.29	0.46
1:B:399:VAL:HA	1:B:402:LEU:HD21	1.98	0.46
1:B:441:SER:C	1:B:443:ASN:H	2.23	0.46
1:B:185:ASP:O	1:B:188:ASN:HB3	2.15	0.46
1:B:579:LEU:HA	1:B:583:VAL:HB	1.98	0.46
1:A:447:VAL:CG1	1:A:448:LYS:N	2.79	0.46
1:B:85:PHE:N	1:B:85:PHE:CD1	2.83	0.46
1:B:161:ILE:HD12	1:B:248:LEU:CD2	2.45	0.46
1:B:214:LEU:HB2	1:B:251:ALA:HB1	1.98	0.46
1:B:383:ARG:C	1:B:385:ALA:N	2.73	0.46
1:A:93:ALA:O	1:A:97:VAL:HG23	2.16	0.46
1:A:373:LYS:HA	1:A:376:ARG:NH2	2.31	0.46
1:A:395:LEU:C	1:A:397:THR:N	2.74	0.46
1:A:457:LEU:HD13	1:A:494:GLN:CB	2.44	0.46
1:B:153:GLN:NE2	1:B:183:GLU:HA	2.31	0.46
1:B:404:LEU:HD22	1:B:404:LEU:O	2.15	0.46
1:B:412:ASN:OD1	1:B:415:GLU:HG2	2.16	0.46
1:A:86:LEU:HD22	1:A:87:LYS:N	2.16	0.46
1:A:329:ARG:CZ	1:A:385:ALA:O	2.64	0.46
1:A:412:ASN:OD1	1:A:415:GLU:HG2	2.16	0.46
1:B:149:LYS:HZ3	1:B:190:MET:CE	2.25	0.46
1:B:438:CYS:SG	1:B:447:VAL:HG23	2.56	0.46
1:B:556:VAL:O	1:B:560:MET:HG3	2.15	0.46
1:B:602:PRO:O	1:B:603:ALA:HB2	2.15	0.46
1:A:86:LEU:HD13	1:A:87:LYS:N	2.30	0.46
1:A:389:HIS:CB	1:A:433:VAL:HG11	2.46	0.46
1:A:392:ASP:O	1:A:393:SER:HB2	2.16	0.46
1:B:192:ALA:O	1:B:196:GLN:HG3	2.16	0.46
1:B:330:ARG:O	1:B:334:VAL:HG23	2.16	0.46
1:B:446:GLY:O	1:B:450:VAL:HG23	2.16	0.46
1:A:85:PHE:N	1:A:85:PHE:CD1	2.84	0.45
1:A:124:MET:HB3	1:A:124:MET:HE2	1.77	0.45
1:A:350:GLU:CD	1:A:367:ALA:HB1	2.41	0.45
1:A:390:VAL:O	1:A:394:PHE:HB2	2.17	0.45
1:A:583:VAL:HG13	1:A:617:LEU:HB2	1.98	0.45
1:B:124:MET:HE2	1:B:124:MET:HB3	1.77	0.45
1:B:389:HIS:CB	1:B:433:VAL:HG11	2.47	0.45
1:B:398:ASN:C	1:B:402:LEU:HD22	2.40	0.45
1:B:508:ILE:CD1	1:B:555:VAL:HG12	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:SER:O	1:A:121:ARG:HB3	2.15	0.45
1:B:291:VAL:HG22	1:B:293:PRO:CD	2.45	0.45
1:B:351:TYR:CB	1:B:368:ILE:HG12	2.44	0.45
1:A:577:LYS:HG2	1:A:581:ASN:ND2	2.31	0.45
1:B:579:LEU:HD21	1:B:622:ILE:HD13	1.98	0.45
1:B:173:LEU:HG	1:B:222:TYR:HE1	1.81	0.45
1:B:400:PRO:HB2	1:B:423:PHE:HD1	1.81	0.45
1:B:431:ILE:O	1:B:434:ALA:HB3	2.17	0.45
1:A:412:ASN:O	1:A:416:VAL:HG23	2.17	0.45
1:A:447:VAL:HG13	1:A:448:LYS:N	2.32	0.45
1:B:394:PHE:O	1:B:395:LEU:C	2.59	0.45
1:B:395:LEU:C	1:B:397:THR:N	2.74	0.45
1:B:407:ALA:HB1	1:B:415:GLU:HG3	1.98	0.45
1:B:518:HIS:HB3	1:B:548:ARG:NH1	2.31	0.45
1:A:553:ILE:HD12	1:A:554:HIS:N	2.31	0.45
1:B:86:LEU:H	1:B:86:LEU:CD1	2.28	0.45
1:B:583:VAL:HG13	1:B:617:LEU:HB3	1.98	0.45
1:A:360:ARG:HH11	1:A:360:ARG:HG3	1.82	0.45
1:A:394:PHE:O	1:A:396:GLU:N	2.49	0.45
1:B:104:MET:HE3	1:B:108:ALA:HB2	1.99	0.45
1:B:394:PHE:O	1:B:396:GLU:N	2.49	0.45
1:A:237:TYR:CZ	1:A:470:ALA:HB1	2.51	0.45
1:A:399:VAL:HA	1:A:402:LEU:HD21	1.98	0.45
1:A:496:ARG:HG3	1:A:497:VAL:N	2.32	0.45
1:A:612:ILE:O	1:A:616:ARG:HG3	2.17	0.45
1:B:392:ASP:O	1:B:393:SER:HB2	2.16	0.45
1:B:582:THR:O	1:B:586:ARG:HG2	2.17	0.45
1:A:344:LEU:HD23	1:A:347:LEU:CD2	2.46	0.45
1:A:373:LYS:HA	1:A:376:ARG:CZ	2.47	0.45
1:A:383:ARG:C	1:A:385:ALA:N	2.74	0.45
1:A:390:VAL:HG13	1:A:551:ARG:NH2	2.31	0.45
1:B:309:LEU:O	1:B:313:ILE:HG13	2.17	0.45
1:B:530:LEU:HD22	1:B:611:PHE:CD1	2.52	0.45
1:B:542:ALA:CB	1:B:591:VAL:HG11	2.46	0.45
1:A:387:MET:CE	1:A:506:THR:HB	2.42	0.45
1:B:214:LEU:C	1:B:214:LEU:HD23	2.42	0.45
1:B:358:LYS:HB3	1:B:365:ASN:OD1	2.16	0.45
1:A:214:LEU:C	1:A:214:LEU:HD23	2.42	0.44
1:A:316:ALA:C	1:A:319:MET:HE1	2.42	0.44
1:B:86:LEU:CG	1:B:87:LYS:H	2.30	0.44
1:B:374:LYS:O	1:B:377:ASP:OD1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:GLU:O	1:A:92:VAL:HG23	2.17	0.44
1:A:220:ILE:HG22	1:A:244:ILE:CD1	2.46	0.44
1:A:394:PHE:O	1:A:395:LEU:C	2.59	0.44
1:A:583:VAL:HG12	1:A:584:MET:N	2.32	0.44
1:A:598:LEU:HA	1:A:603:ALA:HA	1.97	0.44
1:B:86:LEU:HD13	1:B:87:LYS:N	2.32	0.44
1:B:93:ALA:HA	1:B:137:ARG:NE	2.32	0.44
1:A:90:LEU:CA	1:A:141:LEU:HD11	2.47	0.44
1:A:601:ASP:CB	1:A:602:PRO:CD	2.95	0.44
1:B:577:LYS:HG2	1:B:581:ASN:ND2	2.32	0.44
1:A:186:LYS:HA	1:A:189:ILE:HD12	2.00	0.44
1:B:420:ALA:O	1:B:424:ARG:HB2	2.18	0.44
1:B:583:VAL:HG12	1:B:584:MET:N	2.32	0.44
1:B:290:ILE:HG22	1:B:291:VAL:N	2.33	0.44
1:B:329:ARG:NH1	1:B:385:ALA:O	2.51	0.44
1:B:93:ALA:O	1:B:97:VAL:HG23	2.17	0.44
1:B:423:PHE:CZ	1:B:464:VAL:HG11	2.52	0.44
1:A:290:ILE:HG22	1:A:291:VAL:N	2.33	0.44
1:A:347:LEU:HD13	1:A:368:ILE:HG23	1.98	0.44
1:B:512:LEU:HD11	1:B:629:VAL:HG21	1.99	0.44
1:A:347:LEU:O	1:A:351:TYR:HB2	2.18	0.43
1:A:354:ASN:O	1:A:358:LYS:HB2	2.18	0.43
1:A:586:ARG:HG2	1:A:586:ARG:H	1.54	0.43
1:B:112:ALA:O	1:B:115:PRO:HD3	2.18	0.43
1:B:118:SER:O	1:B:121:ARG:HB3	2.17	0.43
1:B:292:ASP:OD1	1:B:293:PRO:HD3	2.17	0.43
1:B:373:LYS:HA	1:B:376:ARG:CZ	2.48	0.43
1:B:412:ASN:O	1:B:416:VAL:HG23	2.17	0.43
1:B:351:TYR:O	1:B:353:GLY:N	2.48	0.43
1:A:216:LYS:O	1:A:219:PRO:HD2	2.18	0.43
1:A:329:ARG:NH1	1:A:385:ALA:O	2.51	0.43
1:A:497:VAL:HG23	1:A:498:LEU:H	1.82	0.43
1:B:405:ILE:HG22	1:B:409:LYS:HE3	2.00	0.43
1:B:497:VAL:HG23	1:B:498:LEU:H	1.82	0.43
1:B:595:VAL:O	1:B:598:LEU:HD12	2.18	0.43
1:B:601:ASP:CB	1:B:602:PRO:CD	2.96	0.43
1:B:621:GLY:O	1:B:625:ILE:HG13	2.19	0.43
1:A:161:ILE:CD1	1:A:180:LEU:HD21	2.45	0.43
1:A:579:LEU:HD13	1:A:621:GLY:HA3	2.00	0.43
1:B:360:ARG:HG3	1:B:360:ARG:HH11	1.83	0.43
1:A:395:LEU:HD11	1:A:550:ALA:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:ARG:HA	1:A:584:MET:CE	2.40	0.43
1:B:90:LEU:CA	1:B:141:LEU:HD11	2.48	0.43
1:B:237:TYR:OH	1:B:479:LEU:HD22	2.18	0.43
1:A:192:ALA:O	1:A:196:GLN:HG3	2.19	0.43
1:A:516:GLU:OE1	1:A:623:ARG:HG2	2.18	0.43
1:B:93:ALA:HB1	1:B:138:LEU:HD13	2.00	0.43
1:B:153:GLN:HE22	1:B:183:GLU:HA	1.83	0.43
1:B:568:TYR:HE1	1:B:628:ALA:O	2.02	0.43
1:A:93:ALA:HA	1:A:137:ARG:NE	2.33	0.43
1:A:423:PHE:CZ	1:A:464:VAL:HG11	2.54	0.43
1:A:579:LEU:HD21	1:A:622:ILE:HD13	2.00	0.43
1:A:104:MET:HE3	1:A:108:ALA:HB2	2.01	0.43
1:A:304:SER:O	1:A:305:LEU:C	2.62	0.43
1:A:591:VAL:O	1:A:595:VAL:HG23	2.18	0.43
1:B:216:LYS:O	1:B:219:PRO:HD2	2.18	0.43
1:B:243:LEU:O	1:B:247:GLN:HG3	2.19	0.43
1:B:398:ASN:C	1:B:400:PRO:HD2	2.44	0.43
1:B:401:LEU:HD21	1:B:488:LYS:HG3	2.01	0.43
1:A:214:LEU:O	1:A:214:LEU:HD23	2.19	0.43
1:A:398:ASN:C	1:A:400:PRO:HD2	2.44	0.43
1:A:440:ILE:O	1:A:441:SER:CB	2.66	0.43
1:B:591:VAL:O	1:B:595:VAL:HG23	2.18	0.43
1:A:312:ILE:O	1:A:312:ILE:HG22	2.18	0.42
1:A:420:ALA:O	1:A:424:ARG:HB2	2.18	0.42
1:B:214:LEU:O	1:B:214:LEU:HD23	2.19	0.42
1:B:424:ARG:O	1:B:428:ASN:OD1	2.37	0.42
1:B:441:SER:C	1:B:443:ASN:N	2.77	0.42
1:A:154:LEU:O	1:A:158:GLU:HG3	2.18	0.42
1:A:154:LEU:CD1	1:A:187:LEU:HD21	2.41	0.42
1:A:214:LEU:HB2	1:A:251:ALA:HB1	2.01	0.42
1:B:390:VAL:HG13	1:B:551:ARG:NH2	2.33	0.42
1:B:401:LEU:C	1:B:403:VAL:H	2.27	0.42
1:A:85:PHE:CG	1:A:86:LEU:N	2.87	0.42
1:A:308:ARG:NH1	1:B:320:ALA:HB3	2.34	0.42
1:B:86:LEU:CD1	1:B:86:LEU:N	2.82	0.42
1:B:154:LEU:CD1	1:B:187:LEU:HD21	2.45	0.42
1:B:231:HIS:N	1:B:232:PRO:HD3	2.34	0.42
1:A:299:GLU:C	1:A:300:ARG:HG2	2.44	0.42
1:A:621:GLY:O	1:A:625:ILE:HG13	2.18	0.42
1:A:451:ARG:HH12	1:B:308:ARG:CD	2.31	0.42
1:A:467:ALA:HB2	1:A:487:PHE:CD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:VAL:HA	1:B:402:LEU:CD2	2.49	0.42
1:B:538:LEU:HD21	1:B:594:ALA:HB3	2.02	0.42
1:A:424:ARG:O	1:A:428:ASN:OD1	2.37	0.42
1:A:535:VAL:HA	1:A:538:LEU:HB3	2.01	0.42
1:B:329:ARG:HG2	1:B:385:ALA:O	2.20	0.42
1:B:377:ASP:O	1:B:378:LEU:C	2.62	0.42
1:A:230:GLN:NE2	1:A:479:LEU:HD12	2.34	0.42
1:A:388:ASP:OD2	1:A:514:VAL:HG11	2.20	0.42
1:A:441:SER:C	1:A:443:ASN:H	2.28	0.42
1:B:302:ARG:HH21	1:B:309:LEU:CD2	2.33	0.42
1:A:161:ILE:HD12	1:A:248:LEU:HD21	2.01	0.42
1:A:568:TYR:HE1	1:A:628:ALA:O	2.03	0.42
1:B:207:MET:HG2	1:B:258:ALA:HB1	2.01	0.42
1:B:302:ARG:HH21	1:B:309:LEU:CG	2.30	0.42
1:A:86:LEU:N	1:A:86:LEU:CD1	2.82	0.42
1:A:231:HIS:N	1:A:232:PRO:HD3	2.35	0.42
1:A:358:LYS:HB3	1:A:365:ASN:OD1	2.20	0.42
1:A:611:PHE:CD1	1:A:611:PHE:C	2.97	0.42
1:B:329:ARG:HH12	1:B:389:HIS:N	2.13	0.42
1:B:387:MET:CE	1:B:506:THR:HB	2.45	0.42
1:B:447:VAL:CG1	1:B:448:LYS:N	2.81	0.42
1:B:612:ILE:O	1:B:616:ARG:HG3	2.19	0.42
1:A:584:MET:HB3	1:A:585:PRO:HD3	2.02	0.42
1:B:389:HIS:NE2	1:B:429:LYS:HE2	2.34	0.42
1:A:329:ARG:HG2	1:A:385:ALA:O	2.20	0.41
1:A:395:LEU:O	1:A:397:THR:HG22	2.20	0.41
1:A:538:LEU:HD21	1:A:594:ALA:HB3	2.01	0.41
1:B:154:LEU:O	1:B:158:GLU:HG3	2.20	0.41
1:B:353:GLY:O	1:B:364:LEU:HD23	2.20	0.41
1:B:373:LYS:HA	1:B:376:ARG:HE	1.85	0.41
1:B:460:LEU:O	1:B:464:VAL:HG23	2.20	0.41
1:A:336:GLU:OE1	1:A:336:GLU:HA	2.20	0.41
1:A:404:LEU:HD22	1:A:404:LEU:O	2.20	0.41
1:A:454:ALA:N	1:A:498:LEU:HD13	2.35	0.41
1:B:234:VAL:HG22	1:B:474:LYS:NZ	2.31	0.41
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.89	0.41
1:A:508:ILE:HG23	1:A:509:ASP:H	1.85	0.41
1:A:556:VAL:O	1:A:560:MET:HG3	2.21	0.41
1:B:123:ASN:HA	1:B:126:ARG:HH21	1.84	0.41
1:B:304:SER:O	1:B:305:LEU:C	2.63	0.41
1:B:383:ARG:HG2	1:B:440:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:CG	1:A:87:LYS:H	2.30	0.41
1:A:304:SER:C	1:A:305:LEU:HD23	2.46	0.41
1:A:497:VAL:HG23	1:A:498:LEU:N	2.34	0.41
1:B:329:ARG:NH1	1:B:388:ASP:CB	2.83	0.41
1:A:218:VAL:CB	1:A:219:PRO:HD3	2.49	0.41
1:A:247:GLN:O	1:A:250:GLN:HB3	2.21	0.41
1:A:326:ARG:NH2	1:A:518:HIS:CD2	2.88	0.41
1:A:519:ILE:CD1	1:A:548:ARG:HB3	2.46	0.41
1:A:560:MET:SD	1:A:572:VAL:HG11	2.60	0.41
1:B:167:ALA:HB3	1:B:173:LEU:HD13	2.02	0.41
1:B:433:VAL:HA	1:B:436:LEU:HD12	2.01	0.41
1:B:464:VAL:HG21	1:B:491:TRP:CE3	2.55	0.41
1:A:182:PRO:HG2	1:A:183:GLU:H	1.85	0.41
1:B:440:ILE:O	1:B:441:SER:CB	2.66	0.41
1:A:446:GLY:O	1:A:450:VAL:HG23	2.20	0.41
1:B:312:ILE:O	1:B:312:ILE:HG22	2.21	0.41
1:A:90:LEU:HG	1:B:111:PHE:CE2	2.55	0.41
1:A:595:VAL:O	1:A:598:LEU:HD12	2.21	0.41
1:B:395:LEU:CD1	1:B:550:ALA:HB3	2.50	0.41
1:A:210:ALA:O	1:A:251:ALA:HB1	2.21	0.41
1:A:296:PHE:CE1	1:A:316:ALA:HB3	2.56	0.41
1:A:329:ARG:NH2	1:A:386:VAL:HA	2.36	0.41
1:A:459:ALA:O	1:A:462:PRO:HD2	2.20	0.41
1:B:296:PHE:HE1	1:B:316:ALA:HB3	1.85	0.41
1:B:296:PHE:CE1	1:B:316:ALA:HB3	2.56	0.41
1:B:391:SER:HB3	1:B:548:ARG:CG	2.47	0.41
1:B:395:LEU:O	1:B:397:THR:HG22	2.20	0.41
1:B:535:VAL:HG11	1:B:598:LEU:HD11	2.03	0.41
1:B:628:ALA:HB1	1:B:631:MET:HE2	2.01	0.41
1:A:407:ALA:HB1	1:A:415:GLU:HG3	2.03	0.41
1:A:628:ALA:CA	1:A:631:MET:HE2	2.51	0.41
1:B:371:MET:O	1:B:375:THR:HG23	2.20	0.41
1:A:97:VAL:HG22	1:A:134:ALA:O	2.21	0.40
1:A:150:LEU:O	1:A:154:LEU:HB2	2.22	0.40
1:A:230:GLN:CD	1:A:479:LEU:HD12	2.46	0.40
1:B:440:ILE:O	1:B:440:ILE:CD1	2.68	0.40
1:B:568:TYR:O	1:B:572:VAL:HG23	2.20	0.40
1:A:87:LYS:HZ2	1:B:116:CYS:HA	1.86	0.40
1:A:217:ASN:O	1:A:218:VAL:C	2.63	0.40
1:B:161:ILE:CD1	1:B:180:LEU:HD21	2.46	0.40
1:B:217:ASN:O	1:B:218:VAL:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:VAL:HG13	1:B:448:LYS:N	2.35	0.40
1:B:497:VAL:HG23	1:B:498:LEU:N	2.36	0.40
1:A:186:LYS:O	1:A:190:MET:HG3	2.20	0.40
1:A:302:ARG:HH21	1:A:309:LEU:CG	2.34	0.40
1:A:405:ILE:CG2	1:A:409:LYS:HE3	2.51	0.40
1:A:414:LYS:HG3	1:A:415:GLU:H	1.86	0.40
1:A:526:CYS:HG	1:A:541:THR:HG1	1.67	0.40
1:A:588:THR:O	1:A:592:GLU:HG2	2.22	0.40
1:B:220:ILE:HG22	1:B:244:ILE:CD1	2.48	0.40
1:B:336:GLU:OE1	1:B:336:GLU:HA	2.22	0.40
1:B:460:LEU:HD12	1:B:463:GLN:NE2	2.37	0.40
1:B:182:PRO:HG2	1:B:183:GLU:H	1.86	0.40
1:A:306:GLU:O	1:A:310:GLU:HB2	2.22	0.40
1:A:415:GLU:O	1:A:419:TYR:HB2	2.21	0.40
1:A:628:ALA:HA	1:A:631:MET:HE2	2.03	0.40
1:B:85:PHE:CG	1:B:86:LEU:N	2.90	0.40
1:B:161:ILE:HD12	1:B:248:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

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	516/912 (57%)	444 (86%)	49 (10%)	23 (4%)	2	17
1	B	516/912 (57%)	447 (87%)	48 (9%)	21 (4%)	2	18
All	All	1032/1824 (57%)	891 (86%)	97 (9%)	44 (4%)	2	17

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	LEU

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Mol	Chain	Res	Type
1	A	291	VAL
1	A	292	ASP
1	A	301	PHE
1	A	393	SER
1	A	441	SER
1	A	583	VAL
1	B	86	LEU
1	B	291	VAL
1	B	292	ASP
1	B	301	PHE
1	B	393	SER
1	B	441	SER
1	B	583	VAL
1	A	321	ASP
1	A	395	LEU
1	A	601	ASP
1	A	603	ALA
1	B	321	ASP
1	B	395	LEU
1	B	601	ASP
1	B	603	ALA
1	A	300	ARG
1	A	305	LEU
1	A	352	MET
1	A	376	ARG
1	B	300	ARG
1	B	305	LEU
1	B	376	ARG
1	A	353	GLY
1	A	390	VAL
1	A	477	SER
1	A	609	ASN
1	B	352	MET
1	B	353	GLY
1	B	390	VAL
1	B	609	ASN
1	A	598	LEU
1	A	630	LEU
1	B	598	LEU
1	B	630	LEU
1	A	261	ALA
1	A	403	VAL

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Mol	Chain	Res	Type
1	B	403	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	431/766 (56%)	394 (91%)	37 (9%)	10	29
1	B	431/766 (56%)	394 (91%)	37 (9%)	10	29
All	All	862/1532 (56%)	788 (91%)	74 (9%)	10	29

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	87	LYS
1	A	89	GLU
1	A	132	LEU
1	A	133	SER
1	A	141	LEU
1	A	149	LYS
1	A	169	ASN
1	A	190	MET
1	A	300	ARG
1	A	321	ASP
1	A	336	GLU
1	A	344	LEU
1	A	347	LEU
1	A	350	GLU
1	A	362	ASP
1	A	377	ASP
1	A	388	ASP
1	A	398	ASN
1	A	399	VAL
1	A	402	LEU
1	A	404	LEU

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Mol	Chain	Res	Type
1	A	406	GLU
1	A	410	ASN
1	A	440	ILE
1	A	445	GLU
1	A	449	LEU
1	A	487	PHE
1	A	508	ILE
1	A	539	ASP
1	A	569	THR
1	A	578	LEU
1	A	584	MET
1	A	586	ARG
1	A	598	LEU
1	A	599	SER
1	A	601	ASP
1	B	86	LEU
1	B	89	GLU
1	B	132	LEU
1	B	133	SER
1	B	141	LEU
1	B	149	LYS
1	B	169	ASN
1	B	190	MET
1	B	221	LEU
1	B	300	ARG
1	B	321	ASP
1	B	336	GLU
1	B	344	LEU
1	B	347	LEU
1	B	362	ASP
1	B	377	ASP
1	B	388	ASP
1	B	398	ASN
1	B	399	VAL
1	B	402	LEU
1	B	404	LEU
1	B	406	GLU
1	B	410	ASN
1	B	430	LEU
1	B	440	ILE
1	B	445	GLU
1	B	449	LEU

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Mol	Chain	Res	Type
1	B	487	PHE
1	B	508	ILE
1	B	539	ASP
1	B	569	THR
1	B	578	LEU
1	B	584	MET
1	B	586	ARG
1	B	598	LEU
1	B	599	SER
1	B	601	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	171	GLN
1	A	196	GLN
1	A	203	ASN
1	A	215	GLN
1	A	217	ASN
1	A	226	GLN
1	A	230	GLN
1	A	231	HIS
1	A	247	GLN
1	A	249	GLN
1	A	342	GLN
1	A	354	ASN
1	A	426	HIS
1	A	435	ASN
1	A	456	GLN
1	A	463	GLN
1	A	466	ASN
1	B	100	GLN
1	B	171	GLN
1	B	196	GLN
1	B	203	ASN
1	B	215	GLN
1	B	217	ASN
1	B	226	GLN
1	B	230	GLN
1	B	249	GLN
1	B	342	GLN

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Mol	Chain	Res	Type
1	B	354	ASN
1	B	426	HIS
1	B	435	ASN
1	B	456	GLN
1	B	466	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

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	520/912 (57%)	0.74	57 (10%)	10 18	355, 355, 355, 355	0
1	B	520/912 (57%)	0.84	73 (14%)	6 15	355, 355, 355, 355	0
All	All	1040/1824 (57%)	0.79	130 (12%)	8 16	355, 355, 355, 355	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	504	ASP	5.8
1	A	331	GLU	5.0
1	A	181	LYS	4.7
1	A	121	ARG	4.6
1	A	116	CYS	4.6
1	A	382	LEU	4.1
1	A	223	THR	4.0
1	A	620	ASP	3.9
1	A	504	ASP	3.9
1	A	521	GLU	3.8
1	A	576	THR	3.7
1	A	525	LYS	3.7
1	B	144	MET	3.7
1	B	337	CYS	3.7
1	A	332	ARG	3.6
1	A	384	LYS	3.5
1	A	189	ILE	3.4
1	B	306	GLU	3.4
1	B	307	GLU	3.4
1	B	349	SER	3.4
1	B	609	ASN	3.2
1	B	618	VAL	3.2
1	B	623	ARG	3.2
1	B	177	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	382	LEU	3.1
1	B	118	SER	3.1
1	B	223	THR	3.1
1	B	332	ARG	3.1
1	B	161	ILE	3.1
1	A	615	SER	3.1
1	A	498	LEU	3.0
1	B	517	ASN	3.0
1	A	517	ASN	3.0
1	A	128	ALA	3.0
1	B	368	ILE	3.0
1	A	248	LEU	3.0
1	A	90	LEU	2.9
1	B	248	LEU	2.9
1	B	121	ARG	2.9
1	B	318	LEU	2.9
1	B	348	LEU	2.9
1	B	215	GLN	2.9
1	A	219	PRO	2.8
1	A	538	LEU	2.8
1	B	510	ASP	2.8
1	A	629	VAL	2.8
1	B	304	SER	2.8
1	A	177	TYR	2.8
1	B	255	ILE	2.8
1	A	311	SER	2.8
1	A	619	TYR	2.8
1	B	355	ALA	2.8
1	B	351	TYR	2.8
1	B	347	LEU	2.7
1	A	91	VAL	2.7
1	B	120	LYS	2.7
1	B	315	GLY	2.7
1	B	437	ALA	2.7
1	B	562	ASN	2.7
1	A	395	LEU	2.7
1	B	379	ARG	2.7
1	B	293	PRO	2.7
1	A	587	PHE	2.7
1	A	222	TYR	2.6
1	B	384	LYS	2.6
1	B	627	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	591	VAL	2.6
1	A	333	ILE	2.6
1	B	141	LEU	2.6
1	A	328	ASP	2.6
1	B	336	GLU	2.6
1	B	149	LYS	2.5
1	A	118	SER	2.5
1	B	378	LEU	2.5
1	B	122	GLY	2.5
1	B	333	ILE	2.5
1	B	619	TYR	2.5
1	B	365	ASN	2.5
1	B	262	THR	2.5
1	B	440	ILE	2.5
1	B	301	PHE	2.4
1	A	250	GLN	2.4
1	A	510	ASP	2.4
1	B	186	LYS	2.4
1	A	586	ARG	2.4
1	B	346	ASP	2.4
1	B	164	LEU	2.4
1	B	622	ILE	2.3
1	B	323	SER	2.3
1	A	161	ILE	2.3
1	B	620	ASP	2.3
1	B	243	LEU	2.3
1	A	327	ASP	2.3
1	B	505	ILE	2.3
1	A	131	LEU	2.3
1	A	300	ARG	2.3
1	B	110	GLU	2.3
1	B	525	LYS	2.3
1	A	571	LYS	2.3
1	A	308	ARG	2.2
1	A	595	VAL	2.2
1	A	193	LYS	2.2
1	B	483	ASN	2.2
1	B	559	GLU	2.2
1	B	433	VAL	2.2
1	B	313	ILE	2.2
1	B	314	SER	2.1
1	A	612	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	214	LEU	2.1
1	B	344	LEU	2.1
1	A	135	VAL	2.1
1	B	352	MET	2.1
1	B	558	SER	2.1
1	A	608	GLU	2.1
1	A	622	ILE	2.1
1	B	218	VAL	2.1
1	B	507	SER	2.1
1	B	521	GLU	2.1
1	A	616	ARG	2.1
1	A	610	GLU	2.1
1	A	337	CYS	2.1
1	A	513	ALA	2.1
1	A	252	VAL	2.1
1	B	135	VAL	2.1
1	A	164	LEU	2.0
1	B	216	LYS	2.0
1	B	128	ALA	2.0
1	B	239	ALA	2.0
1	A	618	VAL	2.0
1	A	129	ARG	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.