



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:01 AM UTC

PDB ID : 5VCH / pdb_00005vch
Title : Crystal structure of full-length Kluyveromyces lactis Kap123
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Deposited on : 2017-03-31
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

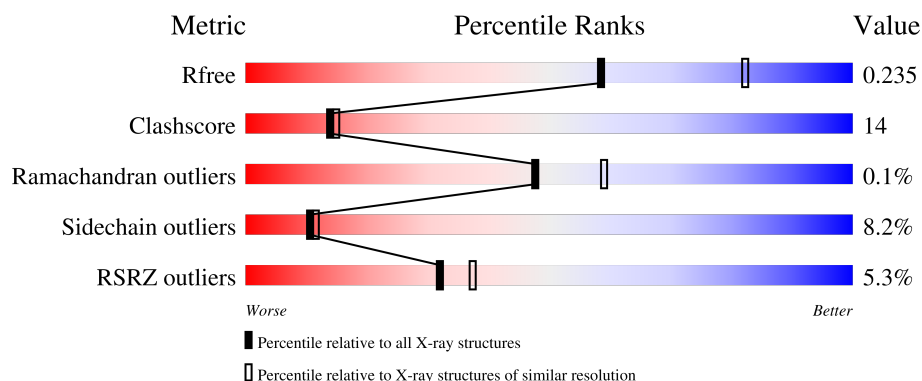
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	1116	5% 65% 23% • 9%
1	B	1116	5% 65% 23% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16287 atoms, of which 38 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 Kap123.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	1020	Total	C	H	N	O	S	Se	0	1	0
			7930	5026	38	1288	1555	12	11			
1	B	1027	Total	C	N	O	S	Se		0	1	0
			7947	5061	1298	1567	10	11				

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q6CMF0
A	-1	ASN	-	expression tag	UNP Q6CMF0
A	0	ALA	-	expression tag	UNP Q6CMF0
A	1	MSE	-	expression tag	UNP Q6CMF0
B	-2	SER	-	expression tag	UNP Q6CMF0
B	-1	ASN	-	expression tag	UNP Q6CMF0
B	0	ALA	-	expression tag	UNP Q6CMF0
B	1	MSE	-	expression tag	UNP Q6CMF0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	195	Total	O	0	0
			195	195		
2	B	215	Total	O	0	0
			215	215		

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.

Chain A:

Residue	Conservation
SER	High
ASN	High
ALA	High
ASP	High
GLN	High
GLY	High
PHE	High
VAL	High
ALA	High
GLN	High
LEU	High
GLU	High
GLN	High
ALA	High
LEU	High
GLY	High
ALA	High
ILE	High
VAL	High
GLN	High
PRO	High
THR	High
GLY	High
SER	High
LEU	High
LYS	High
ASP	High
ALA	High
THR	High
THR	High
GLN	High
LEU	High
GLY	High
SER	High
GLN	High
PHE	High
THR	High
THR	High
GLN	High
SER	High
GLN	High
ALA	High
ALA	High
P42	High
A43	High
I44	High
I45	High
H46	High
Q49	High
N50	High
S51	High
S52	High
N53	High
H54	High
G55	High
L59	High
E63	High
A64	High
R65	High
MSE	High
K66	High
Q67	High
V68	High
S69	High
K70	High
V191	High
S192	High
S193	High
L194	High
I195	High
E198	High
G199	High
A77	High
A78	High
T79	High
N201	High
N202	High
Q80	High
S82	High
V83	High
K84	High
Q85	High
S86	High
L87	High
A108	High
S109	High
I110	High
G111	High
S112	High
E113	High
GLU	High
LEU	High
GLN	High
ASP	High
GLU	High
LYS	High
W120	High
P121	High
E122	High
P125	High
L41	High
N135	High
Q248	High
L249	High
T250	High
L150	High
N154	High
A155	High
L157	High
A158	High
L159	High
H160	High
I161	High
E164	High
R289	High
K292	High
K297	High
E313	High
V316	High
E317	High
N322	High
E323	High
D324	High
G199	High
A199	High
GLY	High
GLU	High
ASN	High
GLU	High
N332	High
T333	High
P334	High
R340	High
S343	High
V354	High
R500	High
A501	High
H361	High
K365	High
F372	High
I377	High
S382	High
V383	High
P389	High
V413	High
V423	High
Q424	High
Q430	High
R435	High
M560	High
L441	High
P442	High
R455	High
A563	High
V564	High
I445	High
D449	High
V454	High
K458	High
L462	High
F470	High
H473	High
N474	High
D475	High
I476	High
A483	High
M484	High
N485	High
K486	High
L487	High
F488	High
Q489	High
E492	High
L499	High
A501	High
I507	High
F518	High
K523	High
T524	High
S525	High
V526	High
Q527	High
Y528	High
F532	High
K550	High
A551	High
L552	High
T553	High
F554	High
S558	High
T559	High
M560	High
L561	High
R562	High
A563	High
V564	High
I445	High
A573	High
E574	High
V577	High</

Chain B: 5% 65% 23% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.05Å 88.12Å 102.01Å 79.19° 80.03° 70.98°	Depositor
Resolution (Å)	33.00 – 2.35 33.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.8 (33.00-2.35) 97.8 (33.00-2.35)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.210 , 0.235 0.211 , 0.235	Depositor DCC
R_{free} test set	2000 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16287	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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	0.56	10/8000 (0.1%)	0.67	12/10842 (0.1%)
1	B	0.47	9/8059 (0.1%)	0.61	3/10924 (0.0%)
All	All	0.52	19/16059 (0.1%)	0.64	15/21766 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	681	LYS	C-O	-9.35	1.15	1.24
1	A	854	VAL	C-O	-8.43	1.14	1.24
1	B	973	ILE	C-O	-7.75	1.15	1.24
1	A	608	LYS	C-O	-7.25	1.14	1.24
1	A	856	GLY	C-O	-7.13	1.14	1.24
1	B	972	GLU	C-O	-6.71	1.16	1.24
1	A	679	ALA	C-O	-6.66	1.14	1.24
1	B	975	ASP	C-O	-6.52	1.16	1.24
1	B	971	LYS	C-O	-6.50	1.16	1.24
1	B	970	THR	C-O	-6.20	1.16	1.24
1	B	967	ASP	C-O	-6.14	1.18	1.24
1	A	678	ILE	C-O	-6.04	1.16	1.24
1	A	677	ALA	C-O	-5.71	1.17	1.24
1	A	607	GLY	C-O	-5.46	1.16	1.23
1	A	609	ASP	C-O	-5.36	1.17	1.24
1	B	967	ASP	CA-C	-5.30	1.48	1.53
1	A	857	PHE	C-O	-5.23	1.17	1.24
1	B	972	GLU	N-CA	-5.20	1.40	1.46
1	B	970	THR	N-CA	-5.19	1.40	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	853	LEU	N-CA-C	13.00	125.53	111.36
1	A	678	ILE	CB-CA-C	-11.57	92.31	111.29
1	A	679	ALA	CB-CA-C	-9.20	95.77	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	967	ASP	N-CA-C	8.02	120.50	108.31
1	A	684	PHE	N-CA-C	-7.21	102.49	112.30
1	A	680	SER	N-CA-C	-6.65	104.34	113.18
1	A	895	ARG	CB-CA-C	-6.61	108.96	116.63
1	A	681	LYS	CB-CA-C	-5.88	109.81	116.63
1	A	683	HIS	CB-CA-C	-5.85	100.70	110.81
1	A	678	ILE	CG1-CB-CG2	-5.58	93.96	110.70
1	A	682	GLU	N-CA-C	5.26	122.01	110.80
1	B	969	ALA	CA-C-N	5.24	127.73	120.29
1	B	969	ALA	C-N-CA	5.24	127.73	120.29
1	A	605	VAL	N-CA-C	5.23	116.70	111.00
1	A	686	GLU	N-CA-C	-5.16	106.83	113.23

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	7892	38	7978	221	1
1	B	7947	0	8015	241	1
2	A	195	0	0	5	0
2	B	215	0	0	14	0
All	All	16249	38	15993	457	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 14.

All (457) 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:479:TYR:HB3	1:A:483:LEU:HD23	1.30	1.14
1:B:736:PRO:HD2	1:B:789:MSE:HE3	1.34	1.08
1:A:161:ILE:HD11	1:A:194:LEU:HB3	1.32	1.08
1:B:689[B]:GLU:HG3	1:B:690:PRO:HD3	1.30	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:707:GLU:HG3	1:B:768:MSE:CE	1.90	1.01
1:B:707:GLU:HG3	1:B:768:MSE:HE1	1.43	1.00
1:B:779:MSE:HA	1:B:779:MSE:HE2	1.43	1.00
1:B:875:LYS:H	1:B:875:LYS:HD3	1.27	0.99
1:A:343:SER:HB2	1:A:383:VAL:HG22	1.45	0.98
1:B:1092:LYS:O	1:B:1095:ASN:ND2	1.96	0.98
1:B:969:ALA:O	2:B:1201:HOH:O	1.80	0.98
1:B:193:SER:O	1:B:197:GLU:HG2	1.65	0.96
1:B:439:GLN:NE2	2:B:1204:HOH:O	2.01	0.94
1:B:161:ILE:HG21	1:B:195:ILE:HD11	1.53	0.91
1:A:254:ILE:HD13	1:A:289:ARG:HD2	1.53	0.91
1:A:473:HIS:ND1	2:A:1201:HOH:O	2.04	0.89
1:A:484:MSE:HE1	1:A:507:ILE:HG23	1.55	0.89
1:B:736:PRO:CD	1:B:789:MSE:HE3	2.04	0.87
1:B:516:SER:OG	2:B:1202:HOH:O	1.93	0.86
1:A:382:SER:O	1:A:424:GLN:HG2	1.76	0.86
1:B:779:MSE:HE1	1:B:782:LEU:HD12	1.58	0.85
1:B:96:LYS:HD2	1:B:97:ASP:N	1.90	0.85
1:A:449:ASP:OD1	1:A:486:LYS:NZ	2.09	0.85
1:B:96:LYS:HD2	1:B:97:ASP:H	1.40	0.84
1:A:435:ARG:NH1	1:A:968:GLU:HG3	1.92	0.84
1:A:479:TYR:HB3	1:A:483:LEU:CD2	2.08	0.84
1:B:689[B]:GLU:HG3	1:B:690:PRO:CD	2.10	0.82
1:B:736:PRO:HA	2:B:1275:HOH:O	1.80	0.82
1:A:707:GLU:HG3	1:A:768:MSE:CE	2.09	0.82
1:A:161:ILE:CD1	1:A:194:LEU:HB3	2.10	0.82
1:B:44:LEU:HD12	1:B:67:GLN:HE22	1.45	0.81
1:B:998:LEU:HB3	1:B:1002:ILE:HD12	1.62	0.81
1:A:191:VAL:O	1:A:195:ILE:HG22	1.78	0.81
1:B:1093:HIS:O	1:B:1097:GLN:HG3	1.81	0.81
1:B:382:SER:O	1:B:424:GLN:HG2	1.81	0.81
1:B:1026:LEU:HD23	1:B:1090:LEU:HD22	1.63	0.80
1:A:121:PRO:HD2	1:A:122:GLU:OE1	1.82	0.80
1:A:858:ALA:HB2	1:A:894:MSE:HE1	1.62	0.80
1:A:343:SER:HB2	1:A:383:VAL:CG2	2.12	0.79
1:B:265:ALA:O	1:B:275:ARG:NH2	2.15	0.79
1:A:678:ILE:O	1:A:678:ILE:HG22	1.83	0.78
1:A:474:ASN:O	1:A:478:LYS:NZ	2.17	0.77
1:B:779:MSE:HA	1:B:779:MSE:CE	2.15	0.77
1:B:693:LYS:HE2	1:B:693:LYS:HA	1.67	0.76
1:A:254:ILE:CD1	1:A:289:ARG:HD2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:HG	1:A:67:GLN:HG2	1.68	0.76
1:B:486:LYS:O	1:B:489:GLN:HG3	1.86	0.76
1:B:192:SER:HB3	1:B:209:PHE:CE2	2.21	0.75
1:A:1072:LEU:HD23	1:A:1075:ARG:HH11	1.51	0.75
1:B:586:THR:HG23	1:B:588:SER:H	1.51	0.75
1:B:779:MSE:CE	1:B:782:LEU:HD12	2.17	0.75
1:B:479:TYR:HB3	1:B:483:LEU:HD12	1.69	0.75
1:B:813:ALA:N	2:B:1203:HOH:O	1.97	0.74
1:B:195:ILE:HD12	1:B:205:TYR:HB3	1.68	0.74
1:B:86:SER:O	1:B:90:SER:OG	2.05	0.74
1:B:1040:ALA:O	1:B:1044:ILE:HG23	1.88	0.74
1:B:1108:LEU:HA	1:B:1111:VAL:CG1	2.18	0.73
1:A:206:ALA:HB1	1:A:248:GLN:O	1.88	0.73
1:A:1091:LEU:CB	1:A:1112:ILE:HD11	2.19	0.73
1:B:562:ARG:HD2	1:B:601:ASN:OD1	1.89	0.73
1:B:469:GLU:OE2	2:B:1205:HOH:O	2.05	0.73
1:A:361:HIS:O	1:A:365:MSE:HG3	1.89	0.73
1:B:737:SER:O	1:B:791:ASN:HA	1.89	0.72
1:B:707:GLU:HG3	1:B:768:MSE:HE2	1.72	0.72
1:B:1108:LEU:HA	1:B:1111:VAL:HG12	1.72	0.72
1:A:1113:ALA:O	2:A:1202:HOH:O	2.08	0.72
1:A:41:LEU:HB2	1:A:67:GLN:HG2	1.72	0.71
1:A:65:ARG:O	1:A:68:VAL:HG23	1.90	0.71
1:A:1040:ALA:O	1:A:1044:ILE:HG23	1.91	0.71
1:A:1072:LEU:HD23	1:A:1075:ARG:NH1	2.05	0.71
1:B:161:ILE:CG2	1:B:195:ILE:HD11	2.20	0.71
1:B:84:LYS:HD3	1:B:120:TRP:CD2	2.26	0.71
1:B:323:GLU:HB3	1:B:498:LYS:HE3	1.72	0.71
1:A:768:MSE:HE2	1:A:768:MSE:HA	1.71	0.71
1:A:435:ARG:HH11	1:A:968:GLU:HG3	1.54	0.70
1:B:1089:GLU:HA	1:B:1092:LYS:HD2	1.72	0.70
1:A:586:THR:HG21	1:A:591:LEU:HD23	1.73	0.70
1:A:1108:LEU:HA	1:A:1111:VAL:CG1	2.21	0.70
1:B:707:GLU:CG	1:B:768:MSE:CE	2.68	0.70
1:A:1108:LEU:HA	1:A:1111:VAL:HG12	1.74	0.70
1:B:219:VAL:O	1:B:223:THR:HG23	1.92	0.70
1:A:746:LEU:O	1:A:750:GLN:HG3	1.92	0.69
1:A:875:LYS:HD2	1:A:875:LYS:O	1.93	0.69
1:A:206:ALA:HA	1:A:249:LEU:HD13	1.75	0.68
1:B:479:TYR:O	1:B:482:PRO:HD2	1.94	0.68
1:B:1093:HIS:HB3	1:B:1097:GLN:NE2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:LYS:O	1:B:697:GLU:HG3	1.93	0.67
1:B:746:LEU:O	1:B:750:GLN:HG3	1.94	0.67
1:B:271:ASP:O	1:B:275:ARG:HG3	1.94	0.67
1:B:736:PRO:HD2	1:B:789:MSE:CE	2.20	0.67
1:B:161:ILE:HG21	1:B:195:ILE:CD1	2.24	0.67
1:B:115:LEU:HD22	1:B:156:ASN:HB2	1.76	0.67
1:B:458:LYS:HE2	1:B:498:LYS:NZ	2.10	0.66
1:A:1091:LEU:HB2	1:A:1112:ILE:HD11	1.78	0.66
1:B:735:VAL:O	2:B:1206:HOH:O	2.13	0.66
1:B:92:PHE:HA	1:B:100:ARG:NH2	2.11	0.66
1:B:785:PRO:HG3	1:B:852:ASN:HB3	1.77	0.66
1:B:84:LYS:HD3	1:B:120:TRP:CE2	2.32	0.65
1:A:475:ASP:HA	1:A:478:LYS:CE	2.26	0.65
1:B:1042:LYS:HE3	1:B:1046:ILE:HD11	1.77	0.65
1:B:875:LYS:H	1:B:875:LYS:CD	1.98	0.65
1:B:1027:LYS:HE2	2:B:1268:HOH:O	1.95	0.65
1:B:717:VAL:HG22	1:B:748:VAL:HG12	1.77	0.64
1:A:984:CYS:O	1:A:988:MSE:HG3	1.98	0.64
1:A:475:ASP:HA	1:A:478:LYS:HE2	1.79	0.64
1:B:121:PRO:HD2	1:B:122:GLU:OE2	1.96	0.64
1:B:707:GLU:CG	1:B:768:MSE:HE1	2.25	0.64
1:B:1101:ALA:HA	1:B:1104:GLN:HB3	1.80	0.64
1:A:707:GLU:CG	1:A:768:MSE:CE	2.75	0.63
1:A:741:VAL:HG13	1:A:745:ALA:HB3	1.80	0.63
1:B:707:GLU:CG	1:B:768:MSE:HE2	2.28	0.63
1:B:583:ALA:O	1:B:586:THR:HB	1.98	0.63
1:B:854:VAL:HG11	1:B:895:ARG:NH2	2.14	0.63
1:A:192:SER:O	1:A:195:ILE:HG23	1.99	0.63
1:A:684:PHE:O	1:A:684:PHE:CD2	2.52	0.63
1:A:333:THR:HG22	1:A:334:PRO:HD2	1.80	0.63
1:A:707:GLU:HG3	1:A:768:MSE:HE1	1.80	0.62
1:A:156:ASN:HA	1:A:159:LEU:HD13	1.80	0.62
1:B:1085:GLN:O	1:B:1089:GLU:HG2	1.99	0.62
1:B:1104:GLN:O	1:B:1104:GLN:HG3	2.00	0.62
1:B:195:ILE:HD12	1:B:205:TYR:CB	2.29	0.62
1:A:192:SER:HA	1:A:195:ILE:CG2	2.29	0.62
1:A:220:LEU:HB2	1:A:235:ILE:HG21	1.82	0.62
1:A:526:VAL:HG23	1:A:560:MSE:HE1	1.81	0.62
1:B:1088:ILE:HG12	1:B:1111:VAL:CG2	2.29	0.61
1:A:41:LEU:CG	1:A:67:GLN:HG2	2.30	0.61
1:B:222:ALA:O	1:B:226:GLU:HG2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HD23	1:A:157:LEU:HD13	1.83	0.61
1:B:192:SER:HB3	1:B:209:PHE:CZ	2.35	0.61
1:B:586:THR:CG2	1:B:588:SER:H	2.13	0.61
1:A:740:TYR:CZ	1:A:786:ILE:HB	2.36	0.61
1:B:112:SER:HA	1:B:154:ASN:HD22	1.65	0.61
1:A:41:LEU:CB	1:A:67:GLN:HG2	2.29	0.60
1:A:195:ILE:HD13	1:A:205:TYR:HB2	1.83	0.60
1:A:586:THR:HG22	1:A:588:SER:H	1.67	0.60
1:B:177:SER:O	1:B:181:ARG:HG3	2.01	0.60
1:B:84:LYS:HG2	1:B:120:TRP:CH2	2.37	0.60
1:B:862:THR:HG21	2:B:1404:HOH:O	2.02	0.59
1:B:586:THR:HG23	1:B:587:ASP:N	2.17	0.59
1:B:195:ILE:CD1	1:B:205:TYR:HB3	2.31	0.59
1:A:586:THR:CG2	1:A:588:SER:H	2.15	0.58
1:A:1058:ILE:O	1:A:1062:THR:HG23	2.03	0.58
1:B:919:GLU:HB2	1:B:973:ILE:HD12	1.84	0.58
1:A:79:THR:O	1:A:79:THR:OG1	2.22	0.58
1:A:108:ALA:O	1:A:111:GLY:N	2.36	0.58
1:B:1026:LEU:CD2	1:B:1090:LEU:HD22	2.32	0.58
1:A:192:SER:HA	1:A:195:ILE:HG23	1.85	0.58
1:A:707:GLU:CG	1:A:768:MSE:HE2	2.34	0.58
1:B:1071:ASN:O	1:B:1075:ARG:HG2	2.04	0.58
1:A:316:VAL:HG22	1:A:413:VAL:HG11	1.86	0.58
1:B:260:LEU:C	1:B:260:LEU:HD23	2.29	0.57
1:A:1091:LEU:HB3	1:A:1112:ILE:HD11	1.85	0.57
1:B:441:LEU:O	1:B:445:ILE:HG12	2.03	0.57
1:B:213:ILE:HG21	1:B:253:THR:HG21	1.85	0.57
1:A:135:ASN:HB3	1:A:138:ILE:HD12	1.87	0.57
1:B:1081:GLU:O	1:B:1085:GLN:HG2	2.04	0.57
1:A:77:ALA:O	1:A:80:GLN:HG2	2.05	0.56
1:A:343:SER:CB	1:A:383:VAL:HG22	2.29	0.56
1:A:754:GLU:OE2	1:A:796:HIS:NE2	2.27	0.56
1:A:939:VAL:O	1:A:942:ILE:HG13	2.06	0.56
1:B:998:LEU:HB3	1:B:1002:ILE:CD1	2.33	0.56
1:B:1090:LEU:O	1:B:1094:LEU:HD13	2.05	0.56
1:A:1072:LEU:HA	1:A:1075:ARG:NH1	2.20	0.56
1:B:44:LEU:CD1	1:B:67:GLN:HE22	2.16	0.56
1:A:473:HIS:O	1:A:476:ILE:HG22	2.06	0.56
1:B:902:GLN:HB3	1:B:937:PHE:CZ	2.41	0.56
1:B:1058:ILE:O	1:B:1062:THR:HG23	2.06	0.56
1:A:684:PHE:O	1:A:688:VAL:HG23	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LYS:NZ	1:B:114:GLU:OE1	2.35	0.55
1:B:561:GLY:O	1:B:564:VAL:O	2.23	0.55
1:B:877:LYS:HD2	1:B:877:LYS:C	2.32	0.55
1:B:231:ASN:O	1:B:235:ILE:HG12	2.06	0.55
1:B:255:ALA:O	1:B:259:LYS:HG3	2.07	0.55
1:A:954:LEU:HG	1:A:981:VAL:HG11	1.88	0.55
1:B:1042:LYS:HE3	1:B:1046:ILE:CD1	2.36	0.55
1:A:423:VAL:CG2	1:A:462:LEU:HD22	2.36	0.55
1:A:219:VAL:O	1:A:223:THR:HG23	2.07	0.55
1:B:1093:HIS:HB3	1:B:1097:GLN:HE21	1.71	0.55
1:A:204:GLN:HE22	1:B:959:GLU:CG	2.19	0.55
1:A:271:ASP:O	1:A:275:ARG:HG3	2.06	0.55
1:A:492:GLU:OE2	1:A:528:TYR:HE2	1.89	0.55
1:B:705:LEU:O	1:B:705:LEU:HG	2.06	0.54
1:A:781:ARG:NH1	2:A:1208:HOH:O	2.40	0.54
1:A:858:ALA:CB	1:A:894:MSE:HE1	2.36	0.54
1:B:875:LYS:HD3	1:B:875:LYS:N	2.10	0.54
1:A:558:SER:HB3	1:A:598:PHE:CD2	2.42	0.54
1:B:944:SER:HB2	1:B:945:PRO:HD3	1.90	0.54
1:A:41:LEU:HB2	1:A:67:GLN:CG	2.38	0.54
1:A:735:VAL:HG13	1:A:789:MSE:SE	2.57	0.54
1:B:128:LEU:HD23	1:B:167:LEU:HD22	1.90	0.54
1:B:919:GLU:OE1	1:B:973:ILE:CD1	2.56	0.54
1:B:954:LEU:HG	1:B:981:VAL:HG11	1.91	0.54
1:A:84:LYS:HE2	1:A:120:TRP:CE3	2.43	0.53
1:A:192:SER:HB3	1:A:209:PHE:CE2	2.44	0.53
1:B:740:TYR:CZ	1:B:786:ILE:HB	2.44	0.53
1:B:1089:GLU:O	1:B:1092:LYS:HB2	2.09	0.53
1:B:47:ILE:O	1:B:51:SER:HB2	2.08	0.53
1:B:84:LYS:HG2	1:B:120:TRP:CZ2	2.44	0.53
1:B:512:PHE:CZ	1:B:1068:ARG:HD3	2.43	0.53
1:A:573:ALA:O	1:A:577:VAL:HG23	2.09	0.53
1:A:160:HIS:HB2	1:A:164:PHE:CE2	2.43	0.53
1:A:707:GLU:CG	1:A:768:MSE:HE1	2.39	0.53
1:A:1088:ILE:HG12	1:A:1111:VAL:CG2	2.38	0.53
1:B:307:LEU:HG	1:B:365:MSE:HE1	1.91	0.53
1:A:289:ARG:HG2	1:A:289:ARG:HH11	1.74	0.53
1:A:1071:ASN:HB2	1:A:1075:ARG:NH2	2.24	0.52
1:A:562:ARG:HD2	1:A:601:ASN:OD1	2.09	0.52
1:B:135:ASN:HB3	1:B:138:ILE:HD12	1.91	0.52
1:B:761:ILE:HD11	1:B:799:GLN:HE21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LYS:HE2	1:B:297:LYS:HD3	1.90	0.52
1:A:1002:ILE:HB	1:A:1003:PRO:HD3	1.92	0.52
1:A:618:ILE:N	1:A:619:PRO:HD2	2.24	0.52
1:A:614:LEU:HD22	1:A:618:ILE:HD11	1.91	0.52
1:A:233:LYS:HD3	1:A:277:PHE:CZ	2.45	0.52
1:A:1002:ILE:HG21	1:A:1035:THR:HG22	1.92	0.52
1:B:188:LEU:HD21	1:B:212:LEU:HD13	1.92	0.52
1:B:630:TYR:CZ	1:B:658:VAL:HG22	2.45	0.52
1:B:1101:ALA:HA	1:B:1104:GLN:CB	2.39	0.52
1:A:122:GLU:C	1:A:125:PRO:HD2	2.35	0.51
1:A:717:VAL:HG22	1:A:748:VAL:HG12	1.92	0.51
1:B:1061:GLU:OE2	1:B:1072:LEU:HD22	2.11	0.51
1:B:220:LEU:HB2	1:B:235:ILE:HG21	1.92	0.51
1:A:789:MSE:HE3	1:A:794:SER:HA	1.93	0.51
1:B:698:GLN:O	1:B:702:SER:HB3	2.10	0.51
1:B:948:LYS:O	1:B:952:GLU:HG3	2.11	0.51
1:B:276:VAL:HG13	1:B:337:THR:HG21	1.93	0.51
1:A:169:ALA:HA	1:A:212:LEU:HD22	1.93	0.51
1:A:289:ARG:HG2	1:A:289:ARG:NH1	2.26	0.51
1:B:315:ASP:OD2	1:B:318:ASP:HB2	2.10	0.51
1:A:781:ARG:NH2	1:A:844:ASP:OD1	2.44	0.51
1:A:1057:ARG:NH1	1:A:1058:ILE:HG13	2.26	0.51
1:A:618:ILE:HD13	1:A:687:TYR:CG	2.46	0.50
1:B:585:LYS:O	2:B:1207:HOH:O	2.19	0.50
1:B:161:ILE:HD13	1:B:195:ILE:HD13	1.92	0.50
1:B:768:MSE:HE2	1:B:768:MSE:HA	1.93	0.50
1:A:246:ASP:OD1	1:A:247:SER:N	2.44	0.50
1:A:297:LYS:NZ	1:B:297:LYS:HB2	2.27	0.50
1:A:602:MSE:HE2	1:A:602:MSE:HA	1.94	0.50
1:B:1070:GLU:H	1:B:1070:GLU:CD	2.20	0.50
1:B:693:LYS:NZ	1:B:697:GLU:HG2	2.26	0.50
1:A:45:ILE:HD13	1:A:83:VAL:CG1	2.42	0.50
1:A:159:LEU:HD12	1:A:159:LEU:N	2.27	0.50
1:B:297:LYS:CG	1:B:297:LYS:O	2.59	0.50
1:A:705:LEU:HG	1:A:705:LEU:O	2.11	0.49
1:A:959:GLU:OE1	1:B:208:LYS:HE3	2.12	0.49
1:A:156:ASN:O	1:A:159:LEU:HD13	2.11	0.49
1:B:501:ALA:HB1	1:B:552:LEU:HD12	1.94	0.49
1:A:161:ILE:HD11	1:A:194:LEU:CB	2.23	0.49
1:B:630:TYR:HE1	1:B:703:TYR:CE1	2.31	0.49
1:B:1094:LEU:HG	1:B:1098:PHE:HE2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:MSE:HE3	1:A:488:PHE:HE2	1.78	0.49
1:A:586:THR:CG2	1:A:587:ASP:N	2.76	0.49
1:A:1027:LYS:HE2	1:A:1031:GLU:OE1	2.13	0.49
1:B:495:GLN:OE1	1:B:495:GLN:HA	2.11	0.49
1:B:630:TYR:CE2	1:B:658:VAL:HG22	2.48	0.49
1:A:707:GLU:HG3	1:A:768:MSE:HE2	1.88	0.49
1:A:354:VAL:O	1:A:358:ILE:HG13	2.13	0.49
1:A:484:MSE:HE2	1:A:518:PHE:CE1	2.47	0.48
1:A:802:ARG:CB	1:A:802:ARG:HH21	2.26	0.48
1:B:96:LYS:CE	1:B:98:ALA:H	2.26	0.48
1:B:551:ALA:HB1	1:B:594:SER:HB3	1.93	0.48
1:B:717:VAL:HG22	1:B:748:VAL:CG1	2.43	0.48
1:B:857:PHE:CE2	1:B:861:PHE:HB2	2.48	0.48
1:A:964:THR:HG21	1:A:970:THR:HG22	1.93	0.48
1:B:943:TYR:CD2	1:B:995:LEU:HB2	2.48	0.48
1:B:43:ALA:O	1:B:47:ILE:HG22	2.13	0.48
1:B:428:ASN:ND2	2:B:1221:HOH:O	2.39	0.48
1:A:475:ASP:HA	1:A:478:LYS:NZ	2.28	0.48
1:A:766:THR:HG22	1:A:814:CYS:SG	2.54	0.48
1:A:789:MSE:CE	1:A:794:SER:HB3	2.43	0.48
1:B:761:ILE:HD11	1:B:799:GLN:NE2	2.29	0.48
1:B:480:LEU:O	1:B:484:MSE:HG2	2.14	0.48
1:A:561:GLY:O	1:A:564:VAL:O	2.32	0.48
1:B:726:LEU:HD23	1:B:783:PHE:HD1	1.78	0.48
1:A:195:ILE:HG12	1:A:249:LEU:HD11	1.95	0.48
1:B:486:LYS:HA	1:B:489:GLN:HG2	1.95	0.48
1:A:727:LYS:HD3	1:A:730:GLU:OE2	2.14	0.48
1:A:526:VAL:HG23	1:A:560:MSE:CE	2.44	0.47
1:B:96:LYS:NZ	1:B:98:ALA:H	2.12	0.47
1:B:479:TYR:HB3	1:B:483:LEU:CD1	2.42	0.47
1:B:586:THR:CG2	1:B:587:ASP:N	2.76	0.47
1:B:473:HIS:O	1:B:476:ILE:HG22	2.14	0.47
1:B:1042:LYS:CE	1:B:1046:ILE:HD11	2.44	0.47
1:B:1095:ASN:HB3	1:B:1102:VAL:CG1	2.44	0.47
1:A:423:VAL:HG21	1:A:462:LEU:HD22	1.96	0.47
1:B:430:GLN:HB3	1:B:470:PHE:CE2	2.49	0.47
1:B:1094:LEU:CG	1:B:1098:PHE:HE2	2.28	0.47
1:A:45:ILE:O	1:A:49:GLN:HG2	2.15	0.47
1:A:475:ASP:OD1	1:A:478:LYS:HE2	2.15	0.47
1:B:457:TYR:CD1	1:B:499:LEU:HD13	2.49	0.47
1:A:254:ILE:HD13	1:A:289:ARG:CD	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:ASP:OD1	1:B:486:LYS:NZ	2.43	0.47
1:B:1108:LEU:O	1:B:1111:VAL:HG13	2.15	0.47
1:B:685:LEU:HA	1:B:685:LEU:HD22	1.68	0.47
1:A:69:SER:OG	1:A:70:LYS:N	2.46	0.47
1:A:492:GLU:OE2	1:A:528:TYR:CE2	2.68	0.47
1:B:430:GLN:H	1:B:430:GLN:HG3	1.46	0.47
1:B:766:THR:HG23	1:B:838:LEU:HD22	1.96	0.47
1:A:581:TYR:OH	1:A:616:THR:HG22	2.15	0.47
1:A:156:ASN:CA	1:A:159:LEU:HD13	2.45	0.46
1:A:225:ARG:CZ	1:A:225:ARG:HB2	2.46	0.46
1:B:466:GLY:HA3	2:B:1349:HOH:O	2.15	0.46
1:B:1085:GLN:HA	1:B:1088:ILE:HD12	1.97	0.46
1:A:789:MSE:HE1	1:A:794:SER:HB3	1.98	0.46
1:B:58:GLN:NE2	1:B:98:ALA:HB1	2.30	0.46
1:A:501:ALA:HB1	1:A:552:LEU:HD12	1.96	0.46
1:A:532:PHE:O	1:A:550:LYS:HG3	2.16	0.46
1:B:41:LEU:HD22	1:B:45:ILE:HD12	1.98	0.46
1:B:693:LYS:HE2	1:B:693:LYS:CA	2.42	0.46
1:A:857:PHE:CE2	1:A:861:PHE:HB2	2.50	0.46
1:A:454:VAL:HG23	1:A:499:LEU:HD11	1.98	0.46
1:B:217:VAL:HG13	1:B:260:LEU:HD11	1.96	0.46
1:B:258:VAL:HG21	1:B:293:ILE:HD11	1.97	0.46
1:B:948:LYS:NZ	1:B:952:GLU:OE2	2.49	0.46
1:B:248:GLN:O	1:B:248:GLN:HG3	2.16	0.46
1:A:586:THR:HG23	1:A:587:ASP:N	2.31	0.46
1:A:628:GLU:OE2	1:A:630:TYR:HB2	2.16	0.46
1:B:213:ILE:N	1:B:214:PRO:HD2	2.30	0.46
1:B:260:LEU:HD23	1:B:260:LEU:O	2.16	0.46
1:A:182:SER:O	1:A:186:GLN:HG3	2.16	0.45
1:A:801[C]:CYS:SG	2:A:1222:HOH:O	2.61	0.45
1:B:781:ARG:HH22	1:B:844:ASP:CG	2.23	0.45
1:A:289:ARG:HD3	1:A:292:LYS:HD3	1.97	0.45
1:A:430:GLN:H	1:A:430:GLN:HG3	1.48	0.45
1:A:877:LYS:C	1:A:877:LYS:HD2	2.41	0.45
1:A:55:GLY:O	1:A:59:LEU:HD13	2.15	0.45
1:A:156:ASN:HA	1:A:159:LEU:CD1	2.46	0.45
1:A:678:ILE:HD13	1:A:719:ALA:HB2	1.98	0.45
1:A:802:ARG:HB3	1:A:802:ARG:NH2	2.31	0.45
1:B:687:TYR:C	1:B:690:PRO:HD2	2.42	0.45
1:A:169:ALA:HB2	1:A:212:LEU:HD21	1.98	0.45
1:B:260:LEU:HD23	1:B:264:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:991:LYS:HG3	1:B:992:HIS:CD2	2.51	0.45
1:A:707:GLU:HA	1:A:768:MSE:HE1	1.99	0.45
1:B:47:ILE:HD13	1:B:60:ALA:HB2	1.99	0.45
1:B:830:ASP:O	1:B:830:ASP:OD1	2.34	0.45
1:A:246:ASP:OD1	1:A:246:ASP:C	2.60	0.45
1:A:707:GLU:HG2	1:A:768:MSE:HE2	1.99	0.45
1:A:895:ARG:HA	1:A:934:TYR:CE2	2.52	0.45
1:A:313:GLU:HA	1:A:372:PHE:CD1	2.52	0.44
1:A:322:ASN:OD1	1:A:322:ASN:C	2.60	0.44
1:A:441:LEU:HB2	1:A:442:PRO:HD3	1.98	0.44
1:B:260:LEU:C	1:B:260:LEU:CD2	2.90	0.44
1:B:558:SER:HB3	1:B:598:PHE:CD2	2.53	0.44
1:A:192:SER:HB3	1:A:209:PHE:CZ	2.52	0.44
1:A:727:LYS:HB2	1:A:730:GLU:CD	2.43	0.44
1:A:1100:GLY:O	1:A:1104:GLN:HG2	2.18	0.44
1:B:496:SER:O	1:B:500:ARG:HG3	2.17	0.44
1:B:905:LEU:O	1:B:909:ILE:HG13	2.18	0.44
1:B:854:VAL:HG11	1:B:895:ARG:HH21	1.82	0.44
1:B:1042:LYS:HE3	1:B:1046:ILE:CG1	2.48	0.44
1:A:112:SER:HA	1:A:154:ASN:HD22	1.83	0.44
1:B:817:ILE:O	1:B:817:ILE:HG13	2.16	0.44
1:A:122:GLU:OE1	1:A:122:GLU:N	2.46	0.44
1:A:435:ARG:HB3	1:A:435:ARG:CZ	2.47	0.44
1:B:1088:ILE:HG12	1:B:1111:VAL:HG23	1.99	0.44
1:A:40:ALA:C	1:A:42:PRO:HD2	2.43	0.44
1:A:584:ILE:HG23	1:A:596:TYR:CZ	2.52	0.44
1:A:1037:ILE:HD13	1:A:1037:ILE:HA	1.64	0.44
1:B:96:LYS:HD2	1:B:96:LYS:C	2.40	0.44
1:B:122:GLU:C	1:B:125:PRO:HD2	2.43	0.44
1:A:63:GLU:HA	1:A:66:LYS:HD2	2.00	0.43
1:A:588:SER:HB3	1:A:591:LEU:HB2	2.00	0.43
1:A:944:SER:HB3	1:A:945:PRO:HD3	2.00	0.43
1:B:1026:LEU:CD2	1:B:1090:LEU:HB2	2.48	0.43
1:A:245:LEU:HB2	1:A:250:THR:CG2	2.47	0.43
1:A:340:ARG:HH11	1:A:340:ARG:HA	1.83	0.43
1:A:1044:ILE:HG13	1:A:1045:ALA:N	2.32	0.43
1:A:204:GLN:NE2	1:B:959:GLU:CD	2.76	0.43
1:A:441:LEU:O	1:A:445:ILE:HG12	2.17	0.43
1:B:65:ARG:HD2	1:B:109:SER:OG	2.17	0.43
1:B:1063:ASN:ND2	2:B:1209:HOH:O	2.28	0.43
1:A:430:GLN:HB3	1:A:470:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:PHE:HZ	1:A:579:ALA:HB1	1.84	0.43
1:A:968:GLU:HA	1:A:971:LYS:HB3	2.00	0.43
1:A:905:LEU:O	1:A:909:ILE:HG13	2.19	0.43
1:B:586:THR:HG21	1:B:591:LEU:HD23	2.00	0.43
1:B:874:SER:O	1:B:880:ARG:HD3	2.18	0.43
1:B:1083:ILE:O	1:B:1087:VAL:HG23	2.18	0.43
1:A:193:SER:HB2	2:A:1372:HOH:O	2.18	0.43
1:B:430:GLN:HB3	1:B:470:PHE:CD2	2.54	0.43
1:A:484:MSE:CE	1:A:507:ILE:HG23	2.38	0.43
1:A:948:LYS:O	1:A:952:GLU:HG3	2.19	0.43
1:B:693:LYS:HZ3	1:B:697:GLU:HG2	1.83	0.43
1:B:542:LEU:HD23	1:B:542:LEU:HA	1.82	0.43
1:B:581:TYR:O	1:B:585:LYS:HG2	2.19	0.43
1:A:120:TRP:HD1	1:A:122:GLU:CD	2.27	0.43
1:A:159:LEU:N	1:A:159:LEU:CD1	2.82	0.43
1:B:49:GLN:HB3	1:B:50:ASN:ND2	2.34	0.43
1:B:975:ASP:HB3	1:B:1013:THR:HG22	2.01	0.43
1:A:169:ALA:HA	1:A:212:LEU:CD2	2.49	0.42
1:A:799:GLN:O	1:A:803:GLU:HG2	2.19	0.42
1:B:354:VAL:O	1:B:358:ILE:HG13	2.19	0.42
1:A:473:HIS:NE2	1:A:1063:ASN:OD1	2.53	0.42
1:B:259:LYS:HG2	1:B:298:LEU:HD21	2.00	0.42
1:B:940:SER:HA	1:B:995:LEU:HD13	2.00	0.42
1:B:1060:LEU:O	1:B:1064:SER:HB3	2.18	0.42
1:A:915:ASP:O	1:A:921:ARG:HD2	2.19	0.42
1:A:921:ARG:HB3	1:A:953:ILE:HD11	2.01	0.42
1:A:41:LEU:C	1:A:41:LEU:CD2	2.93	0.42
1:A:585:LYS:HE3	1:A:585:LYS:HB3	1.87	0.42
1:B:726:LEU:HD23	1:B:783:PHE:CD1	2.54	0.42
1:A:231:ASN:O	1:A:235:ILE:HG12	2.19	0.42
1:B:397:ASP:HB3	1:B:967:ASP:HB2	2.02	0.42
1:B:584:ILE:CD1	1:B:599:ILE:HD12	2.50	0.42
1:B:872:CYS:O	1:B:880:ARG:HD2	2.20	0.42
1:A:377:ILE:HD12	1:A:377:ILE:HA	1.91	0.42
1:B:586:THR:HG21	1:B:591:LEU:HB3	2.02	0.42
1:B:1041:PRO:O	1:B:1044:ILE:HG13	2.20	0.42
1:B:74:SER:C	1:B:75:LEU:HD22	2.44	0.42
1:B:762:GLU:OE2	1:B:762:GLU:HA	2.20	0.42
1:B:1112:ILE:HD12	1:B:1112:ILE:HA	1.85	0.42
1:A:289:ARG:HH11	1:A:289:ARG:CG	2.32	0.42
1:A:430:GLN:HB3	1:A:470:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:LYS:H	1:A:478:LYS:HG3	1.64	0.42
1:B:915:ASP:O	1:B:921:ARG:HD2	2.20	0.42
1:A:581:TYR:CZ	1:A:616:THR:HG22	2.55	0.41
1:B:458:LYS:HE2	1:B:498:LYS:HZ2	1.81	0.41
1:B:1042:LYS:HE3	1:B:1046:ILE:HG13	2.02	0.41
1:B:192:SER:O	1:B:196:GLU:HG2	2.21	0.41
1:B:343:SER:HB2	1:B:383:VAL:HB	2.02	0.41
1:B:709:ALA:O	1:B:713:MSE:HG3	2.20	0.41
1:B:998:LEU:HD22	1:B:1002:ILE:HD11	2.02	0.41
1:A:817:ILE:O	1:A:817:ILE:HG22	2.21	0.41
1:A:895:ARG:HA	1:A:934:TYR:CD2	2.55	0.41
1:A:480:LEU:O	1:A:484:MSE:HB2	2.20	0.41
1:A:932:ILE:O	1:A:991:LYS:HE2	2.20	0.41
1:A:1039:GLU:OE1	1:A:1039:GLU:HA	2.20	0.41
1:B:100:ARG:HH21	1:B:141:THR:HG21	1.85	0.41
1:B:332:ASN:HD22	1:B:332:ASN:HA	1.57	0.41
1:B:500:ARG:O	1:B:504:VAL:HG23	2.20	0.41
1:B:781:ARG:NH2	1:B:844:ASP:OD1	2.52	0.41
1:B:895:ARG:NH1	2:B:1237:HOH:O	2.53	0.41
1:B:90:SER:O	1:B:94:GLU:HB2	2.21	0.41
1:B:96:LYS:HE3	1:B:98:ALA:H	1.85	0.41
1:B:1112:ILE:N	1:B:1112:ILE:HD13	2.35	0.41
1:A:192:SER:C	1:A:195:ILE:HG23	2.45	0.41
1:A:389:PRO:HD2	1:A:833:GLU:OE2	2.21	0.41
1:B:939:VAL:O	1:B:942:ILE:HG13	2.21	0.41
1:A:192:SER:CA	1:A:195:ILE:HG23	2.51	0.41
1:A:686:GLU:H	1:A:686:GLU:HG3	1.67	0.41
1:B:926:TYR:CZ	1:B:930:LEU:HD11	2.55	0.41
1:A:83:VAL:O	1:A:87:LEU:HD12	2.21	0.41
1:A:202:ASN:HB3	1:A:205:TYR:CD2	2.55	0.41
1:A:551:ALA:HB1	1:A:594:SER:HB3	2.03	0.41
1:A:1057:ARG:HH12	1:A:1058:ILE:HG13	1.86	0.41
1:A:781:ARG:HH21	1:A:844:ASP:CG	2.28	0.40
1:A:894:MSE:CB	1:A:898:ASN:HB2	2.51	0.40
1:B:122:GLU:OE2	1:B:122:GLU:N	2.42	0.40
1:B:810:GLY:HA2	1:B:815:GLN:NE2	2.36	0.40
1:A:580:ALA:O	1:A:584:ILE:HG12	2.21	0.40
1:A:689:GLU:HB2	1:A:690:PRO:HD3	2.02	0.40
1:B:627:GLN:CD	1:B:662:ILE:HD12	2.46	0.40
1:B:901:ILE:O	1:B:905:LEU:HB2	2.21	0.40
1:B:853:LEU:HA	1:B:853:LEU:HD12	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:ASN:OD1	1:A:1063:ASN:C	2.64	0.40
1:B:757:LEU:HA	1:B:757:LEU:HD13	1.81	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:ASP:OD1	1:B:1110:GLN:NE2[1_546]	1.86	0.34

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	1010/1116 (90%)	981 (97%)	26 (3%)	3 (0%)	36	43
1	B	1018/1116 (91%)	993 (98%)	25 (2%)	0	100	100
All	All	2028/2232 (91%)	1974 (97%)	51 (2%)	3 (0%)	48	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	682	GLU
1	A	854	VAL
1	A	78	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	877/946 (93%)	806 (92%)	71 (8%)	11	12
1	B	881/946 (93%)	807 (92%)	74 (8%)	10	11
All	All	1758/1892 (93%)	1613 (92%)	145 (8%)	10	11

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	52	SER
1	A	67	GLN
1	A	79	THR
1	A	80	GLN
1	A	82	SER
1	A	85	GLN
1	A	86	SER
1	A	109	SER
1	A	110	ILE
1	A	113	GLU
1	A	159	LEU
1	A	194	LEU
1	A	195	ILE
1	A	198	GLU
1	A	200	GLU
1	A	226	GLU
1	A	247	SER
1	A	260	LEU
1	A	268	SER
1	A	289	ARG
1	A	292	LYS
1	A	316	VAL
1	A	317	GLU
1	A	333	THR
1	A	383	VAL
1	A	413	VAL
1	A	458	LYS
1	A	478	LYS
1	A	483	LEU
1	A	484	MSE
1	A	489	GLN
1	A	523	LYS
1	A	524	THR

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Mol	Chain	Res	Type
1	A	574	GLU
1	A	586	THR
1	A	608	LYS
1	A	616	THR
1	A	657	THR
1	A	658	VAL
1	A	681	LYS
1	A	682	GLU
1	A	685	LEU
1	A	686	GLU
1	A	692	LEU
1	A	697	GLU
1	A	703	TYR
1	A	725	ASN
1	A	741	VAL
1	A	754	GLU
1	A	757	LEU
1	A	802	ARG
1	A	829	LEU
1	A	830	ASP
1	A	863	THR
1	A	873	GLN
1	A	875	LYS
1	A	904	LEU
1	A	906	GLU
1	A	919	GLU
1	A	956	VAL
1	A	964	THR
1	A	965	GLU
1	A	966	ASP
1	A	999	GLU
1	A	1005	LEU
1	A	1021	ILE
1	A	1037	ILE
1	A	1044	ILE
1	A	1061	GLU
1	A	1111	VAL
1	B	41	LEU
1	B	47	ILE
1	B	49	GLN
1	B	59	LEU
1	B	66	LYS

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Mol	Chain	Res	Type
1	B	74	SER
1	B	76	ASP
1	B	89	ASN
1	B	90	SER
1	B	96	LYS
1	B	97	ASP
1	B	115	LEU
1	B	118	LYS
1	B	137	LYS
1	B	175	SER
1	B	211	SER
1	B	260	LEU
1	B	268	SER
1	B	290	LYS
1	B	332	ASN
1	B	413	VAL
1	B	435	ARG
1	B	439	GLN
1	B	446	ASP
1	B	452	LYS
1	B	456	ILE
1	B	489	GLN
1	B	538	GLN
1	B	539	ILE
1	B	540	GLU
1	B	564	VAL
1	B	585	LYS
1	B	586	THR
1	B	678	ILE
1	B	685	LEU
1	B	689[A]	GLU
1	B	689[B]	GLU
1	B	693	LYS
1	B	725	ASN
1	B	741	VAL
1	B	757	LEU
1	B	765	GLU
1	B	779	MSE
1	B	781	ARG
1	B	789	MSE
1	B	817	ILE
1	B	853	LEU

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Mol	Chain	Res	Type
1	B	860	VAL
1	B	863	THR
1	B	875	LYS
1	B	902	GLN
1	B	905	LEU
1	B	906	GLU
1	B	955	SER
1	B	999	GLU
1	B	1002	ILE
1	B	1021	ILE
1	B	1037	ILE
1	B	1044	ILE
1	B	1052	GLU
1	B	1059	GLU
1	B	1061	GLU
1	B	1068	ARG
1	B	1069	GLU
1	B	1072	LEU
1	B	1083	ILE
1	B	1085	GLN
1	B	1094	LEU
1	B	1095	ASN
1	B	1099	ASN
1	B	1102	VAL
1	B	1104	GLN
1	B	1111	VAL
1	B	1112	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	80	GLN
1	A	93	ASN
1	A	204	GLN
1	A	248	GLN
1	A	415	GLN
1	A	424	GLN
1	A	453	HIS
1	A	494	GLN
1	A	531	GLN
1	A	859	GLN

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Mol	Chain	Res	Type
1	A	914	ASN
1	A	993	GLN
1	A	1032	GLN
1	A	1096	GLN
1	A	1097	GLN
1	B	67	GLN
1	B	93	ASN
1	B	156	ASN
1	B	173	ASN
1	B	186	GLN
1	B	322	ASN
1	B	332	ASN
1	B	439	GLN
1	B	485	ASN
1	B	531	GLN
1	B	538	GLN
1	B	799	GLN
1	B	902	GLN
1	B	1097	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	1009/1116 (90%)	0.29	54 (5%)	31	37	9, 39, 76, 119	1 (0%)
1	B	1016/1116 (91%)	0.28	54 (5%)	32	37	13, 39, 79, 108	1 (0%)
All	All	2025/2232 (90%)	0.29	108 (5%)	32	37	9, 39, 77, 119	2 (0%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1113	ALA	6.7
1	B	1098	PHE	5.7
1	B	817	ILE	4.6
1	A	964	THR	4.5
1	B	1110	GLN	4.1
1	B	1112	ILE	4.0
1	A	59	LEU	3.9
1	A	41	LEU	3.8
1	B	1100	GLY	3.8
1	B	75	LEU	3.8
1	A	40	ALA	3.7
1	A	55	GLY	3.6
1	A	963	ALA	3.6
1	A	42	PRO	3.6
1	A	703	TYR	3.5
1	B	1099	ASN	3.4
1	B	1000	HIS	3.4
1	A	45	ILE	3.3
1	A	581	TYR	3.2
1	B	73	GLY	3.1
1	B	1101	ALA	3.1
1	A	195	ILE	3.1
1	B	1103	ALA	3.0
1	A	204	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	64	ALA	3.0
1	B	79	THR	3.0
1	A	76	ASP	3.0
1	B	830	ASP	3.0
1	B	968	GLU	2.9
1	A	43	ALA	2.9
1	B	703	TYR	2.9
1	A	53	ASN	2.9
1	A	54	ASP	2.9
1	B	657	THR	2.9
1	A	829	LEU	2.9
1	A	657	THR	2.8
1	B	76	ASP	2.8
1	A	1075	ARG	2.8
1	B	831	ALA	2.7
1	B	67	GLN	2.7
1	A	46	HIS	2.7
1	B	966	ASP	2.7
1	B	48	LEU	2.6
1	B	60	ALA	2.6
1	A	564	VAL	2.6
1	B	324	ASP	2.6
1	A	79	THR	2.6
1	B	59	LEU	2.6
1	B	41	LEU	2.5
1	B	81	THR	2.5
1	B	330	GLU	2.5
1	A	44	LEU	2.5
1	B	736	PRO	2.5
1	A	78	ALA	2.4
1	A	965	GLU	2.4
1	A	52	SER	2.4
1	A	68	VAL	2.4
1	A	249	LEU	2.4
1	A	1072	LEU	2.4
1	B	962	LEU	2.4
1	B	94	GLU	2.4
1	A	65	ARG	2.4
1	A	1099	ASN	2.4
1	A	435	ARG	2.3
1	A	1071	ASN	2.3
1	B	89	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	332	ASN	2.3
1	B	581	TYR	2.3
1	B	77	ALA	2.3
1	A	201	ILE	2.3
1	A	859	GLN	2.3
1	A	658	VAL	2.3
1	A	1038	ASN	2.3
1	A	574	GLU	2.3
1	A	817	ILE	2.3
1	A	70	LYS	2.2
1	A	324	ASP	2.2
1	B	95	GLY	2.2
1	B	57	LYS	2.2
1	A	112	SER	2.2
1	B	855	GLY	2.2
1	A	69	SER	2.2
1	A	630	TYR	2.2
1	B	630	TYR	2.2
1	B	1095	ASN	2.2
1	B	51	SER	2.2
1	B	47	ILE	2.1
1	A	1069	GLU	2.1
1	B	999	GLU	2.1
1	A	51	SER	2.1
1	B	50	ASN	2.1
1	B	97	ASP	2.1
1	B	203	PRO	2.1
1	B	1085	GLN	2.1
1	B	969	ALA	2.1
1	A	87	LEU	2.1
1	A	685	LEU	2.1
1	B	72	TRP	2.1
1	A	81	THR	2.1
1	A	155	ALA	2.1
1	A	679	ALA	2.1
1	A	473	HIS	2.1
1	B	1097	GLN	2.0
1	B	735	VAL	2.0
1	B	854	VAL	2.0
1	B	70	LYS	2.0
1	A	1113	ALA	2.0
1	B	56	ILE	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.