Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2022 – 03:07 AM EST

PDB ID	:	5VCH
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 following versions of software and data (see references ⓘ) were used in the production of this report:

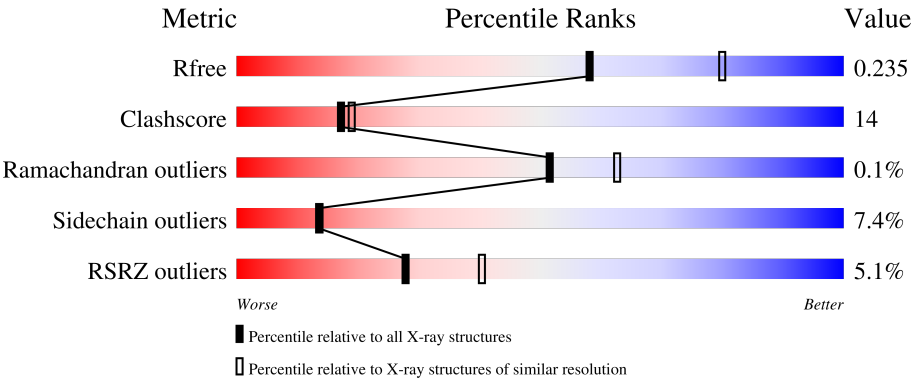
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (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 <=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	4% 66% 23% · 9%
1	B	1116	5% 66% 23% · 8%

2 Entry composition (i)

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.

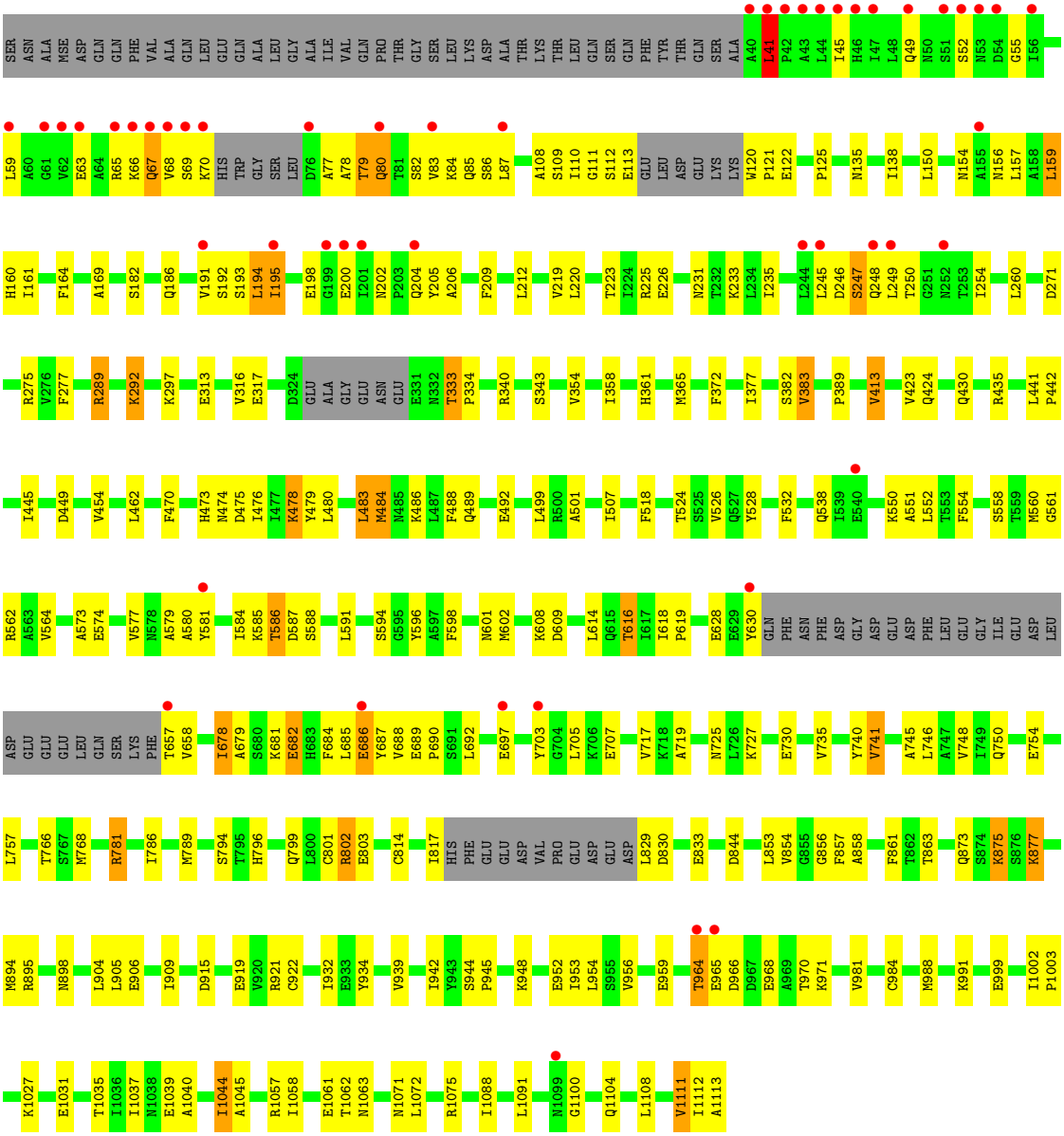
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	195	Total	O	0	0
			195	195		
2	B	215	Total	O	0	0
			215	215		

3 Residue-property plots (i)

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.

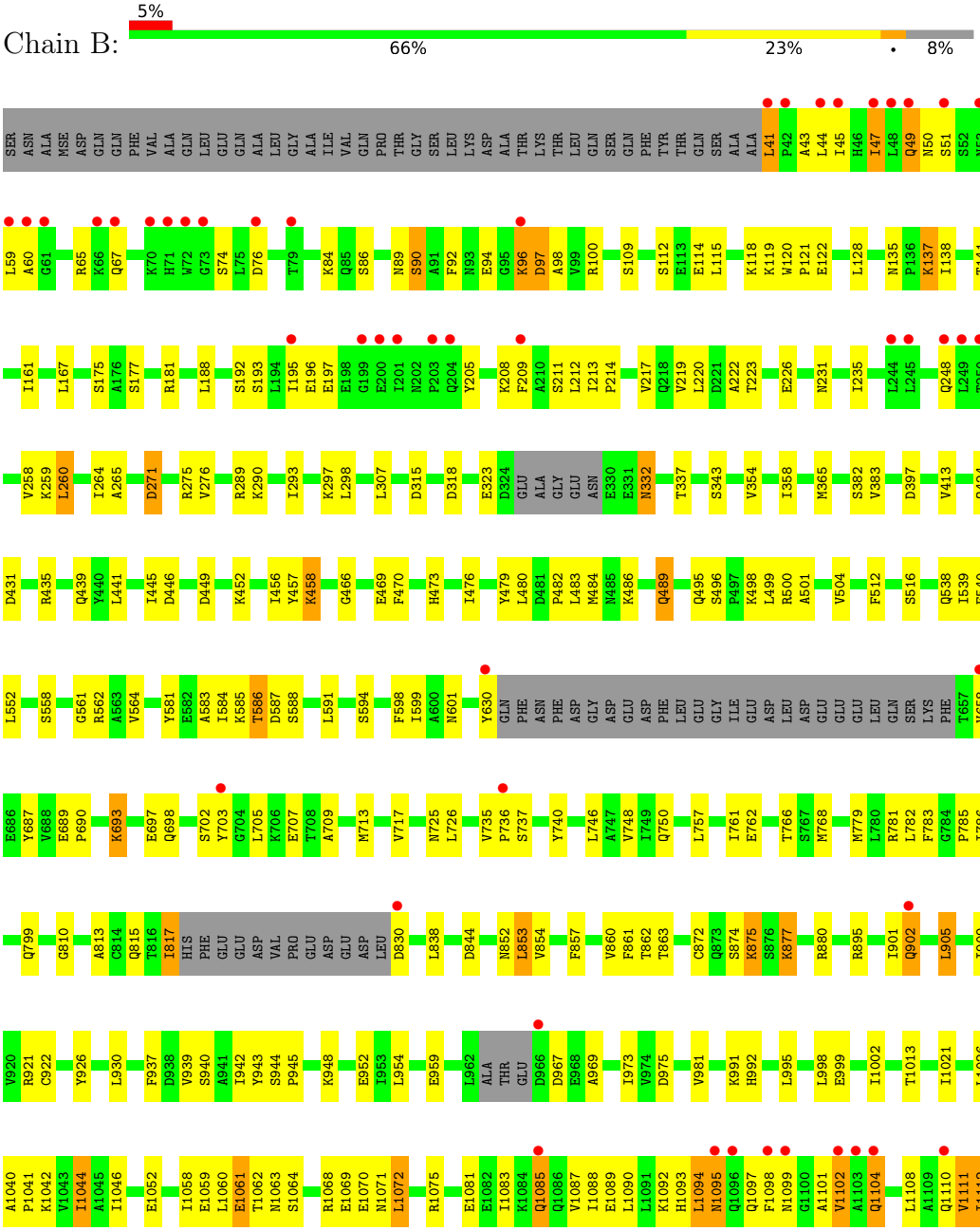
- Molecule 1: Kap123

Chain A: 



• Molecule 1: Kap123

Chain B:



4 Data and refinement statistics (i)

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 43.83 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.8 (33.00-2.35) 97.8 (43.83-2.35)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.210 , 0.235 0.210 , 0.235	Depositor DCC
R_{free} test set	2000 reflections (1.93%)	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 , 57.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.53	1/8000 (0.0%)	0.65	6/10842 (0.1%)
1	B	0.46	0/8059	0.61	0/10924
All	All	0.50	1/16059 (0.0%)	0.63	6/21766 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	856	GLY	C-O	-5.78	1.14	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	678	ILE	CB-CA-C	-9.64	92.31	111.60
1	A	679	ALA	CB-CA-C	-9.55	95.77	110.10
1	A	678	ILE	CG1-CB-CG2	-7.93	93.96	111.40
1	A	679	ALA	N-CA-CB	5.63	117.98	110.10
1	A	41	LEU	CA-CB-CG	5.54	128.03	115.30
1	A	853	LEU	N-CA-C	5.38	125.53	111.00

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	211	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7947	0	8015	235	1
2	A	195	0	0	4	0
2	B	215	0	0	14	0
All	All	16249	38	15993	442	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 (442) 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
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: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: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:516:SER:OG	2:B:1202:HOH:O	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:705:LEU:O	1:B:705:LEU:HG	2.06	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:260:LEU:C	1:B:260:LEU:HD23	2.29	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
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: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:B:877:LYS:HD2	1:B:877:LYS:C	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:MSE:HE2	1:A:602:MSE:HA	1.94	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:122:GLU:C	1:A:125:PRO:HD2	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1070:GLU:H	1:B:1070:GLU:CD	2.20	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: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: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: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
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: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:441:LEU:HB2	1:A:442:PRO:HD3	1.98	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: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: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: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:441:LEU:O	1:A:445:ILE:HG12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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:137:LYS:O	1:B:137:LYS:HG3	2.20	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: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: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: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:458:LYS:HE2	1:B:498:LYS:HZ2	1.81	0.41
1:B:781:ARG:HH22	1:B:844:ASP:CG	2.23	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:877:LYS:C	1:A:877:LYS:HD2	2.41	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:901:ILE:O	1:B:905:LEU:HB2	2.21	0.40
1:B:687:TYR:C	1:B:690:PRO:HD2	2.42	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:246:ASP:OD1	1:A:246:ASP:C	2.60	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%)	41 47
1	B	1018/1116 (91%)	993 (98%)	25 (2%)	0	100 100
All	All	2028/2232 (91%)	1974 (97%)	51 (2%)	3 (0%)	51 63

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%)	810 (92%)	67 (8%)	13	13
1	B	881/946 (93%)	818 (93%)	63 (7%)	14	14
All	All	1758/1892 (93%)	1628 (93%)	130 (7%)	13	14

All (130) 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	289	ARG
1	A	292	LYS
1	A	317	GLU
1	A	333	THR
1	A	383	VAL
1	A	413	VAL
1	A	478	LYS
1	A	483	LEU
1	A	484	MSE
1	A	489	GLN
1	A	524	THR
1	A	538	GLN
1	A	574	GLU
1	A	586	THR
1	A	608	LYS

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Mol	Chain	Res	Type
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	757	LEU
1	A	781	ARG
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	877	LYS
1	A	904	LEU
1	A	906	GLU
1	A	919	GLU
1	A	922	CYS
1	A	956	VAL
1	A	964	THR
1	A	965	GLU
1	A	966	ASP
1	A	999	GLU
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	74	SER
1	B	76	ASP
1	B	89	ASN
1	B	90	SER
1	B	96	LYS

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Mol	Chain	Res	Type
1	B	97	ASP
1	B	118	LYS
1	B	119	LYS
1	B	137	LYS
1	B	175	SER
1	B	211	SER
1	B	260	LEU
1	B	271	ASP
1	B	289	ARG
1	B	290	LYS
1	B	332	ASN
1	B	413	VAL
1	B	431	ASP
1	B	435	ARG
1	B	446	ASP
1	B	452	LYS
1	B	456	ILE
1	B	458	LYS
1	B	489	GLN
1	B	538	GLN
1	B	539	ILE
1	B	540	GLU
1	B	586	THR
1	B	678	ILE
1	B	685	LEU
1	B	693	LYS
1	B	725	ASN
1	B	789	MSE
1	B	817	ILE
1	B	853	LEU
1	B	860	VAL
1	B	863	THR
1	B	875	LYS
1	B	877	LYS
1	B	902	GLN
1	B	905	LEU
1	B	922	CYS
1	B	999	GLU
1	B	1021	ILE
1	B	1037	ILE
1	B	1044	ILE
1	B	1052	GLU

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Mol	Chain	Res	Type
1	B	1059	GLU
1	B	1061	GLU
1	B	1069	GLU
1	B	1072	LEU
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 (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	80	GLN
1	A	204	GLN
1	A	240	ASN
1	A	248	GLN
1	A	852	ASN
1	A	993	GLN
1	A	1032	GLN
1	A	1097	GLN
1	B	49	GLN
1	B	67	GLN
1	B	332	ASN
1	B	439	GLN
1	B	799	GLN
1	B	873	GLN
1	B	1097	GLN

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 monosaccharides 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, 95^{th} 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%)	0.25	50 (4%)	28	41	17, 39, 76, 119	0
1	B	1016/1116 (91%)	0.23	53 (5%)	27	39	13, 39, 79, 108	0
All	All	2025/2232 (90%)	0.24	103 (5%)	28	40	13, 39, 77, 119	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1113	ALA	6.3
1	A	43	ALA	5.6
1	B	1098	PHE	5.6
1	A	54	ASP	5.2
1	B	703	TYR	4.9
1	B	47	ILE	4.8
1	A	42	PRO	4.7
1	B	1103	ALA	4.7
1	B	41	LEU	4.5
1	A	70	LYS	4.5
1	B	73	GLY	4.5
1	A	59	LEU	4.5
1	A	62	VAL	4.5
1	B	249	LEU	4.5
1	A	703	TYR	4.5
1	A	61	GLY	4.3
1	A	200	GLU	4.2
1	A	69	SER	4.1
1	A	965	GLU	4.1
1	A	41	LEU	4.0
1	A	76	ASP	4.0
1	A	56	ILE	3.9
1	A	155	ALA	3.8
1	A	199	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	245	LEU	3.8
1	A	195	ILE	3.7
1	B	1110	GLN	3.7
1	B	199	GLY	3.7
1	A	45	ILE	3.6
1	A	630	TYR	3.6
1	A	964	THR	3.6
1	A	657	THR	3.5
1	A	245	LEU	3.5
1	B	59	LEU	3.4
1	B	44	LEU	3.4
1	B	48	LEU	3.4
1	B	155	ALA	3.4
1	B	70	LYS	3.4
1	B	209	PHE	3.4
1	A	46	HIS	3.3
1	B	49	GLN	3.3
1	A	44	LEU	3.3
1	A	201	ILE	3.3
1	A	53	ASN	3.3
1	A	52	SER	3.2
1	A	65	ARG	3.2
1	B	630	TYR	3.2
1	B	79	THR	3.1
1	B	72	TRP	3.1
1	A	248	GLN	3.1
1	B	248	GLN	3.1
1	B	658	VAL	3.0
1	B	60	ALA	3.0
1	B	200	GLU	3.0
1	B	736	PRO	3.0
1	A	63	GLU	3.0
1	A	40	ALA	2.9
1	B	902	GLN	2.9
1	A	1099	ASN	2.8
1	B	71	HIS	2.8
1	B	1096	GLN	2.8
1	B	57	LYS	2.8
1	A	204	GLN	2.8
1	B	1102	VAL	2.7
1	B	45	ILE	2.7
1	B	966	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	66	LYS	2.6
1	B	195	ILE	2.6
1	A	49	GLN	2.6
1	A	67	GLN	2.6
1	A	68	VAL	2.5
1	B	830	ASP	2.5
1	B	244	LEU	2.5
1	A	83	VAL	2.4
1	B	42	PRO	2.4
1	B	204	GLN	2.4
1	B	203	PRO	2.4
1	A	697	GLU	2.3
1	B	51	SER	2.3
1	A	252	ASN	2.3
1	B	53	ASN	2.3
1	B	67	GLN	2.3
1	A	51	SER	2.2
1	B	1104	GLN	2.2
1	B	61	GLY	2.2
1	A	249	LEU	2.2
1	A	686	GLU	2.2
1	B	54	ASP	2.2
1	A	66	LYS	2.2
1	A	540	GLU	2.2
1	A	581	TYR	2.1
1	B	250	THR	2.1
1	B	201	ILE	2.1
1	B	76	ASP	2.1
1	B	1095	ASN	2.1
1	A	191	VAL	2.1
1	B	96	LYS	2.1
1	A	47	ILE	2.1
1	A	80	GLN	2.1
1	A	87	LEU	2.0
1	A	244	LEU	2.0
1	B	1085	GLN	2.0
1	B	1099	ASN	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 monosaccharides 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.