WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 10:53 PM EDT

PDB ID	:	3KHZ
Title	:	Crystal Structure of R350A mutant of Staphylococcus aureus metallopeptidase (Sapep/DapE) in the apo-form
Authors	:	Girish, T.S.; Gopal, B.
Deposited on	:	2009-10-31
Resolution	:	2.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

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 2.50 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	Percentile Ranks	Value
Rfree		0.267
Clashscore		31
Ramachandran outliers		0.2%
Sidechain outliers		13.0%
RSRZ outliers		0.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
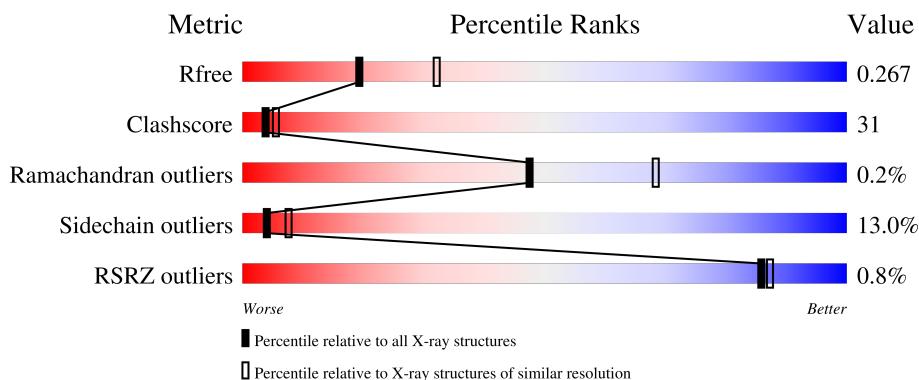
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	492	54% · 27% · 6% · 12%
1	B	492	52% · 29% · 7% · 12%
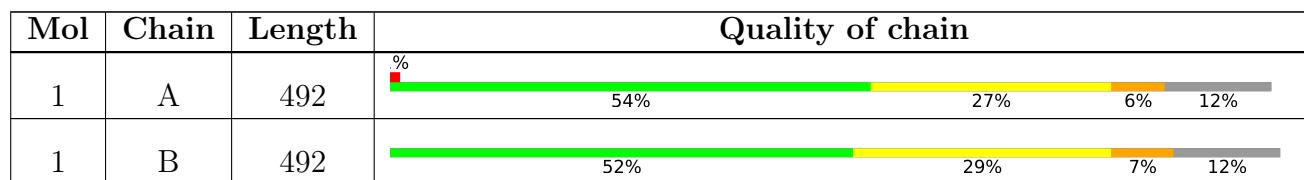
2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 6880 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 Putative dipeptidase SACOL1801.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total 3382	C 2154	N 558	O 655	S 15	17	0	0
1	B	435	Total 3385	C 2153	N 552	O 664	S 16	2	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q5HF23
A	-21	GLY	-	expression tag	UNP Q5HF23
A	-20	SER	-	expression tag	UNP Q5HF23
A	-19	SER	-	expression tag	UNP Q5HF23
A	-18	HIS	-	expression tag	UNP Q5HF23
A	-17	HIS	-	expression tag	UNP Q5HF23
A	-16	HIS	-	expression tag	UNP Q5HF23
A	-15	HIS	-	expression tag	UNP Q5HF23
A	-14	HIS	-	expression tag	UNP Q5HF23
A	-13	HIS	-	expression tag	UNP Q5HF23
A	-12	SER	-	expression tag	UNP Q5HF23
A	-11	SER	-	expression tag	UNP Q5HF23
A	-10	GLY	-	expression tag	UNP Q5HF23
A	-9	LEU	-	expression tag	UNP Q5HF23
A	-8	VAL	-	expression tag	UNP Q5HF23
A	-7	PRO	-	expression tag	UNP Q5HF23
A	-6	ARG	-	expression tag	UNP Q5HF23
A	-5	GLY	-	expression tag	UNP Q5HF23
A	-4	SER	-	expression tag	UNP Q5HF23
A	-3	HIS	-	expression tag	UNP Q5HF23
A	-2	MET	-	expression tag	UNP Q5HF23
A	-1	ALA	-	expression tag	UNP Q5HF23
A	0	SER	-	expression tag	UNP Q5HF23
A	350	ALA	ARG	engineered mutation	UNP Q5HF23
B	-22	MET	-	expression tag	UNP Q5HF23

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	GLY	-	expression tag	UNP Q5HF23
B	-20	SER	-	expression tag	UNP Q5HF23
B	-19	SER	-	expression tag	UNP Q5HF23
B	-18	HIS	-	expression tag	UNP Q5HF23
B	-17	HIS	-	expression tag	UNP Q5HF23
B	-16	HIS	-	expression tag	UNP Q5HF23
B	-15	HIS	-	expression tag	UNP Q5HF23
B	-14	HIS	-	expression tag	UNP Q5HF23
B	-13	HIS	-	expression tag	UNP Q5HF23
B	-12	SER	-	expression tag	UNP Q5HF23
B	-11	SER	-	expression tag	UNP Q5HF23
B	-10	GLY	-	expression tag	UNP Q5HF23
B	-9	LEU	-	expression tag	UNP Q5HF23
B	-8	VAL	-	expression tag	UNP Q5HF23
B	-7	PRO	-	expression tag	UNP Q5HF23
B	-6	ARG	-	expression tag	UNP Q5HF23
B	-5	GLY	-	expression tag	UNP Q5HF23
B	-4	SER	-	expression tag	UNP Q5HF23
B	-3	HIS	-	expression tag	UNP Q5HF23
B	-2	MET	-	expression tag	UNP Q5HF23
B	-1	ALA	-	expression tag	UNP Q5HF23
B	0	SER	-	expression tag	UNP Q5HF23
B	350	ALA	ARG	engineered mutation	UNP Q5HF23

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	69	Total　O 69　　69	0	0
2	B	44	Total　O 44　　44	0	0

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: Putative dipeptidase SACOL1801

Chain A:

• Molecule 1: Putative dipeptidase SACOL1801

Chain B:
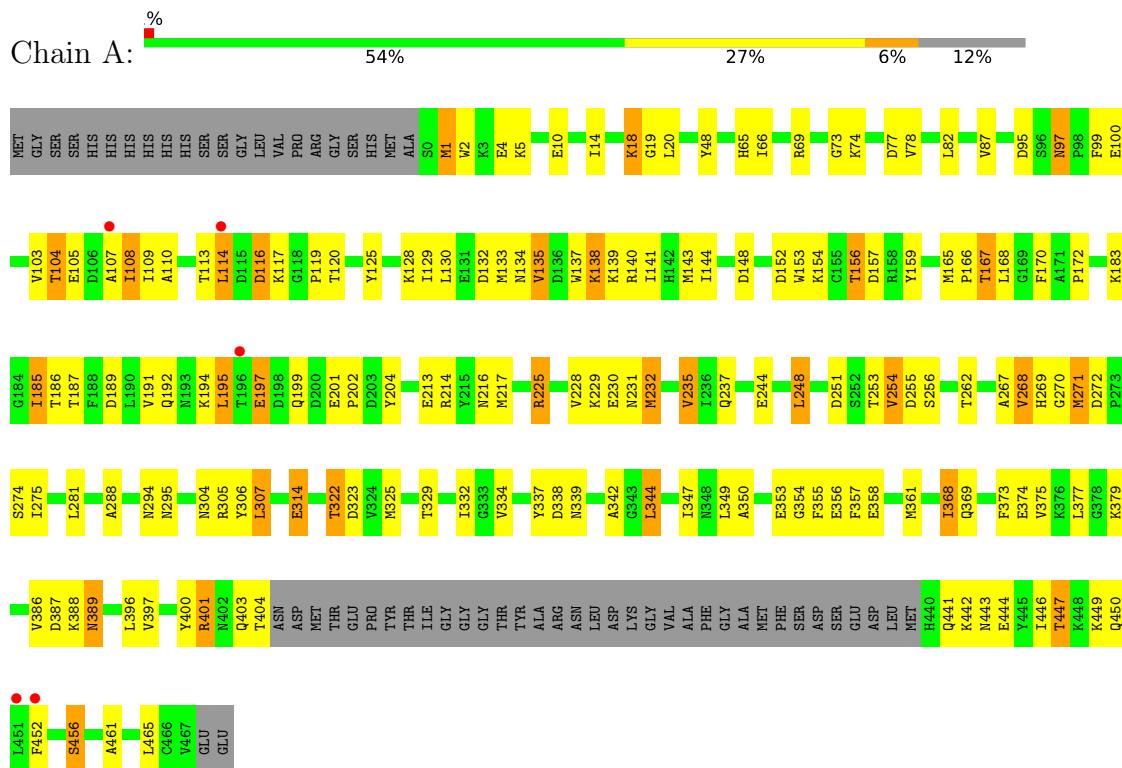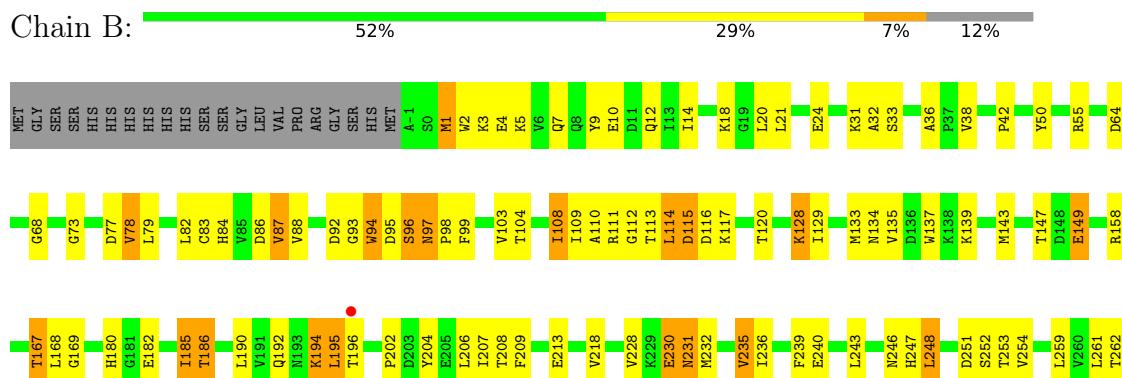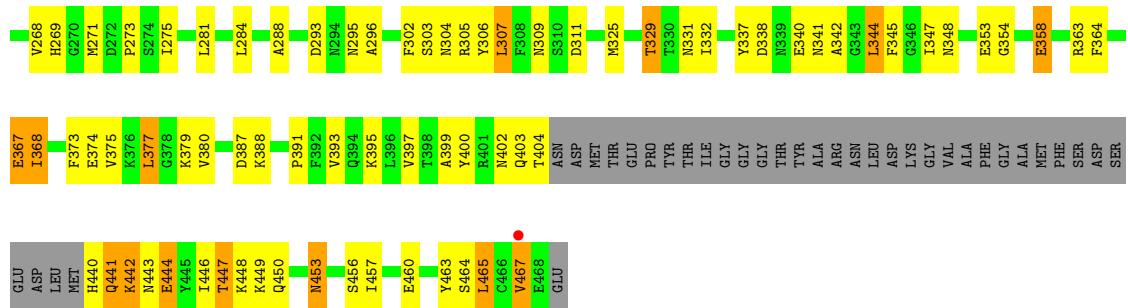
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.75Å 133.52Å 67.71Å 90.00° 95.59° 90.00°	Depositor
Resolution (Å)	49.02 – 2.50 49.02 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.02-2.50) 100.0 (49.02-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.24 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.208 , 0.269 0.215 , 0.267	Depositor DCC
R_{free} test set	1984 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6880	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.68	0/3457	0.72	4/4691 (0.1%)
1	B	0.67	0/3460	0.70	1/4700 (0.0%)
All	All	0.67	0/6917	0.71	5/9391 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	248	LEU	CA-CB-CG	5.84	128.73	115.30
1	A	272	ASP	N-CA-C	-5.67	95.68	111.00
1	A	344	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	116	ASP	CB-CA-C	5.33	121.07	110.40
1	B	94	TRP	CB-CA-C	-5.17	100.06	110.40

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	3382	0	3220	197	0
1	B	3385	0	3195	208	0
2	A	69	0	0	5	0
2	B	44	0	0	6	0
All	All	6880	0	6415	404	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 31.

All (404) 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:108:ILE:HD12	1:A:109:ILE:N	1.45	1.31
1:B:93:GLY:N	1:B:442:LYS:HD2	1.44	1.28
1:A:108:ILE:HD12	1:A:108:ILE:C	1.49	1.24
1:A:357:PHE:CE1	1:A:361:MET:CE	2.32	1.12
1:A:447:THR:HG22	1:A:450:GLN:H	1.00	1.11
1:A:217:MET:HE2	1:A:269:HIS:HA	1.30	1.10
1:B:92:ASP:O	1:B:442:LYS:HD3	1.51	1.09
1:A:386:VAL:HG22	1:A:389:ASN:HB2	1.37	1.06
1:A:195:LEU:HD12	1:A:197:GLU:HG3	1.34	1.06
1:A:20:LEU:HG	1:A:117:LYS:HD3	1.38	1.05
1:A:217:MET:CE	1:A:269:HIS:HA	1.86	1.04
1:B:92:ASP:HB2	1:B:93:GLY:HA2	1.38	1.03
1:A:271:MET:HA	1:A:271:MET:CE	1.89	1.02
1:B:395:LYS:HE3	1:B:465:LEU:CD1	1.88	1.02
1:A:447:THR:CG2	1:A:450:GLN:H	1.73	1.01
1:B:186:THR:HG22	1:B:379:LYS:O	1.60	1.01
1:B:93:GLY:H	1:B:442:LYS:HD2	0.88	1.00
1:A:186:THR:HG23	1:A:379:LYS:O	1.62	1.00
1:B:194:LYS:H	1:B:194:LYS:HD3	1.27	0.98
1:B:354:GLY:HA2	2:B:472:HOH:O	1.62	0.98
1:B:395:LYS:HE3	1:B:465:LEU:HD11	1.45	0.98
1:B:447:THR:HG22	1:B:450:GLN:H	1.27	0.97
1:B:93:GLY:N	1:B:442:LYS:CD	2.26	0.97
1:B:375:VAL:HG12	1:B:377:LEU:CD1	1.95	0.96
1:A:108:ILE:C	1:A:108:ILE:CD1	2.30	0.96
1:A:447:THR:HG22	1:A:450:GLN:N	1.79	0.96
1:B:95:ASP:N	1:B:443:ASN:HD21	1.63	0.95
1:A:108:ILE:CD1	1:A:109:ILE:N	2.29	0.95
1:A:271:MET:HE1	1:A:350:ALA:HB2	1.48	0.94
1:B:12:GLN:HG3	2:B:476:HOH:O	1.68	0.93
1:B:186:THR:HG21	1:B:380:VAL:HG22	1.46	0.93
1:A:195:LEU:HB2	1:A:295:ASN:HD21	1.32	0.93
1:A:386:VAL:CG2	1:A:389:ASN:HB2	1.99	0.92
1:A:104:THR:HG22	1:A:107:ALA:H	1.32	0.91
1:A:104:THR:HG23	1:A:105:GLU:N	1.83	0.91
1:B:186:THR:HG23	1:B:380:VAL:HA	1.49	0.91
1:B:180:HIS:ND1	1:B:325:MET:HE2	1.86	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:THR:CG2	1:B:380:VAL:HG22	2.01	0.91
1:B:21:LEU:CD1	1:B:108:ILE:HD11	2.01	0.90
1:B:95:ASP:H	1:B:443:ASN:HD21	0.90	0.89
1:A:322:THR:CG2	1:A:325:MET:H	1.86	0.88
1:A:357:PHE:CE1	1:A:361:MET:HE1	2.08	0.88
1:B:93:GLY:H	1:B:442:LYS:CD	1.80	0.88
1:B:111:ARG:NH2	1:B:440:HIS:HA	1.89	0.88
1:B:268:VAL:HG11	1:B:275:ILE:HG22	1.56	0.87
1:A:78:VAL:H	1:A:167:THR:HG22	1.38	0.87
1:B:129:ILE:HG22	1:B:133:MET:HE3	1.57	0.86
1:B:375:VAL:HG12	1:B:377:LEU:HD12	1.55	0.86
1:A:195:LEU:CB	1:A:295:ASN:HD21	1.88	0.86
1:B:447:THR:CG2	1:B:450:GLN:H	1.87	0.86
1:B:440:HIS:O	1:B:441:GLN:O	1.93	0.86
1:B:186:THR:CG2	1:B:380:VAL:HA	2.05	0.85
1:B:113:THR:HB	1:B:446:ILE:HG22	1.59	0.85
1:A:185:ILE:HD13	1:A:185:ILE:C	1.96	0.85
1:A:322:THR:HG21	1:A:325:MET:CB	2.06	0.85
1:A:403:GLN:O	1:A:404:THR:CB	2.24	0.85
1:A:195:LEU:CD1	1:A:197:GLU:HG3	2.08	0.84
1:A:357:PHE:HE1	1:A:361:MET:CE	1.90	0.83
1:B:149:GLU:HG2	2:B:509:HOH:O	1.78	0.83
1:B:440:HIS:C	1:B:441:GLN:O	2.15	0.82
1:A:271:MET:HA	1:A:271:MET:HE3	1.59	0.82
1:B:393:VAL:O	1:B:397:VAL:HG23	1.80	0.82
1:A:78:VAL:HG13	1:A:166:PRO:HA	1.62	0.81
1:A:323:ASP:HB2	2:A:536:HOH:O	1.80	0.81
1:B:94:TRP:CZ3	1:B:443:ASN:HA	2.15	0.81
1:A:97:ASN:HD22	1:A:97:ASN:C	1.84	0.80
1:B:95:ASP:H	1:B:443:ASN:ND2	1.75	0.80
1:B:447:THR:HG22	1:B:450:GLN:N	1.95	0.80
1:B:5:LYS:HD2	1:B:133:MET:CE	2.13	0.79
1:A:78:VAL:H	1:A:167:THR:CG2	1.93	0.79
1:B:20:LEU:HG	1:B:117:LYS:HD3	1.64	0.79
1:B:5:LYS:HD2	1:B:133:MET:HE2	1.64	0.79
1:A:357:PHE:CE1	1:A:361:MET:HE3	2.15	0.78
1:A:104:THR:CG2	1:A:105:GLU:N	2.43	0.78
1:A:104:THR:HG23	1:A:105:GLU:H	1.48	0.78
1:B:73:GLY:HA2	1:B:137:TRP:CG	2.19	0.78
1:A:137:TRP:C	1:A:138:LYS:HD2	2.04	0.77
1:B:92:ASP:O	1:B:442:LYS:CD	2.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:MET:O	1:B:236:ILE:HG13	1.84	0.77
1:B:92:ASP:C	1:B:442:LYS:HD3	2.05	0.77
1:B:94:TRP:HA	1:B:443:ASN:ND2	1.99	0.77
1:B:21:LEU:HD12	1:B:108:ILE:HD11	1.67	0.77
1:B:447:THR:CG2	1:B:449:LYS:N	2.47	0.76
1:B:97:ASN:HD22	1:B:99:PHE:H	1.31	0.76
1:A:329:THR:OG1	1:A:350:ALA:HB3	1.86	0.76
1:A:271:MET:HA	1:A:271:MET:HE2	1.67	0.76
1:B:92:ASP:C	1:B:442:LYS:CD	2.53	0.76
1:B:447:THR:HG22	1:B:449:LYS:N	2.00	0.76
1:B:204:TYR:CE2	1:B:235:VAL:HG11	2.20	0.75
1:B:204:TYR:OH	1:B:235:VAL:HG13	1.86	0.75
1:B:194:LYS:H	1:B:194:LYS:CD	1.95	0.75
1:B:92:ASP:HB2	1:B:93:GLY:CA	2.17	0.74
1:A:307:LEU:HG	1:A:332:ILE:HD12	1.70	0.74
1:A:386:VAL:CG2	1:A:386:VAL:O	2.35	0.74
1:A:137:TRP:CZ3	1:A:141:ILE:HD11	2.22	0.74
1:B:180:HIS:ND1	1:B:325:MET:CE	2.50	0.74
1:B:231:ASN:HD22	1:B:232:MET:H	1.34	0.74
1:B:395:LYS:HE3	1:B:465:LEU:HD13	1.70	0.74
1:A:97:ASN:ND2	1:A:99:PHE:H	1.86	0.73
1:B:447:THR:HG23	1:B:449:LYS:H	1.51	0.73
1:A:130:LEU:O	1:A:135:VAL:HG13	1.88	0.73
1:B:329:THR:HG22	2:B:485:HOH:O	1.89	0.73
1:A:116:ASP:O	1:A:119:PRO:HD2	1.89	0.72
1:A:322:THR:CG2	1:A:325:MET:N	2.52	0.72
1:A:271:MET:CE	1:A:350:ALA:HB2	2.19	0.72
1:B:447:THR:CG2	1:B:449:LYS:H	2.02	0.71
1:A:357:PHE:HE1	1:A:361:MET:HE1	1.48	0.70
1:A:1:MET:HG3	1:A:2:TRP:N	2.07	0.70
1:A:195:LEU:HD12	1:A:197:GLU:CG	2.19	0.70
1:A:357:PHE:CZ	1:A:361:MET:HE3	2.26	0.69
1:B:1:MET:SD	1:B:1:MET:C	2.71	0.69
1:A:357:PHE:CZ	1:A:361:MET:CE	2.75	0.69
1:A:368:ILE:HG22	1:A:373:PHE:O	1.93	0.69
1:A:232:MET:HE1	1:A:254:VAL:HB	1.75	0.69
1:B:92:ASP:CB	1:B:93:GLY:HA2	2.09	0.69
1:B:213:GLU:OE2	1:B:213:GLU:HA	1.93	0.69
1:B:447:THR:HB	1:B:450:GLN:HG3	1.75	0.69
1:A:195:LEU:CD1	1:A:197:GLU:CG	2.71	0.68
1:A:307:LEU:HG	1:A:332:ILE:CD1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:TRP:HA	1:B:443:ASN:HD22	1.56	0.68
1:A:368:ILE:CG2	1:A:373:PHE:O	2.42	0.68
1:B:194:LYS:HD3	1:B:194:LYS:N	2.06	0.68
1:B:377:LEU:CD1	1:B:377:LEU:N	2.56	0.68
1:B:269:HIS:ND1	1:B:271:MET:HB2	2.09	0.68
1:A:194:LYS:HE2	1:A:339:ASN:O	1.94	0.68
1:B:7:GLN:O	1:B:10:GLU:HG3	1.94	0.67
1:B:32:ALA:HA	1:B:36:ALA:O	1.93	0.67
1:B:375:VAL:CG1	1:B:377:LEU:CD1	2.71	0.67
1:B:2:TRP:NE1	1:B:460:GLU:HG3	2.10	0.67
1:A:186:THR:HG22	1:A:187:THR:H	1.58	0.67
1:B:196:THR:HG22	1:B:196:THR:O	1.94	0.67
1:B:204:TYR:CE2	1:B:235:VAL:CG1	2.78	0.67
1:B:235:VAL:HG23	1:B:236:ILE:H	1.60	0.67
1:A:322:THR:HG22	1:A:325:MET:N	2.10	0.67
1:B:78:VAL:H	1:B:167:THR:CG2	2.08	0.67
1:B:235:VAL:HG23	1:B:236:ILE:N	2.11	0.66
1:B:302:PHE:HE1	1:B:368:ILE:HG12	1.59	0.66
1:B:364:PHE:CZ	1:B:368:ILE:CD1	2.78	0.66
1:A:191:VAL:HG22	1:A:344:LEU:HD23	1.76	0.66
1:B:87:VAL:HG11	1:B:111:ARG:HG3	1.78	0.66
1:A:447:THR:HG23	1:A:449:LYS:H	1.60	0.66
1:A:386:VAL:HG22	1:A:386:VAL:O	1.94	0.65
1:B:38:VAL:HG23	1:B:42:PRO:HG2	1.77	0.65
1:A:195:LEU:HD12	1:A:195:LEU:C	2.18	0.65
1:A:78:VAL:HG13	1:A:78:VAL:O	1.97	0.64
1:A:138:LYS:HD2	1:A:138:LYS:N	2.13	0.64
1:B:111:ARG:NH1	1:B:444:GLU:OE1	2.26	0.64
1:A:281:LEU:HD11	1:A:332:ILE:HG13	1.81	0.63
1:A:349:LEU:C	1:A:349:LEU:HD23	2.18	0.63
1:B:97:ASN:ND2	1:B:99:PHE:H	1.95	0.63
1:B:180:HIS:CE1	1:B:325:MET:HE2	2.33	0.63
1:A:231:ASN:OD1	1:A:232:MET:N	2.30	0.63
1:A:97:ASN:C	1:A:97:ASN:ND2	2.53	0.62
1:B:231:ASN:HD22	1:B:232:MET:N	1.98	0.62
1:B:94:TRP:CE3	1:B:443:ASN:HA	2.35	0.61
1:A:201:GLU:HG3	1:A:202:PRO:HD2	1.82	0.61
1:A:186:THR:HG22	1:A:187:THR:N	2.15	0.61
1:B:377:LEU:N	1:B:377:LEU:HD13	2.15	0.61
1:A:137:TRP:CZ3	1:A:141:ILE:CD1	2.84	0.61
1:B:111:ARG:HD3	1:B:444:GLU:OE1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:THR:CG2	1:B:380:VAL:CG2	2.78	0.61
1:B:195:LEU:HB2	1:B:295:ASN:HD21	1.65	0.61
1:A:114:LEU:CD1	1:A:446:ILE:HG13	2.31	0.61
1:A:65:HIS:HD2	2:A:493:HOH:O	1.84	0.60
1:B:377:LEU:HD13	1:B:377:LEU:H	1.66	0.60
1:A:403:GLN:HE22	1:A:456:SER:CB	2.14	0.60
1:A:447:THR:HB	1:A:450:GLN:HG3	1.83	0.60
1:A:217:MET:HE1	1:A:269:HIS:HA	1.76	0.60
1:A:228:VAL:HG12	1:A:230:GLU:O	2.02	0.60
1:B:344:LEU:CD1	1:B:344:LEU:C	2.70	0.60
1:B:329:THR:CG2	2:B:485:HOH:O	2.47	0.59
1:A:403:GLN:HE22	1:A:456:SER:HB2	1.67	0.59
1:B:77:ASP:HA	1:B:167:THR:HG21	1.83	0.59
1:A:447:THR:CG2	1:A:449:LYS:N	2.65	0.59
1:B:113:THR:HB	1:B:446:ILE:CG2	2.30	0.59
1:B:246:ASN:O	1:B:248:LEU:HD13	2.02	0.58
1:A:204:TYR:CE2	1:A:235:VAL:HG11	2.39	0.58
1:A:225:ARG:NH2	2:A:503:HOH:O	2.36	0.58
1:A:103:VAL:HG12	1:A:103:VAL:O	2.01	0.58
1:B:288:ALA:HB2	1:B:304:ASN:ND2	2.19	0.57
1:B:338:ASP:OD2	1:B:338:ASP:C	2.42	0.57
1:A:154:LYS:C	1:A:156:THR:H	2.06	0.57
1:A:255:ASP:C	1:A:255:ASP:OD1	2.41	0.57
1:A:447:THR:HG23	1:A:449:LYS:N	2.19	0.57
1:B:447:THR:HB	1:B:450:GLN:CG	2.34	0.57
1:A:357:PHE:CE1	1:A:361:MET:HE2	2.36	0.57
1:B:97:ASN:HD22	1:B:97:ASN:C	2.08	0.57
1:B:204:TYR:HE2	1:B:235:VAL:HG11	1.69	0.56
1:B:246:ASN:O	1:B:247:HIS:HB2	2.05	0.56
1:A:78:VAL:CG1	1:A:166:PRO:HA	2.34	0.56
1:A:156:THR:HG22	1:A:157:ASP:OD1	2.06	0.56
1:A:110:ALA:O	1:A:113:THR:HG23	2.06	0.56
1:B:84:HIS:HD2	1:B:86:ASP:OD1	1.89	0.56
1:A:5:LYS:HD3	1:A:133:MET:HE1	1.87	0.56
1:B:5:LYS:HD2	1:B:133:MET:HE1	1.88	0.56
1:B:358:GLU:H	1:B:358:GLU:CD	2.10	0.55
1:A:69:ARG:HD3	1:A:159:TYR:OH	2.07	0.55
1:B:3:LYS:NZ	1:B:403:GLN:O	2.29	0.55
1:B:375:VAL:CG1	1:B:377:LEU:HD11	2.37	0.55
1:A:5:LYS:HD3	1:A:133:MET:CE	2.37	0.55
1:A:375:VAL:HG12	1:A:377:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:GLU:OE2	1:B:213:GLU:CA	2.53	0.54
1:B:344:LEU:C	1:B:344:LEU:HD12	2.28	0.54
1:A:66:ILE:HD11	1:A:148:ASP:HB2	1.89	0.54
1:A:104:THR:HG22	1:A:107:ALA:N	2.13	0.54
1:A:400:TYR:C	1:A:400:TYR:CD2	2.81	0.54
1:A:267:ALA:O	1:A:268:VAL:HG23	2.08	0.54
1:B:190:LEU:CD1	1:B:347:ILE:CD1	2.85	0.54
1:B:375:VAL:CG1	1:B:377:LEU:HD12	2.33	0.54
1:A:137:TRP:HZ3	1:A:141:ILE:HD11	1.68	0.54
1:B:87:VAL:CG1	1:B:88:VAL:N	2.70	0.54
1:A:194:LYS:CE	1:A:339:ASN:O	2.56	0.53
1:B:109:ILE:O	1:B:110:ALA:HB2	2.08	0.53
1:B:82:LEU:N	1:B:82:LEU:HD23	2.23	0.53
1:A:14:ILE:HG22	1:A:18:LYS:HE2	1.88	0.53
1:A:168:LEU:N	1:A:168:LEU:HD23	2.23	0.53
1:B:77:ASP:CA	1:B:167:THR:HG21	2.39	0.53
1:A:154:LYS:C	1:A:156:THR:N	2.61	0.53
1:A:288:ALA:HB2	1:A:304:ASN:ND2	2.24	0.53
1:A:187:THR:HA	1:A:347:ILE:O	2.09	0.53
1:A:77:ASP:OD2	1:A:139:LYS:HE3	2.09	0.53
1:B:64:ASP:OD2	1:B:158:ARG:NH1	2.42	0.53
1:B:259:LEU:HD21	1:B:261:LEU:HD21	1.89	0.53
1:A:217:MET:CE	1:A:269:HIS:CA	2.75	0.52
1:B:185:ILE:HD11	1:B:348:ASN:OD1	2.09	0.52
1:A:5:LYS:CD	1:A:133:MET:HE2	2.39	0.52
1:B:186:THR:HG22	1:B:380:VAL:HA	1.91	0.52
1:B:337:TYR:HA	1:B:342:ALA:O	2.10	0.52
1:B:442:LYS:O	1:B:443:ASN:C	2.42	0.52
1:A:185:ILE:HD13	1:A:186:THR:N	2.25	0.52
1:A:186:THR:CG2	1:A:379:LYS:O	2.46	0.52
1:A:275:ILE:HG22	1:A:275:ILE:O	2.08	0.52
1:A:97:ASN:HD22	1:A:99:PHE:H	1.56	0.52
1:B:168:LEU:N	1:B:168:LEU:HD23	2.24	0.52
1:B:404:THR:HG22	1:B:453:ASN:HD21	1.75	0.52
1:A:195:LEU:HB3	1:A:295:ASN:HD21	1.74	0.52
1:A:78:VAL:N	1:A:167:THR:CG2	2.69	0.52
1:A:189:ASP:OD1	1:A:214:ARG:NH2	2.43	0.52
1:B:204:TYR:CZ	1:B:235:VAL:HG13	2.45	0.52
1:A:10:GLU:HG2	1:A:452:PHE:CZ	2.45	0.52
1:B:14:ILE:O	1:B:18:LYS:HG3	2.09	0.52
1:A:73:GLY:HA2	1:A:137:TRP:CG	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LEU:HD12	1:B:347:ILE:CD1	2.40	0.52
1:B:446:ILE:HG13	1:B:447:THR:N	2.24	0.51
1:B:446:ILE:HG13	1:B:447:THR:H	1.75	0.51
1:B:87:VAL:HG13	1:B:88:VAL:N	2.26	0.51
1:B:269:HIS:C	1:B:271:MET:H	2.14	0.51
1:A:337:TYR:HA	1:A:342:ALA:O	2.11	0.50
1:B:446:ILE:CG1	1:B:447:THR:N	2.74	0.50
1:B:50:TYR:OH	1:B:68:GLY:HA3	2.11	0.50
1:B:275:ILE:CG2	1:B:275:ILE:O	2.59	0.50
1:A:275:ILE:O	1:A:275:ILE:CG2	2.59	0.50
1:A:97:ASN:ND2	1:A:100:GLU:H	2.09	0.50
1:B:1:MET:HA	1:B:4:GLU:HG2	1.92	0.50
1:A:120:THR:HG23	1:A:143:MET:CE	2.42	0.50
1:A:217:MET:HE1	1:A:269:HIS:CB	2.42	0.50
1:A:133:MET:HB2	1:A:135:VAL:CG1	2.42	0.49
1:A:271:MET:CE	1:A:271:MET:CA	2.76	0.49
1:B:1:MET:HE1	1:B:5:LYS:HZ1	1.77	0.49
1:A:338:ASP:OD2	1:A:338:ASP:C	2.50	0.49
1:B:73:GLY:HA2	1:B:137:TRP:CD1	2.45	0.49
1:B:367:GLU:O	1:B:367:GLU:HG3	2.11	0.49
1:B:209:PHE:CE1	1:B:284:LEU:CD2	2.95	0.49
1:A:255:ASP:OD1	1:A:256:SER:CB	2.61	0.49
1:B:87:VAL:CG1	1:B:111:ARG:HG3	2.41	0.49
1:A:204:TYR:CE2	1:A:228:VAL:HG13	2.46	0.49
1:B:2:TRP:HE1	1:B:460:GLU:HG3	1.77	0.49
1:B:185:ILE:HG13	1:B:186:THR:N	2.27	0.49
1:A:10:GLU:O	1:A:14:ILE:HG12	2.12	0.49
1:A:82:LEU:HD22	1:A:144:ILE:HB	1.94	0.48
1:A:288:ALA:HB2	1:A:304:ASN:HD21	1.78	0.48
1:A:191:VAL:HG22	1:A:344:LEU:CD2	2.44	0.48
1:B:42:PRO:HB3	1:B:147:THR:HB	1.95	0.48
1:B:186:THR:CG2	1:B:380:VAL:CA	2.86	0.48
1:A:357:PHE:CZ	1:A:361:MET:HE1	2.45	0.48
1:B:5:LYS:CE	1:B:133:MET:HE1	2.44	0.48
1:B:186:THR:HG21	1:B:380:VAL:CG2	2.33	0.48
1:B:24:GLU:HG3	1:B:99:PHE:CZ	2.49	0.48
1:A:114:LEU:HD12	1:A:114:LEU:HA	1.70	0.48
1:A:396:LEU:HD23	1:A:461:ALA:CB	2.43	0.48
1:B:1:MET:CE	1:B:5:LYS:NZ	2.77	0.48
1:B:128:LYS:O	1:B:128:LYS:HD3	2.13	0.48
1:B:305:ARG:HD3	1:B:306:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLU:O	1:A:334:VAL:HG22	2.14	0.48
1:B:251:ASP:OD1	1:B:262:THR:HB	2.14	0.48
1:A:216:ASN:ND2	1:A:270:GLY:HA3	2.28	0.47
1:A:217:MET:HE1	1:B:33:SER:HA	1.96	0.47
1:B:204:TYR:CZ	1:B:235:VAL:CG1	2.97	0.47
1:B:78:VAL:N	1:B:167:THR:CG2	2.77	0.47
1:A:152:ASP:O	1:A:153:TRP:HB2	2.15	0.47
1:B:104:THR:O	1:B:448:LYS:HE3	2.14	0.47
1:B:78:VAL:H	1:B:167:THR:HG22	1.78	0.47
1:B:387:ASP:OD1	1:B:388:LYS:N	2.47	0.47
1:B:113:THR:CB	1:B:446:ILE:HG22	2.38	0.47
1:B:403:GLN:HE22	1:B:456:SER:HB2	1.80	0.47
1:A:97:ASN:ND2	1:A:99:PHE:N	2.58	0.47
1:B:463:TYR:O	1:B:467:VAL:HG23	2.15	0.47
1:A:78:VAL:N	1:A:167:THR:HG22	2.19	0.46
1:B:115:ASP:HA	1:B:116:ASP:HA	1.43	0.46
1:A:192:GLN:HB2	1:A:373:PHE:CZ	2.50	0.46
1:A:201:GLU:HG3	1:A:202:PRO:CD	2.45	0.46
1:A:232:MET:HE1	1:A:254:VAL:CB	2.44	0.46
1:A:337:TYR:C	1:A:337:TYR:CD2	2.87	0.46
1:A:195:LEU:CD1	1:A:195:LEU:C	2.72	0.46
1:B:192:GLN:HB2	1:B:373:PHE:CZ	2.51	0.46
1:A:192:GLN:HB2	1:A:373:PHE:CE1	2.49	0.46
1:B:79:LEU:CD1	1:B:169:GLY:HA2	2.46	0.46
1:B:465:LEU:HA	1:B:465:LEU:HD12	1.47	0.46
1:A:368:ILE:HG23	1:A:373:PHE:HB2	1.98	0.46
1:A:97:ASN:HD22	1:A:99:PHE:N	2.13	0.46
1:A:217:MET:HE1	1:A:269:HIS:CA	2.42	0.45
1:A:314:GLU:H	1:A:314:GLU:HG3	1.39	0.45
1:A:386:VAL:CG2	1:A:389:ASN:CB	2.85	0.45
1:A:170:PHE:CE2	1:A:172:PRO:HG3	2.51	0.45
1:A:199:GLN:HE22	1:A:294:ASN:H	1.64	0.45
1:B:391:PRO:O	1:B:395:LYS:HG2	2.16	0.45
1:A:255:ASP:OD1	1:A:256:SER:HB3	2.17	0.45
1:B:269:HIS:C	1:B:271:MET:N	2.70	0.45
1:A:195:LEU:HD13	1:A:195:LEU:HA	1.42	0.45
1:A:271:MET:CE	1:A:350:ALA:CB	2.93	0.45
1:B:55:ARG:O	1:B:55:ARG:HG2	2.16	0.45
1:A:305:ARG:HD3	1:A:306:TYR:CZ	2.51	0.45
1:A:271:MET:HE3	1:A:271:MET:CA	2.39	0.45
1:B:337:TYR:C	1:B:337:TYR:CD2	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASP:H	1:A:443:ASN:HD21	1.65	0.45
1:B:1:MET:HE2	1:B:5:LYS:HZ3	1.81	0.45
1:B:190:LEU:HD12	1:B:347:ILE:HD11	1.99	0.44
1:A:386:VAL:HG23	1:A:389:ASN:H	1.82	0.44
1:A:185:ILE:C	1:A:185:ILE:CD1	2.71	0.44
1:A:256:SER:O	1:A:256:SER:OG	2.30	0.44
1:B:403:GLN:HE21	1:B:403:GLN:HB3	1.63	0.44
1:B:364:PHE:CE1	1:B:368:ILE:HD12	2.52	0.44
1:B:5:LYS:CD	1:B:133:MET:HE1	2.48	0.44
1:A:387:ASP:OD1	1:A:388:LYS:N	2.51	0.44
1:B:207:ILE:HG22	1:B:208:THR:HG23	1.99	0.44
1:A:400:TYR:O	1:A:403:GLN:O	2.35	0.43
1:B:202:PRO:HG3	1:B:293:ASP:HB3	1.98	0.43
1:B:228:VAL:HG12	1:B:230:GLU:O	2.18	0.43
1:A:114:LEU:HD11	1:A:446:ILE:HG13	2.00	0.43
1:A:5:LYS:CD	1:A:133:MET:CE	2.96	0.43
1:B:281:LEU:HD11	1:B:332:ILE:HG13	1.99	0.43
1:B:353:GLU:HA	1:B:354:GLY:HA2	1.86	0.43
1:A:201:GLU:HG2	1:A:229:LYS:HD2	1.99	0.43
1:A:323:ASP:CB	2:A:536:HOH:O	2.50	0.43
1:B:94:TRP:CA	1:B:443:ASN:ND2	2.76	0.43
1:B:399:ALA:CB	1:B:457:ILE:HG23	2.48	0.43
1:B:209:PHE:CE1	1:B:284:LEU:HD23	2.53	0.43
1:B:112:GLY:H	1:B:444:GLU:CD	2.21	0.43
1:B:2:TRP:HA	1:B:2:TRP:CE3	2.54	0.43
1:A:447:THR:HG22	1:A:449:LYS:N	2.34	0.42
1:A:78:VAL:HG13	1:A:167:THR:H	1.83	0.42
1:A:307:LEU:HG	1:A:332:ILE:HD11	2.01	0.42
1:B:97:ASN:HA	1:B:98:PRO:HD2	1.88	0.42
1:A:165:MET:HE2	1:A:165:MET:HB2	1.90	0.42
1:B:77:ASP:CB	1:B:167:THR:HG21	2.50	0.42
1:B:180:HIS:CG	1:B:325:MET:CE	3.02	0.42
1:A:322:THR:HG21	1:A:325:MET:CA	2.50	0.42
1:A:204:TYR:OH	1:A:235:VAL:HG13	2.20	0.42
1:B:404:THR:HG22	1:B:453:ASN:ND2	2.34	0.42
1:A:368:ILE:O	1:A:369:GLN:C	2.58	0.42
1:A:386:VAL:CG2	1:A:389:ASN:H	2.33	0.42
1:B:84:HIS:CD2	1:B:86:ASP:OD1	2.71	0.42
1:A:97:ASN:ND2	1:A:100:GLU:N	2.68	0.41
1:B:1:MET:HE2	1:B:5:LYS:NZ	2.34	0.41
1:B:108:ILE:HG13	1:B:109:ILE:N	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:PHE:CE2	1:B:243:LEU:HD11	2.55	0.41
1:A:82:LEU:N	1:A:82:LEU:HD23	2.35	0.41
1:A:201:GLU:HA	1:A:202:PRO:HD3	1.90	0.41
1:B:192:GLN:HB2	1:B:373:PHE:CE1	2.56	0.41
1:B:218:VAL:HG22	1:B:331:ASN:OD1	2.20	0.41
1:A:113:THR:OG1	1:A:444:GLU:HG2	2.20	0.41
1:B:400:TYR:HA	1:B:457:ILE:HD13	2.02	0.41
1:A:125:TYR:O	1:A:129:ILE:HG13	2.21	0.41
1:A:403:GLN:HE22	1:A:456:SER:HB3	1.83	0.41
1:B:364:PHE:CZ	1:B:368:ILE:HD11	2.52	0.41
1:B:9:TYR:O	1:B:10:GLU:C	2.57	0.41
1:B:180:HIS:CG	1:B:325:MET:HE3	2.55	0.41
1:B:341:ASN:O	2:B:479:HOH:O	2.22	0.41
1:A:185:ILE:HD13	1:A:185:ILE:O	2.18	0.41
1:B:344:LEU:HD13	1:B:345:PHE:N	2.36	0.41
1:A:19:GLY:HA3	1:A:48:TYR:OH	2.21	0.41
1:B:5:LYS:HE2	1:B:5:LYS:HB2	1.71	0.41
1:A:4:GLU:O	1:A:5:LYS:C	2.59	0.41
1:A:69:ARG:HA	1:A:143:MET:O	2.21	0.41
1:A:170:PHE:CZ	1:A:172:PRO:HG3	2.55	0.41
1:A:322:THR:HG23	1:A:325:MET:H	1.78	0.41
1:A:397:VAL:O	1:A:401:ARG:HG3	2.21	0.41
1:B:114:LEU:HD12	1:B:114:LEU:HA	1.74	0.41
1:B:120:THR:HG23	1:B:143:MET:CE	2.51	0.41
1:A:368:ILE:HD12	1:A:368:ILE:HA	1.75	0.40
1:B:186:THR:HG22	1:B:379:LYS:C	2.35	0.40
1:B:228:VAL:HG21	1:B:232:MET:HE1	2.04	0.40
1:B:273:PRO:HG2	1:B:311:ASP:HB3	2.03	0.40
1:B:303:SER:O	1:B:307:LEU:HB2	2.21	0.40
1:A:132:ASP:C	1:A:134:ASN:H	2.24	0.40
1:B:96:SER:O	1:B:98:PRO:HD3	2.21	0.40
1:A:140:ARG:HD2	2:A:504:HOH:O	2.22	0.40
1:A:353:GLU:HA	1:A:354:GLY:HA2	1.73	0.40
1:A:375:VAL:CG1	1:A:377:LEU:HD12	2.50	0.40
1:B:87:VAL:HG11	1:B:111:ARG:CG	2.50	0.40
1:B:133:MET:O	1:B:134:ASN:C	2.58	0.40
1:B:206:LEU:HB3	1:B:296:ALA:HB2	2.04	0.40
1:A:322:THR:CG2	1:A:325:MET:CA	2.99	0.40
1:B:129:ILE:CG2	1:B:133:MET:HE3	2.39	0.40

There are no symmetry-related clashes.

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	429/492 (87%)	405 (94%)	23 (5%)	1 (0%)	47	68
1	B	431/492 (88%)	407 (94%)	23 (5%)	1 (0%)	47	68
All	All	860/984 (87%)	812 (94%)	46 (5%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	441	GLN
1	A	274	SER

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	354/417 (85%)	310 (88%)	44 (12%)	4	9
1	B	354/417 (85%)	306 (86%)	48 (14%)	3	7
All	All	708/834 (85%)	616 (87%)	92 (13%)	4	7

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	18	LYS
1	A	74	LYS
1	A	87	VAL

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Mol	Chain	Res	Type
1	A	97	ASN
1	A	104	THR
1	A	108	ILE
1	A	114	LEU
1	A	128	LYS
1	A	135	VAL
1	A	138	LYS
1	A	156	THR
1	A	167	THR
1	A	183	LYS
1	A	185	ILE
1	A	195	LEU
1	A	197	GLU
1	A	225	ARG
1	A	232	MET
1	A	235	VAL
1	A	237	GLN
1	A	244	GLU
1	A	248	LEU
1	A	251	ASP
1	A	253	THR
1	A	254	VAL
1	A	262	THR
1	A	268	VAL
1	A	271	MET
1	A	307	LEU
1	A	314	GLU
1	A	322	THR
1	A	355	PHE
1	A	356	GLU
1	A	358	GLU
1	A	368	ILE
1	A	374	GLU
1	A	389	ASN
1	A	401	ARG
1	A	441	GLN
1	A	442	LYS
1	A	447	THR
1	A	456	SER
1	A	465	LEU
1	B	1	MET
1	B	31	LYS

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Mol	Chain	Res	Type
1	B	78	VAL
1	B	83	CYS
1	B	87	VAL
1	B	96	SER
1	B	97	ASN
1	B	103	VAL
1	B	108	ILE
1	B	114	LEU
1	B	115	ASP
1	B	128	LYS
1	B	135	VAL
1	B	139	LYS
1	B	149	GLU
1	B	167	THR
1	B	182	GLU
1	B	185	ILE
1	B	186	THR
1	B	194	LYS
1	B	195	LEU
1	B	230	GLU
1	B	231	ASN
1	B	235	VAL
1	B	240	GLU
1	B	248	LEU
1	B	252	SER
1	B	253	THR
1	B	254	VAL
1	B	307	LEU
1	B	309	ASN
1	B	329	THR
1	B	340	GLU
1	B	344	LEU
1	B	358	GLU
1	B	363	ARG
1	B	367	GLU
1	B	368	ILE
1	B	374	GLU
1	B	377	LEU
1	B	402	ASN
1	B	442	LYS
1	B	444	GLU
1	B	447	THR

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Mol	Chain	Res	Type
1	B	453	ASN
1	B	464	SER
1	B	465	LEU
1	B	467	VAL

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

Mol	Chain	Res	Type
1	A	61	HIS
1	A	65	HIS
1	A	76	ASN
1	A	84	HIS
1	A	97	ASN
1	A	199	GLN
1	A	216	ASN
1	A	237	GLN
1	A	294	ASN
1	A	295	ASN
1	A	339	ASN
1	A	384	HIS
1	A	389	ASN
1	A	402	ASN
1	A	403	GLN
1	A	443	ASN
1	B	76	ASN
1	B	84	HIS
1	B	97	ASN
1	B	231	ASN
1	B	294	ASN
1	B	295	ASN
1	B	339	ASN
1	B	369	GLN
1	B	384	HIS
1	B	389	ASN
1	B	403	GLN
1	B	443	ASN
1	B	453	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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 (i)

6.1　Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	433/492 (88%)	0.12	5 (1%)	79	80	25, 48, 75, 97	5 (1%)
1	B	435/492 (88%)	0.11	2 (0%)	91	91	27, 48, 80, 97	1 (0%)
All	All	868/984 (88%)	0.12	7 (0%)	86	87	25, 48, 76, 97	6 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	452	PHE	4.0
1	A	107	ALA	3.4
1	B	467	VAL	2.9
1	B	196	THR	2.8
1	A	196	THR	2.4
1	A	451	LEU	2.1
1	A	114	LEU	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 ⓘ

There are no such residues in this entry.