



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:07 AM UTC

PDB ID : 3KHX / pdb_00003khx
Title : Crystal structure of Staphylococcus aureus metallopeptidase (Sapep/DapE) in the apo-form
Authors : Girish, T.S.; Gopal, B.
Deposited on : 2009-10-31
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

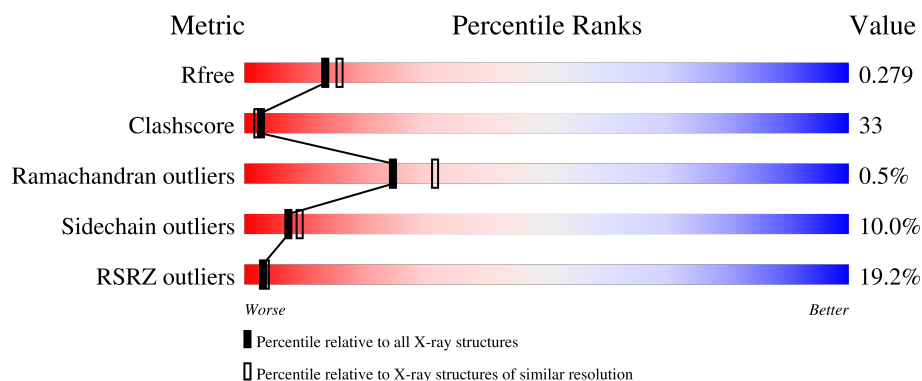
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	492	18% 51% 28% 6% 14%
1	B	492	15% 55% 24% 7% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6716 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	422	Total	C	N	O	S	1	0	0
			3232	2052	531	635	14			
1	B	425	Total	C	N	O	S	0	0	0
			3302	2099	546	642	15			

There are 46 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
B	-22	MET	-	expression tag	UNP Q5HF23
B	-21	GLY	-	expression tag	UNP Q5HF23

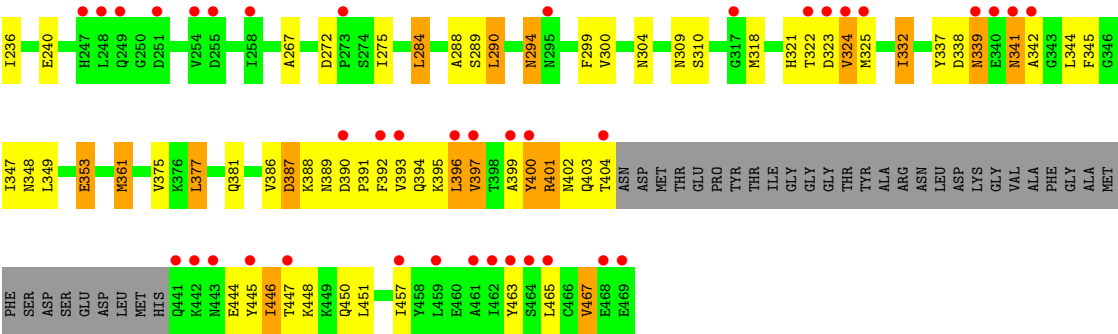
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	SER	-	expression tag	UNP Q5HF23
B	-19	SER	-	expression tag	UNP Q5HF23
B	-18	HIS	-	expression tag	UNP Q5HF23
B	-17	HIS	-	expression tag	UNP Q5HF23
B	-16	HIS	-	expression tag	UNP Q5HF23
B	-15	HIS	-	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

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	92	Total	O	0	0
			92	92		
2	B	90	Total	O	0	0
			90	90		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.82Å 134.17Å 68.28Å 90.00° 94.52° 90.00°	Depositor
Resolution (Å)	60.71 – 2.30 60.71 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (60.71-2.30) 99.3 (60.71-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.246 , 0.278 0.256 , 0.279	Depositor DCC
R_{free} test set	2605 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6716	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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	0.72	0/3298	1.00	16/4478 (0.4%)
1	B	0.65	0/3372	0.93	15/4574 (0.3%)
All	All	0.69	0/6670	0.96	31/9052 (0.3%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	467	VAL	CB-CA-C	-8.22	104.72	111.71
1	A	39	GLY	CA-C-N	7.54	126.81	118.97
1	A	39	GLY	C-N-CA	7.54	126.81	118.97
1	A	211	SER	CB-CA-C	7.43	120.74	110.34
1	B	341	ASN	N-CA-C	7.22	118.84	110.97
1	A	468	GLU	N-CA-C	6.89	119.96	110.24
1	A	1	MET	N-CA-C	-6.86	103.89	111.36
1	A	97	ASN	CA-C-N	6.56	128.04	119.84
1	A	97	ASN	C-N-CA	6.56	128.04	119.84
1	A	169	GLY	N-CA-C	6.46	119.28	110.69
1	B	4	GLU	N-CA-C	6.06	117.75	111.03
1	B	386	VAL	CB-CA-C	-5.94	105.23	111.23
1	B	401	ARG	CB-CA-C	-5.78	101.19	110.79
1	B	158	ARG	N-CA-C	5.74	118.02	111.02
1	A	96	SER	CB-CA-C	5.66	121.19	110.56
1	B	390	ASP	CA-C-N	5.51	125.17	119.05
1	B	390	ASP	C-N-CA	5.51	125.17	119.05
1	B	4	GLU	CB-CA-C	-5.35	102.66	110.95
1	B	107	ALA	N-CA-C	5.29	116.33	108.60
1	B	310	SER	N-CA-C	-5.27	98.06	107.28
1	B	155	CYS	N-CA-C	-5.19	106.05	112.38
1	A	158	ARG	N-CA-C	5.18	117.34	111.02
1	A	28	ASP	CB-CA-C	5.17	118.57	111.23
1	A	267	ALA	CA-C-N	5.13	131.20	121.97
1	A	267	ALA	C-N-CA	5.13	131.20	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ALA	CB-CA-C	-5.10	103.34	113.45
1	A	185	ILE	N-CA-C	5.10	115.26	108.27
1	A	211	SER	N-CA-C	-5.06	99.58	107.93
1	B	294	ASN	N-CA-C	5.05	117.18	111.02
1	B	272	ASP	CA-C-N	5.04	124.65	119.56
1	B	272	ASP	C-N-CA	5.04	124.65	119.56

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	3232	0	3017	211	0
1	B	3302	0	3113	210	0
2	A	92	0	0	8	0
2	B	90	0	0	4	0
All	All	6716	0	6130	421	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 33.

All (421) 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:185:ILE:HB	1:A:350:ARG:NH1	1.28	1.43
1:A:130:LEU:HD21	1:A:459:LEU:CD1	1.55	1.34
1:A:186:THR:CG2	1:A:380:VAL:HG22	1.60	1.32
1:B:5:LYS:N	1:B:5:LYS:HE3	1.50	1.27
1:A:114:LEU:HD11	1:A:445:TYR:O	1.35	1.25
1:B:74:LYS:HD3	1:B:75:GLY:N	1.51	1.23
1:A:130:LEU:CD2	1:A:459:LEU:HD11	1.68	1.22
1:B:12:GLN:HG3	2:B:529:HOH:O	1.35	1.22
1:A:104:THR:CG2	1:A:107:ALA:H	1.57	1.18
1:A:28:ASP:OD2	1:A:31:LYS:HG3	1.44	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:MET:HE1	1:B:52:ILE:HD11	1.16	1.15
1:A:447:THR:CG2	1:A:449:LYS:H	1.61	1.14
1:A:186:THR:HG21	1:A:380:VAL:HG22	1.20	1.13
1:B:113:THR:HB	1:B:446:ILE:HG22	1.30	1.12
1:A:185:ILE:CB	1:A:350:ARG:HH11	1.64	1.10
1:A:104:THR:HG22	1:A:107:ALA:N	1.66	1.10
1:A:310:SER:HB3	2:A:533:HOH:O	1.54	1.07
1:B:392:PHE:CZ	1:B:396:LEU:HD11	1.88	1.07
1:A:130:LEU:HD21	1:A:459:LEU:HD12	1.38	1.05
1:A:130:LEU:CD2	1:A:459:LEU:CD1	2.30	1.05
1:A:377:LEU:HD23	1:A:378:GLY:O	1.57	1.04
1:B:392:PHE:CE2	1:B:396:LEU:CD1	2.41	1.03
1:A:186:THR:CG2	1:A:380:VAL:CG2	2.37	1.03
1:A:387:ASP:OD1	1:A:388:LYS:N	1.92	1.02
1:B:400:TYR:HD2	1:B:401:ARG:N	1.57	1.01
1:A:130:LEU:HD21	1:A:459:LEU:HD11	1.18	1.01
1:A:186:THR:HG23	1:A:380:VAL:HG22	1.41	1.01
1:A:447:THR:HB	1:A:450:GLN:HG3	1.43	1.00
1:A:186:THR:HG21	1:A:380:VAL:CG2	1.91	1.00
1:B:104:THR:CG2	1:B:105:GLU:N	2.21	1.00
1:A:104:THR:HG23	1:A:106:ASP:H	1.24	0.99
1:A:447:THR:HG22	1:A:449:LYS:N	1.78	0.99
1:A:83:CYS:HB3	2:A:510:HOH:O	1.63	0.98
1:A:231:ASN:HD21	1:A:234:ASP:CB	1.75	0.98
1:A:231:ASN:HD21	1:A:234:ASP:HB2	1.24	0.98
1:A:104:THR:HG22	1:A:107:ALA:H	0.82	0.97
1:B:49:MET:HE1	1:B:52:ILE:CD1	1.95	0.97
1:B:49:MET:CE	1:B:52:ILE:HD11	1.94	0.96
1:A:102:VAL:HG22	1:A:109:ILE:HB	1.48	0.96
1:A:191:VAL:HG21	1:A:376:LYS:HE2	1.46	0.96
1:A:377:LEU:CD2	1:A:378:GLY:O	2.14	0.95
1:B:156:THR:O	1:B:161:LYS:HE2	1.67	0.95
1:B:104:THR:HG22	1:B:106:ASP:N	1.80	0.95
1:A:329:THR:HG22	1:A:350:ARG:HB2	1.49	0.95
1:A:185:ILE:CB	1:A:350:ARG:NH1	2.25	0.94
1:A:447:THR:HG22	1:A:450:GLN:H	1.31	0.94
1:B:400:TYR:CD2	1:B:401:ARG:N	2.35	0.93
1:A:447:THR:HG23	1:A:449:LYS:H	1.30	0.93
1:A:231:ASN:ND2	1:A:234:ASP:HB2	1.83	0.93
1:B:88:VAL:HG13	1:B:89:PRO:HD2	1.48	0.93
1:B:104:THR:HG23	1:B:105:GLU:H	1.34	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:THR:CG2	1:A:107:ALA:N	2.27	0.92
1:B:104:THR:HG22	1:B:106:ASP:H	1.32	0.92
1:A:2:TRP:CZ3	1:A:5:LYS:NZ	2.38	0.92
1:B:114:LEU:HD11	1:B:445:TYR:O	1.70	0.91
1:B:114:LEU:HD12	1:B:114:LEU:N	1.84	0.91
1:A:447:THR:HG22	1:A:449:LYS:H	1.34	0.91
1:A:231:ASN:HD21	1:A:234:ASP:CG	1.79	0.91
1:B:5:LYS:HE3	1:B:5:LYS:H	1.23	0.90
1:B:49:MET:CE	1:B:49:MET:HA	2.00	0.90
1:A:447:THR:CG2	1:A:449:LYS:N	2.33	0.90
1:B:74:LYS:HD3	1:B:75:GLY:H	1.37	0.89
1:B:392:PHE:CE2	1:B:396:LEU:HD11	2.06	0.89
1:B:400:TYR:CD2	1:B:400:TYR:C	2.51	0.89
1:B:338:ASP:O	1:B:342:ALA:HB1	1.73	0.89
1:B:395:LYS:HD2	1:B:465:LEU:HD23	1.54	0.89
1:A:2:TRP:HZ3	1:A:5:LYS:NZ	1.71	0.88
1:B:209:PHE:CE1	1:B:284:LEU:HD13	2.09	0.88
1:A:204:TYR:CE2	1:A:235:VAL:HG21	2.10	0.87
1:B:104:THR:HG23	1:B:105:GLU:N	1.88	0.87
1:A:104:THR:HG23	1:A:106:ASP:N	1.91	0.86
1:A:104:THR:HG23	1:A:105:GLU:N	1.91	0.85
1:A:5:LYS:HD2	1:A:133:MET:HE1	1.58	0.85
1:B:236:ILE:O	1:B:240:GLU:HG2	1.77	0.84
1:B:156:THR:C	1:B:161:LYS:HE2	2.03	0.84
1:A:84:HIS:HD2	1:A:86:ASP:OD1	1.60	0.84
1:B:21:LEU:HD21	1:B:113:THR:CG2	2.08	0.83
1:B:103:VAL:O	1:B:103:VAL:HG13	1.79	0.83
1:B:1:MET:O	1:B:4:GLU:CB	2.27	0.83
1:B:113:THR:HB	1:B:446:ILE:CG2	2.09	0.82
1:A:20:LEU:HG	1:A:117:LYS:HD3	1.60	0.82
1:B:63:VAL:CG2	1:B:67:ALA:O	2.27	0.82
1:B:199:GLN:HE22	1:B:294:ASN:H	1.23	0.82
1:B:321:HIS:CE1	1:B:323:ASP:CB	2.62	0.82
1:B:104:THR:HG22	1:B:105:GLU:N	1.95	0.81
1:A:396:LEU:HD22	1:A:461:ALA:CB	2.09	0.81
1:B:74:LYS:HD3	1:B:74:LYS:C	2.00	0.81
1:B:49:MET:HA	1:B:49:MET:HE3	1.62	0.81
1:A:84:HIS:CD2	1:A:86:ASP:OD1	2.33	0.81
1:B:154:LYS:HB3	1:B:156:THR:HG22	1.61	0.81
1:A:186:THR:HG23	1:A:380:VAL:HA	1.62	0.81
1:B:63:VAL:HG23	1:B:67:ALA:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:THR:CG2	1:B:106:ASP:H	1.95	0.80
1:B:290:LEU:N	1:B:290:LEU:HD12	1.94	0.80
1:B:74:LYS:CD	1:B:75:GLY:N	2.41	0.80
1:A:130:LEU:HD23	1:A:459:LEU:HD11	1.62	0.80
1:A:104:THR:CG2	1:A:106:ASP:H	1.95	0.80
1:A:329:THR:CG2	1:A:350:ARG:HB2	2.11	0.80
1:A:168:LEU:HD11	1:A:465:LEU:HD21	1.63	0.79
1:A:5:LYS:HE3	1:A:459:LEU:HD21	1.65	0.78
1:B:114:LEU:HD11	1:B:445:TYR:C	2.07	0.78
1:B:321:HIS:CE1	1:B:323:ASP:HB2	2.18	0.78
1:A:251:ASP:OD1	1:A:262:THR:CG2	2.31	0.78
1:A:114:LEU:HD13	1:A:444:GLU:HG2	1.66	0.77
1:A:316:MET:HG2	1:A:364:PHE:CE1	2.18	0.77
1:B:395:LYS:CD	1:B:465:LEU:HD23	2.14	0.77
1:A:357:PHE:CE1	1:A:361:MET:HE3	2.20	0.77
1:A:28:ASP:CG	1:A:31:LYS:HG3	2.10	0.77
1:B:5:LYS:N	1:B:5:LYS:CE	2.41	0.77
1:B:392:PHE:CZ	1:B:396:LEU:CD1	2.66	0.77
1:B:21:LEU:HD21	1:B:113:THR:HG22	1.65	0.77
1:A:204:TYR:OH	1:A:235:VAL:CG2	2.33	0.76
1:A:251:ASP:O	1:A:262:THR:HG22	1.85	0.76
1:B:139:LYS:HD2	1:B:465:LEU:O	1.85	0.75
1:A:447:THR:HG22	1:A:450:GLN:N	2.01	0.75
1:A:168:LEU:HD11	1:A:465:LEU:CD2	2.17	0.74
1:B:73:GLY:HA2	1:B:137:TRP:CG	2.22	0.74
1:B:323:ASP:N	1:B:324:VAL:CB	2.50	0.74
1:B:392:PHE:HA	1:B:465:LEU:HD21	1.68	0.74
1:A:396:LEU:CD2	1:A:461:ALA:CB	2.66	0.74
1:A:343:GLY:HA2	2:A:477:HOH:O	1.88	0.74
1:A:310:SER:OG	1:A:315:LYS:HB2	1.88	0.74
1:A:317:GLY:HA3	2:A:493:HOH:O	1.86	0.74
1:B:338:ASP:O	1:B:342:ALA:CB	2.36	0.74
1:A:448:LYS:O	1:A:452:PHE:CD2	2.42	0.73
1:B:114:LEU:N	1:B:114:LEU:CD1	2.52	0.72
1:B:322:THR:C	1:B:324:VAL:CB	2.62	0.72
1:B:323:ASP:HA	1:B:324:VAL:C	2.14	0.72
1:B:190:LEU:CD1	1:B:347:ILE:HD11	2.20	0.72
1:B:321:HIS:CE1	1:B:323:ASP:HB3	2.25	0.72
1:A:347:ILE:N	1:A:347:ILE:CD1	2.51	0.71
1:B:15:ASN:O	1:B:18:LYS:HG2	1.90	0.71
1:A:251:ASP:OD1	1:A:262:THR:HG21	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:LYS:CE	1:B:465:LEU:HD23	2.19	0.71
1:B:290:LEU:N	1:B:290:LEU:CD1	2.52	0.71
1:B:126:ALA:O	1:B:130:LEU:HG	1.91	0.70
1:B:74:LYS:HE2	1:B:74:LYS:HA	1.71	0.70
1:B:102:VAL:HG22	1:B:109:ILE:CB	2.22	0.70
1:A:186:THR:HG23	1:A:380:VAL:CG2	2.13	0.70
1:B:49:MET:HA	1:B:49:MET:HE2	1.73	0.70
1:B:49:MET:CE	1:B:52:ILE:CD1	2.61	0.70
1:B:387:ASP:OD2	1:B:387:ASP:N	2.22	0.69
1:B:391:PRO:O	1:B:395:LYS:HE2	1.93	0.69
1:B:209:PHE:CE1	1:B:284:LEU:CD1	2.75	0.69
1:B:1:MET:O	1:B:4:GLU:N	2.25	0.69
1:B:74:LYS:CD	1:B:75:GLY:H	2.02	0.69
1:A:138:LYS:HG2	1:A:466:CYS:O	1.93	0.69
1:A:204:TYR:CZ	1:A:235:VAL:HG21	2.27	0.68
1:A:231:ASN:ND2	1:A:234:ASP:OD2	2.27	0.68
1:B:102:VAL:CG2	1:B:109:ILE:CB	2.71	0.68
1:A:194:LYS:HE3	1:A:342:ALA:HB2	1.76	0.68
1:A:347:ILE:N	1:A:347:ILE:HD13	2.09	0.67
1:B:403:GLN:O	1:B:404:THR:OG1	2.10	0.67
1:A:316:MET:HG2	1:A:364:PHE:CZ	2.29	0.67
1:B:214:ARG:NH1	1:B:217:MET:HG3	2.09	0.67
1:B:275:ILE:O	1:B:275:ILE:HG22	1.94	0.67
1:A:233:THR:O	1:A:237:GLN:HG3	1.95	0.66
1:B:5:LYS:HE3	1:B:5:LYS:CA	2.26	0.66
1:B:103:VAL:O	1:B:103:VAL:CG1	2.43	0.66
1:B:109:ILE:O	1:B:110:ALA:HB2	1.95	0.65
1:B:63:VAL:HG22	1:B:67:ALA:O	1.96	0.65
1:B:27:ARG:HG3	1:B:38:VAL:HB	1.77	0.65
1:A:3:LYS:NZ	2:A:527:HOH:O	2.28	0.65
1:B:209:PHE:CZ	1:B:284:LEU:HD13	2.32	0.65
1:B:7:GLN:O	1:B:10:GLU:HG3	1.97	0.64
1:B:392:PHE:CE2	1:B:396:LEU:HD13	2.31	0.64
1:A:185:ILE:HB	1:A:350:ARG:HH12	1.49	0.64
1:A:396:LEU:CD2	1:A:461:ALA:HB3	2.26	0.64
1:A:447:THR:CG2	1:A:450:GLN:H	2.07	0.64
1:B:113:THR:O	1:B:118:GLY:HA3	1.98	0.64
1:A:377:LEU:HG	1:A:378:GLY:N	2.13	0.64
1:B:209:PHE:O	1:B:210:LYS:HD3	1.98	0.64
1:B:289:SER:C	1:B:290:LEU:HD12	2.23	0.63
1:A:104:THR:CG2	1:A:106:ASP:N	2.57	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:THR:HG23	1:A:143:MET:CE	2.29	0.63
1:A:47:ASP:O	1:A:51:GLU:HG3	1.99	0.62
1:B:154:LYS:CB	1:B:156:THR:CG2	2.78	0.62
1:B:381:GLN:NE2	2:B:496:HOH:O	2.24	0.62
1:B:400:TYR:HA	1:B:457:ILE:HD13	1.82	0.62
1:A:220:ASP:HB2	1:A:265:GLY:O	2.00	0.62
1:A:377:LEU:HD21	1:A:378:GLY:O	2.00	0.62
1:B:20:LEU:HD13	1:B:117:LYS:HB3	1.82	0.62
1:B:5:LYS:H	1:B:5:LYS:CE	2.07	0.62
1:B:18:LYS:NZ	2:B:483:HOH:O	2.32	0.62
1:B:154:LYS:CB	1:B:156:THR:HG22	2.29	0.61
1:A:114:LEU:HD11	1:A:445:TYR:C	2.23	0.61
1:B:154:LYS:HB2	1:B:156:THR:HG23	1.82	0.61
1:A:194:LYS:HE2	1:A:295:ASN:OD1	2.01	0.61
1:A:114:LEU:CD1	1:A:445:TYR:O	2.29	0.61
1:A:396:LEU:HD22	1:A:461:ALA:HB2	1.82	0.61
1:A:217:MET:HA	1:A:268:VAL:O	2.01	0.61
1:B:154:LYS:HB3	1:B:156:THR:CG2	2.31	0.61
1:A:447:THR:CB	1:A:450:GLN:HG3	2.26	0.60
1:A:2:TRP:CE3	1:A:5:LYS:NZ	2.69	0.60
1:A:193:ASN:ND2	1:A:372:GLY:HA2	2.17	0.60
1:B:5:LYS:CE	1:B:5:LYS:CA	2.80	0.60
1:A:252:SER:HA	1:A:260:VAL:O	2.02	0.59
1:B:394:GLN:O	1:B:397:VAL:HG13	2.03	0.59
1:B:392:PHE:HA	1:B:465:LEU:CD2	2.31	0.59
1:B:88:VAL:CG1	1:B:89:PRO:HD2	2.30	0.59
1:A:332:ILE:HD12	1:A:332:ILE:N	2.17	0.59
1:A:78:VAL:H	1:A:167:THR:HG22	1.67	0.59
1:B:341:ASN:CB	1:B:342:ALA:HA	2.33	0.58
1:A:204:TYR:OH	1:A:235:VAL:HG21	2.03	0.58
1:A:194:LYS:HE2	1:A:295:ASN:CG	2.28	0.58
1:B:1:MET:C	1:B:4:GLU:H	2.11	0.58
1:A:216:ASN:O	1:A:269:HIS:HA	2.04	0.57
1:A:10:GLU:HG2	1:A:452:PHE:CE1	2.39	0.57
1:A:113:THR:HB	1:A:446:ILE:HG22	1.85	0.57
1:B:88:VAL:HG13	1:B:89:PRO:CD	2.29	0.57
1:A:14:ILE:O	1:A:18:LYS:HG3	2.04	0.57
1:A:329:THR:HG22	1:A:350:ARG:CB	2.30	0.57
1:A:377:LEU:HD21	1:A:380:VAL:HG23	1.86	0.57
1:A:133:MET:HG3	1:A:135:VAL:HG13	1.85	0.56
1:A:185:ILE:HB	1:A:350:ARG:HH11	0.75	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:C	1:A:344:LEU:HD12	2.29	0.56
1:B:113:THR:C	1:B:114:LEU:HD12	2.29	0.56
1:B:321:HIS:NE2	1:B:323:ASP:HB3	2.21	0.56
1:A:154:LYS:HB3	1:A:156:THR:HG22	1.87	0.56
1:B:74:LYS:CE	1:B:75:GLY:H	2.17	0.56
1:A:353:GLU:OE1	1:A:383:PRO:HB2	2.06	0.56
1:A:463:TYR:O	1:A:467:VAL:HG23	2.06	0.56
1:B:10:GLU:O	1:B:14:ILE:HG12	2.05	0.56
1:A:336:THR:O	1:A:343:GLY:HA2	2.06	0.55
1:A:193:ASN:HD22	1:A:372:GLY:HA2	1.70	0.55
1:A:396:LEU:HD22	1:A:461:ALA:HB3	1.84	0.55
1:A:83:CYS:CB	2:A:510:HOH:O	2.36	0.55
1:B:165:MET:CE	1:B:353:GLU:HG3	2.37	0.55
1:A:2:TRP:HZ3	1:A:5:LYS:HZ1	1.48	0.54
1:B:288:ALA:HB2	1:B:304:ASN:HD21	1.72	0.54
1:B:395:LYS:HD2	1:B:465:LEU:CD2	2.34	0.54
1:A:447:THR:HG22	1:A:449:LYS:CA	2.37	0.54
1:B:201:GLU:CD	1:B:229:LYS:HD3	2.32	0.54
1:A:338:ASP:OD2	1:A:340:GLU:N	2.40	0.54
1:B:154:LYS:HB2	1:B:156:THR:CG2	2.37	0.54
1:B:322:THR:O	1:B:325:MET:N	2.40	0.54
1:A:14:ILE:CG2	1:A:15:ASN:N	2.71	0.54
1:A:111:ARG:NH1	1:A:441:GLN:CB	2.71	0.54
1:A:95:ASP:H	1:A:443:ASN:HD21	1.55	0.53
1:A:14:ILE:HD11	1:A:108:ILE:HG12	1.90	0.53
1:B:129:ILE:O	1:B:133:MET:HG2	2.08	0.53
1:A:204:TYR:HE2	1:A:235:VAL:HG21	1.68	0.53
1:A:65:HIS:HD2	2:A:518:HOH:O	1.90	0.53
1:B:112:GLY:H	1:B:444:GLU:CD	2.17	0.53
1:B:318:MET:HE1	1:B:361:MET:CE	2.39	0.53
1:B:109:ILE:O	1:B:110:ALA:CB	2.58	0.52
1:B:165:MET:HE1	1:B:353:GLU:HG3	1.92	0.52
1:B:190:LEU:HD11	1:B:347:ILE:CD1	2.39	0.52
1:A:104:THR:HG21	1:A:107:ALA:N	2.17	0.52
1:A:14:ILE:HD11	1:A:108:ILE:CG1	2.40	0.52
1:A:377:LEU:HG	1:A:378:GLY:H	1.73	0.52
1:B:403:GLN:C	1:B:404:THR:HG1	2.13	0.52
1:A:82:LEU:N	1:A:82:LEU:HD23	2.24	0.52
1:A:102:VAL:CG2	1:A:109:ILE:HB	2.30	0.52
1:B:168:LEU:H	1:B:168:LEU:HD23	1.75	0.52
1:B:361:MET:HG2	1:B:377:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ARG:HH12	1:A:441:GLN:CB	2.23	0.52
1:A:357:PHE:CE1	1:A:361:MET:CE	2.93	0.52
1:A:448:LYS:O	1:A:452:PHE:HD2	1.93	0.52
1:A:447:THR:CG2	1:A:449:LYS:CB	2.88	0.52
1:A:11:ASP:O	1:A:14:ILE:HG22	2.10	0.52
1:A:367:GLU:O	1:A:367:GLU:CG	2.55	0.52
1:B:82:LEU:HD12	1:B:82:LEU:N	2.25	0.52
1:A:77:ASP:HB2	1:A:139:LYS:HG2	1.91	0.51
1:A:332:ILE:N	1:A:332:ILE:CD1	2.73	0.51
1:B:404:THR:HG22	1:B:404:THR:O	2.09	0.51
1:A:302:PHE:HE1	1:A:368:ILE:HG13	1.75	0.51
1:A:396:LEU:HD13	1:A:457:ILE:HG22	1.92	0.51
1:B:1:MET:O	1:B:4:GLU:CA	2.58	0.51
1:A:28:ASP:OD2	1:A:31:LYS:CG	2.37	0.51
1:A:135:VAL:HB	1:A:467:VAL:HG11	1.93	0.51
1:B:21:LEU:HD21	1:B:113:THR:HG23	1.90	0.51
1:B:463:TYR:CD1	1:B:467:VAL:HG21	2.45	0.51
1:A:102:VAL:CG2	1:A:102:VAL:O	2.59	0.51
1:B:194:LYS:O	1:B:195:LEU:C	2.54	0.51
1:A:186:THR:HG23	1:A:380:VAL:CA	2.37	0.51
1:B:190:LEU:CD1	1:B:347:ILE:CD1	2.88	0.51
1:A:114:LEU:N	1:A:114:LEU:HD12	2.25	0.50
1:A:346:GLY:C	1:A:347:ILE:HD12	2.35	0.50
1:B:168:LEU:HD23	1:B:168:LEU:N	2.27	0.50
1:B:168:LEU:HD12	1:B:391:PRO:HG2	1.94	0.50
1:A:338:ASP:OD2	1:A:340:GLU:HB3	2.12	0.50
1:A:346:GLY:C	1:A:347:ILE:CD1	2.84	0.50
1:A:73:GLY:HA2	1:A:137:TRP:CG	2.46	0.50
1:B:115:ASP:OD2	1:B:115:ASP:N	2.44	0.50
1:B:392:PHE:CA	1:B:465:LEU:HD21	2.37	0.50
1:A:78:VAL:O	1:A:167:THR:HG22	2.12	0.50
1:A:399:ALA:O	1:A:403:GLN:HG3	2.11	0.50
1:B:82:LEU:N	1:B:82:LEU:CD1	2.74	0.50
1:A:402:ASN:OD1	1:A:402:ASN:O	2.30	0.50
1:A:367:GLU:O	1:A:367:GLU:HG3	2.11	0.50
1:B:102:VAL:HG23	1:B:102:VAL:O	2.11	0.50
1:A:102:VAL:CG2	1:A:109:ILE:HD12	2.42	0.49
1:B:275:ILE:O	1:B:275:ILE:CG2	2.60	0.49
1:B:446:ILE:HD11	1:B:451:LEU:HB2	1.93	0.49
1:B:337:TYR:C	1:B:337:TYR:CD2	2.90	0.49
1:B:446:ILE:HG12	1:B:447:THR:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:SER:OG	1:A:315:LYS:CB	2.60	0.49
1:B:387:ASP:C	1:B:389:ASN:H	2.21	0.49
1:B:387:ASP:C	1:B:389:ASN:N	2.69	0.49
1:A:194:LYS:CE	1:A:342:ALA:HB2	2.41	0.49
1:B:113:THR:CB	1:B:446:ILE:HG22	2.21	0.49
1:A:28:ASP:OD2	1:A:31:LYS:HE3	2.13	0.48
1:A:251:ASP:H	1:A:262:THR:HG23	1.76	0.48
1:B:159:TYR:CE2	1:B:163:GLU:HB2	2.48	0.48
1:B:168:LEU:CD1	1:B:391:PRO:HG2	2.43	0.48
1:B:21:LEU:HD12	1:B:21:LEU:HA	1.73	0.48
1:B:190:LEU:HD12	1:B:347:ILE:HD11	1.92	0.48
1:B:339:ASN:O	2:B:530:HOH:O	2.20	0.48
1:A:158:ARG:O	1:A:161:LYS:HB2	2.14	0.48
1:A:337:TYR:HA	1:A:343:GLY:CA	2.42	0.48
1:B:114:LEU:CD1	1:B:445:TYR:O	2.52	0.48
1:B:344:LEU:C	1:B:344:LEU:HD23	2.39	0.48
1:A:103:VAL:O	1:A:103:VAL:HG12	2.13	0.48
1:B:111:ARG:HD3	1:B:444:GLU:OE2	2.14	0.48
1:A:218:VAL:HB	1:A:267:ALA:HA	1.95	0.48
1:A:447:THR:CG2	1:A:449:LYS:CA	2.91	0.48
1:B:165:MET:HE1	1:B:353:GLU:CG	2.44	0.48
1:B:199:GLN:NE2	1:B:294:ASN:CG	2.72	0.48
1:B:323:ASP:CA	1:B:324:VAL:CB	2.91	0.48
1:B:375:VAL:HG12	1:B:377:LEU:HD13	1.96	0.48
1:A:10:GLU:HG2	1:A:452:PHE:CZ	2.49	0.47
1:B:318:MET:HE1	1:B:361:MET:HE1	1.95	0.47
1:B:321:HIS:NE2	1:B:323:ASP:CB	2.77	0.47
1:A:165:MET:HE2	1:A:180:HIS:CD2	2.49	0.47
1:A:357:PHE:CZ	1:A:361:MET:HE3	2.48	0.47
1:B:400:TYR:HD2	1:B:401:ARG:CA	2.24	0.47
1:A:231:ASN:ND2	1:A:234:ASP:CG	2.60	0.47
1:B:179:ILE:O	1:B:180:HIS:C	2.55	0.47
1:B:447:THR:OG1	1:B:450:GLN:HB3	2.15	0.47
1:A:168:LEU:CD1	1:A:465:LEU:HD21	2.40	0.47
1:A:305:ARG:HD3	1:A:306:TYR:CZ	2.50	0.47
1:B:88:VAL:CG1	1:B:89:PRO:CD	2.93	0.46
1:B:190:LEU:HD11	1:B:347:ILE:HD11	1.93	0.46
1:A:341:ASN:O	1:A:342:ALA:HB3	2.15	0.46
1:B:114:LEU:C	1:B:115:ASP:OD2	2.58	0.46
1:B:104:THR:HG22	1:B:105:GLU:C	2.39	0.46
1:A:195:LEU:H	1:A:295:ASN:HD21	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:TYR:CZ	1:A:235:VAL:CG2	2.95	0.46
1:B:10:GLU:O	1:B:14:ILE:CG1	2.63	0.46
1:B:157:ASP:O	1:B:161:LYS:HD3	2.14	0.46
1:B:446:ILE:CD1	1:B:451:LEU:HB2	2.45	0.46
1:B:393:VAL:O	1:B:397:VAL:HG12	2.17	0.45
1:B:81:ILE:C	1:B:82:LEU:HD12	2.41	0.45
1:B:332:ILE:HD13	1:B:332:ILE:N	2.32	0.45
1:B:400:TYR:CD2	1:B:401:ARG:CA	2.99	0.45
1:A:336:THR:O	1:A:343:GLY:CA	2.64	0.45
1:B:399:ALA:HB3	1:B:457:ILE:HG23	1.98	0.45
1:A:114:LEU:HD13	1:A:444:GLU:CG	2.41	0.45
1:B:63:VAL:HG21	1:B:159:TYR:HD1	1.82	0.45
1:A:102:VAL:O	1:A:102:VAL:HG23	2.16	0.45
1:A:185:ILE:N	1:A:381:GLN:O	2.42	0.45
1:A:133:MET:HE2	1:A:133:MET:HB3	1.75	0.45
1:A:94:TRP:CD2	1:A:98:PRO:HG3	2.53	0.44
1:A:349:LEU:C	1:A:349:LEU:HD23	2.42	0.44
1:B:105:GLU:O	1:B:448:LYS:NZ	2.32	0.44
1:B:101:PRO:HA	1:B:109:ILE:O	2.18	0.44
1:A:186:THR:CG2	1:A:380:VAL:HG23	2.42	0.44
1:A:130:LEU:HD23	1:A:459:LEU:CD1	2.32	0.44
1:B:401:ARG:O	1:B:402:ASN:C	2.61	0.44
1:B:388:LYS:C	1:B:389:ASN:HD22	2.25	0.44
1:B:395:LYS:HE2	1:B:465:LEU:HD23	1.97	0.44
1:A:347:ILE:N	1:A:347:ILE:HD12	2.33	0.44
1:B:338:ASP:O	1:B:339:ASN:C	2.59	0.44
1:A:114:LEU:CD1	1:A:114:LEU:N	2.80	0.44
1:A:168:LEU:HD11	1:A:465:LEU:HD22	1.96	0.43
1:B:288:ALA:HB2	1:B:304:ASN:ND2	2.32	0.43
1:B:96:SER:O	1:B:98:PRO:HD3	2.17	0.43
1:A:390:ASP:HA	1:A:391:PRO:HD3	1.88	0.43
1:A:400:TYR:O	1:A:404:THR:N	2.30	0.43
1:B:392:PHE:CB	1:B:465:LEU:HD21	2.48	0.43
1:B:447:THR:OG1	1:B:450:GLN:CB	2.66	0.43
1:B:148:ASP:C	1:B:150:GLU:N	2.75	0.43
1:B:394:GLN:HA	1:B:397:VAL:CG1	2.48	0.43
1:A:236:ILE:O	1:A:240:GLU:HG3	2.19	0.43
1:B:349:LEU:HD23	1:B:349:LEU:C	2.44	0.43
1:A:343:GLY:CA	2:A:477:HOH:O	2.57	0.42
1:A:368:ILE:C	1:A:370:GLN:N	2.77	0.42
1:A:168:LEU:N	1:A:168:LEU:HD23	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:PRO:HB2	1:B:44:LYS:NZ	2.34	0.42
1:B:165:MET:HG3	1:B:178:CYS:SG	2.59	0.42
1:A:185:ILE:HG12	1:A:186:THR:N	2.33	0.42
1:B:88:VAL:CG1	1:B:89:PRO:N	2.80	0.42
1:A:400:TYR:O	1:A:404:THR:HG22	2.20	0.42
1:A:463:TYR:CD1	1:A:467:VAL:HG21	2.54	0.42
1:B:190:LEU:HG	1:B:347:ILE:HD12	2.02	0.42
1:B:392:PHE:HB2	1:B:465:LEU:HD21	2.00	0.42
1:B:228:VAL:HG23	1:B:232:MET:HE2	2.02	0.42
1:A:218:VAL:N	1:A:268:VAL:O	2.39	0.42
1:A:78:VAL:H	1:A:167:THR:CG2	2.32	0.42
1:A:138:LYS:CG	1:A:466:CYS:O	2.67	0.41
1:A:144:ILE:HG22	1:A:153:TRP:CH2	2.55	0.41
1:A:403:GLN:HE21	1:A:403:GLN:HB3	1.64	0.41
1:B:49:MET:CE	1:B:49:MET:CA	2.82	0.41
1:A:19:GLY:HA3	1:A:48:TYR:OH	2.20	0.41
1:A:120:THR:CG2	1:A:143:MET:CE	2.98	0.41
1:A:193:ASN:HD22	1:A:372:GLY:CA	2.33	0.41
1:A:447:THR:HG21	1:A:449:LYS:CB	2.50	0.41
1:B:299:PHE:CE2	1:B:345:PHE:CZ	3.08	0.41
1:B:397:VAL:O	1:B:397:VAL:CG2	2.69	0.41
1:B:24:GLU:O	1:B:24:GLU:CG	2.68	0.41
1:A:187:THR:HA	1:A:347:ILE:O	2.20	0.41
1:B:120:THR:HG23	1:B:143:MET:CE	2.50	0.41
1:B:148:ASP:C	1:B:150:GLU:H	2.28	0.41
1:A:381:GLN:HA	1:A:382:PRO:HD3	1.73	0.41
1:B:220:ASP:HB3	1:B:267:ALA:HB2	2.03	0.41
1:A:3:LYS:HB2	1:A:3:LYS:HE2	1.84	0.41
1:B:6:VAL:O	1:B:7:GLN:C	2.64	0.41
1:A:173:ASP:OD2	1:A:173:ASP:N	2.48	0.41
1:A:398:THR:O	1:A:402:ASN:HB2	2.21	0.41
1:B:154:LYS:C	1:B:156:THR:N	2.73	0.41
1:A:115:ASP:HA	1:A:116:ASP:HA	1.51	0.41
1:A:190:LEU:N	1:A:190:LEU:HD23	2.36	0.41
1:B:100:GLU:HA	1:B:101:PRO:HD2	1.91	0.41
1:B:228:VAL:CG2	1:B:232:MET:HE2	2.51	0.40
1:B:88:VAL:HG12	1:B:89:PRO:N	2.34	0.40
1:B:115:ASP:HA	1:B:116:ASP:HA	1.64	0.40
1:B:4:GLU:C	1:B:5:LYS:HE3	2.34	0.40
1:B:73:GLY:HA2	1:B:137:TRP:CD1	2.57	0.40
1:B:388:LYS:O	1:B:388:LYS:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:TYR:O	1:B:348:ASN:HB2	2.21	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	414/492 (84%)	397 (96%)	15 (4%)	2 (0%)	24	31
1	B	417/492 (85%)	399 (96%)	16 (4%)	2 (0%)	24	31
All	All	831/984 (84%)	796 (96%)	31 (4%)	4 (0%)	24	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	VAL
1	B	110	ALA
1	A	343	GLY
1	B	324	VAL

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	330/418 (79%)	296 (90%)	34 (10%)	7	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	343/418 (82%)	310 (90%)	33 (10%)	8	10
All	All	673/836 (80%)	606 (90%)	67 (10%)	7	9

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	78	VAL
1	A	82	LEU
1	A	84	HIS
1	A	87	VAL
1	A	92	ASP
1	A	102	VAL
1	A	104	THR
1	A	115	ASP
1	A	130	LEU
1	A	185	ILE
1	A	186	THR
1	A	194	LYS
1	A	214	ARG
1	A	227	LEU
1	A	233	THR
1	A	248	LEU
1	A	253	THR
1	A	258	ILE
1	A	307	LEU
1	A	309	ASN
1	A	329	THR
1	A	332	ILE
1	A	340	GLU
1	A	341	ASN
1	A	344	LEU
1	A	347	ILE
1	A	368	ILE
1	A	396	LEU
1	A	398	THR
1	A	447	THR
1	A	448	LYS
1	A	465	LEU
1	A	467	VAL
1	B	1	MET
1	B	5	LYS

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Mol	Chain	Res	Type
1	B	14	ILE
1	B	20	LEU
1	B	21	LEU
1	B	49	MET
1	B	63	VAL
1	B	74	LYS
1	B	82	LEU
1	B	104	THR
1	B	115	ASP
1	B	133	MET
1	B	134	ASN
1	B	151	SER
1	B	156	THR
1	B	161	LYS
1	B	168	LEU
1	B	213	GLU
1	B	214	ARG
1	B	284	LEU
1	B	290	LEU
1	B	300	VAL
1	B	309	ASN
1	B	332	ILE
1	B	339	ASN
1	B	353	GLU
1	B	361	MET
1	B	377	LEU
1	B	387	ASP
1	B	396	LEU
1	B	397	VAL
1	B	400	TYR
1	B	446	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	76	ASN
1	A	84	HIS
1	A	180	HIS
1	A	193	ASN
1	A	231	ASN
1	A	246	ASN

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Mol	Chain	Res	Type
1	A	294	ASN
1	A	295	ASN
1	A	331	ASN
1	A	339	ASN
1	A	370	GLN
1	A	389	ASN
1	A	402	ASN
1	A	403	GLN
1	A	443	ASN
1	B	12	GLN
1	B	76	ASN
1	B	199	GLN
1	B	246	ASN
1	B	297	GLN
1	B	304	ASN
1	B	309	ASN
1	B	366	ASN
1	B	384	HIS
1	B	389	ASN
1	B	403	GLN
1	B	453	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	422/492 (85%)	1.27	89 (21%) 2 3	31, 49, 76, 95	1 (0%)
1	B	425/492 (86%)	1.17	74 (17%) 4 4	29, 47, 83, 110	0
All	All	847/984 (86%)	1.22	163 (19%) 3 3	29, 48, 80, 110	1 (0%)

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	THR	6.9
1	A	405	ASN	5.9
1	B	404	THR	5.5
1	A	267	ALA	5.2
1	A	465	LEU	4.7
1	B	441	GLN	4.6
1	A	327	ASP	4.6
1	B	324	VAL	4.3
1	B	465	LEU	4.3
1	A	265	GLY	4.3
1	B	96	SER	4.2
1	A	269	HIS	4.2
1	B	445	TYR	4.1
1	A	404	THR	4.0
1	A	464	SER	4.0
1	B	323	ASP	4.0
1	A	200	ASP	3.8
1	A	268	VAL	3.8
1	A	400	TYR	3.8
1	B	400	TYR	3.8
1	A	197	GLU	3.7
1	A	397	VAL	3.7
1	A	104	THR	3.6
1	B	462	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	372	GLY	3.6
1	A	393	VAL	3.6
1	A	441	GLN	3.5
1	A	312	PHE	3.5
1	A	390	ASP	3.5
1	A	195	LEU	3.4
1	B	341	ASN	3.4
1	A	96	SER	3.4
1	B	103	VAL	3.4
1	B	195	LEU	3.4
1	B	390	ASP	3.4
1	B	443	ASN	3.4
1	B	255	ASP	3.4
1	B	393	VAL	3.3
1	A	102	VAL	3.3
1	B	396	LEU	3.3
1	A	386	VAL	3.2
1	A	0	SER	3.2
1	A	442	LYS	3.2
1	A	391	PRO	3.1
1	A	354	GLY	3.1
1	B	136	ASP	3.1
1	B	463	TYR	3.1
1	A	310	SER	3.1
1	B	397	VAL	3.0
1	A	91	GLY	3.0
1	A	355	PHE	3.0
1	A	462	ILE	3.0
1	A	160	PHE	2.9
1	A	342	ALA	2.9
1	B	114	LEU	2.9
1	B	104	THR	2.9
1	B	247	HIS	2.9
1	A	198	ASP	2.9
1	A	276	GLY	2.8
1	A	343	GLY	2.8
1	A	7	GLN	2.8
1	A	313	GLY	2.8
1	A	318	MET	2.8
1	B	102	VAL	2.8
1	B	115	ASP	2.8
1	A	173	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	319	LYS	2.7
1	A	6	VAL	2.7
1	B	63	VAL	2.7
1	B	254	VAL	2.7
1	A	134	ASN	2.7
1	A	1	MET	2.7
1	A	357	PHE	2.7
1	B	231	ASN	2.7
1	A	317	GLY	2.7
1	A	469	GLU	2.6
1	B	200	ASP	2.6
1	B	399	ALA	2.6
1	B	340	GLU	2.6
1	A	366	ASN	2.6
1	B	392	PHE	2.6
1	B	258	ILE	2.6
1	A	396	LEU	2.5
1	B	64	ASP	2.5
1	B	468	GLU	2.5
1	B	447	THR	2.5
1	A	358	GLU	2.5
1	A	443	ASN	2.5
1	A	340	GLU	2.5
1	A	371	TYR	2.5
1	A	304	ASN	2.5
1	A	176	PHE	2.4
1	A	452	PHE	2.4
1	B	1	MET	2.4
1	B	325	MET	2.4
1	B	339	ASN	2.4
1	B	180	HIS	2.4
1	B	156	THR	2.4
1	B	78	VAL	2.4
1	B	248	LEU	2.4
1	B	251	ASP	2.4
1	B	442	LYS	2.4
1	B	26	VAL	2.4
1	B	7	GLN	2.4
1	A	468	GLU	2.4
1	A	231	ASN	2.3
1	A	315	LYS	2.3
1	A	373	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	384	HIS	2.3
1	B	295	ASN	2.3
1	B	2	TRP	2.3
1	A	352	PRO	2.3
1	A	382	PRO	2.3
1	B	457	ILE	2.3
1	B	6	VAL	2.3
1	B	135	VAL	2.3
1	B	130	LEU	2.3
1	B	342	ALA	2.3
1	A	201	GLU	2.3
1	B	8	GLN	2.3
1	A	5	LYS	2.3
1	A	2	TRP	2.3
1	A	457	ILE	2.3
1	A	171	ALA	2.2
1	A	215	TYR	2.2
1	B	34	GLU	2.2
1	B	249	GLN	2.2
1	B	464	SER	2.2
1	B	97	ASN	2.2
1	B	469	GLU	2.2
1	B	44	LYS	2.2
1	A	467	VAL	2.2
1	A	392	PHE	2.2
1	B	198	ASP	2.2
1	B	98	PRO	2.2
1	B	133	MET	2.2
1	A	314	GLU	2.2
1	A	351	TYR	2.2
1	B	227	LEU	2.2
1	B	173	ASP	2.2
1	A	93	GLY	2.2
1	B	322	THR	2.2
1	A	377	LEU	2.1
1	A	459	LEU	2.1
1	B	459	LEU	2.1
1	B	89	PRO	2.1
1	B	172	PRO	2.1
1	B	317	GLY	2.1
1	A	463	TYR	2.1
1	A	95	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	103	VAL	2.1
1	B	273	PRO	2.1
1	A	399	ALA	2.1
1	B	461	ALA	2.1
1	A	14	ILE	2.1
1	A	97	ASN	2.1
1	A	339	ASN	2.1
1	A	257	GLY	2.1
1	A	403	GLN	2.1
1	A	309	ASN	2.0
1	A	141	ILE	2.0
1	A	266	LYS	2.0
1	B	3	LYS	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.