Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:58 PM GMT

PDB ID	:	1MWR
Title	:	Structure of SeMet Penicillin binding protein 2a from methicillin resistant Staphylococcus aureus strain 27r (trigonal form) at 2.45 A resolution.
Authors	:	Lim, D.C.; Strynadka, N.C.J.
Deposited on	:	2002-10-01
Resolution	:	2.45 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

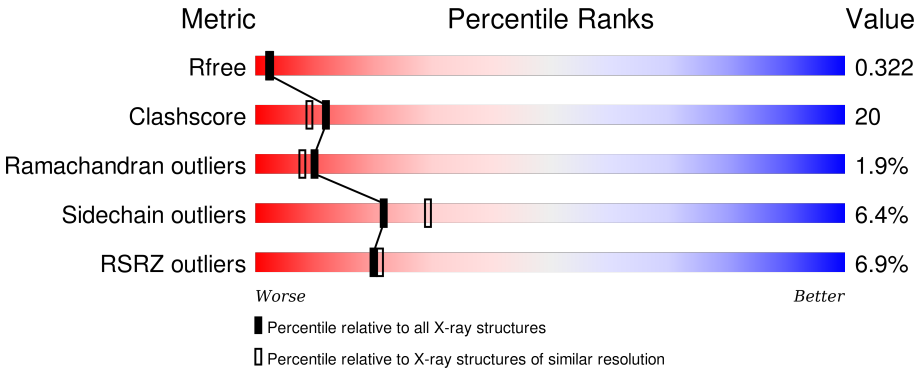
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.45 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}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	646	6% 62% 31%
1	B	646	7% 60% 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10089 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 penicillin-binding protein 2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	Se	0	0	0
			5019	3169	842	993	15			
1	B	629	Total	C	N	O	Se	0	0	0
			5054	3188	850	1001	15			

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Cd	0	0
			2	2		
2	A	2	Total	Cd	0	0
			2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is water.

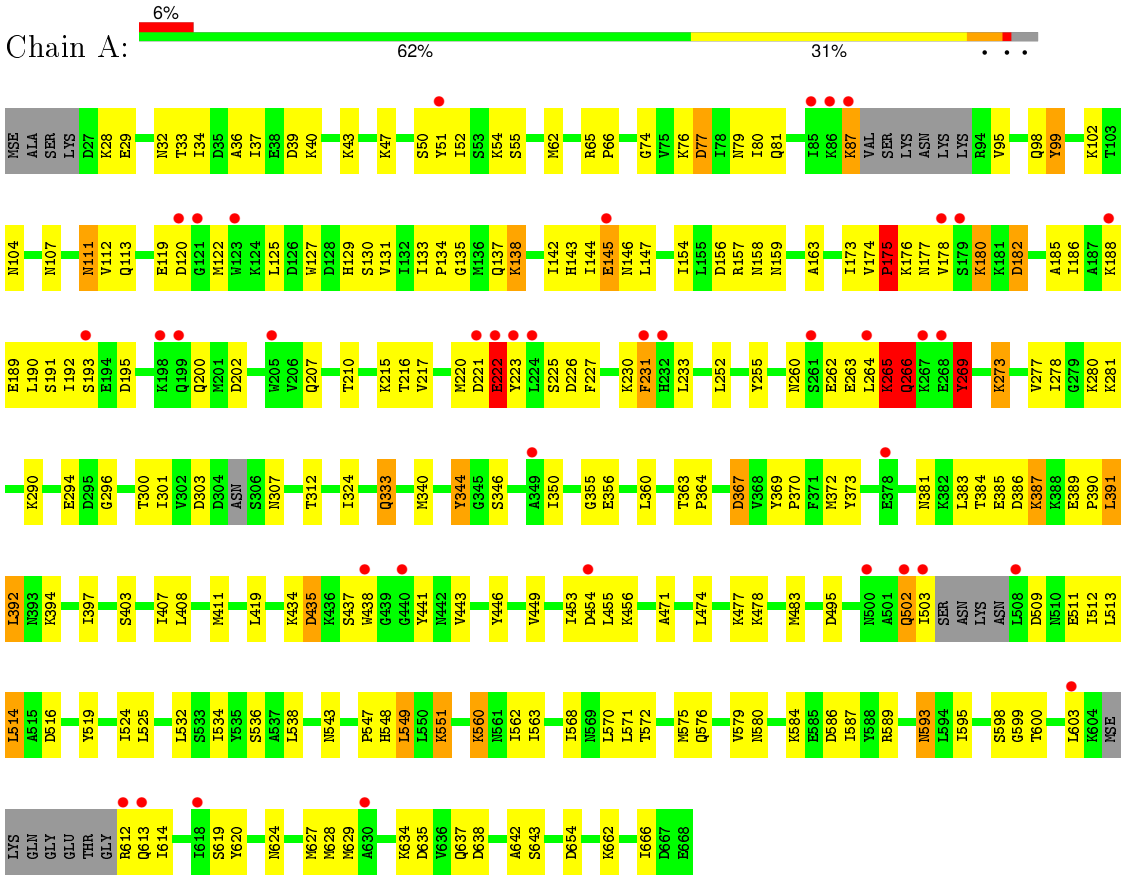
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	2	Total	O	0	0
			2	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

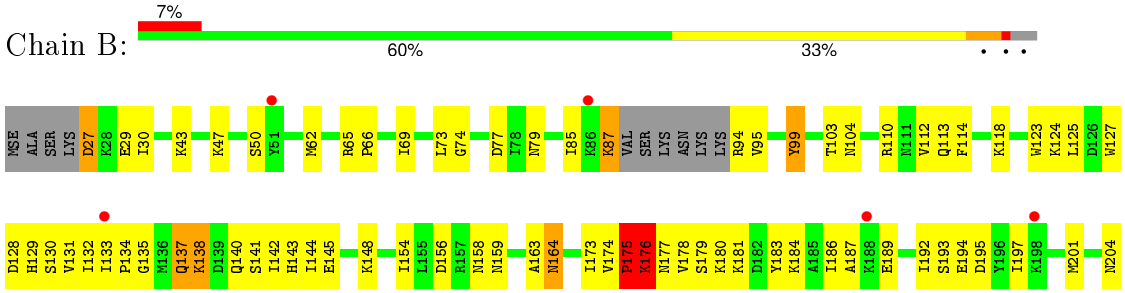
- Molecule 1: penicillin-binding protein 2a

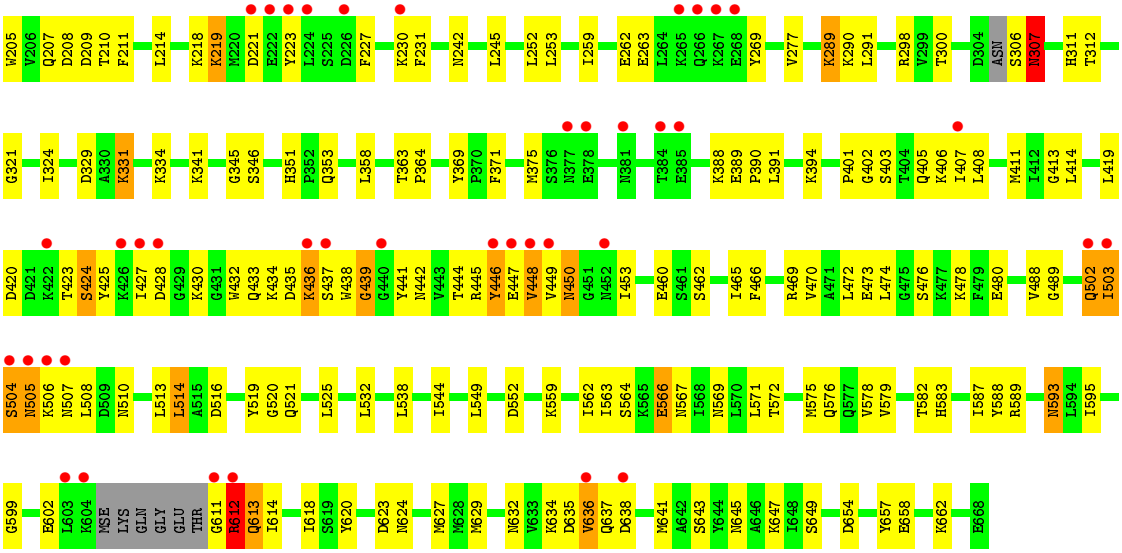
Chain A:



- Molecule 1: penicillin-binding protein 2a

Chain B:




W205 V206 Q207 D208 D209 T210 F211 L214 K218 K219 M220 D221 E222 Y223 L224 S225 D226 F227 K230 F231 N242 L245 L252 L253 I259 E262 E263 L264 K265 Q266 K267 E268 Y269 V277 K289 K290 L291 R298 V299 T300 D304 ASN S306 N307 H311 T312
G321 I324 D329 A330 K331 K334 K341 G345 S346 H351 P352 Q353 L358 T363 P364 Y369 P370 F371 M375 S376 N377 E378 N381 T384 E385 K388 E389 P390 L391 K394 P401 G402 S403 T404 Q405 K406 I407 L408 M411 I412 G413 L414 L419
D420 D421 K422 T423 S424 Y425 K426 I427 D428 G429 K430 G431 W432 Q433 K434 D435 K436 S437 W438 G439 G440 Y441 N442 V443 T444 R445 Y446 E447 V448 V449 N450 G451 N452 I453 E460 S461 S462 I465 F466 R469 V470 A471 L472 E473 L474 G475 S476 K477 K478 F479 E480 V488 G489 Q502 I503
S504 N505 K506 N507 L508 D509 N510 L513 L514 A515 D516 Y519 G520 Q521 L525 L532 L538 I544 L549 D552 K559 I562 I563 S564 K565 E566 N567 I568 N569 L570 L571 T572 M575 Q576 Q577 V578 V579 T582 H583 I587 Y588 R589 N593 L594 I595
G599 E602 L603 K604 MSE LYS GLN GLY GLU THR G611 R612 Q613 I614 I618 S619 Y620 D623 N624 M627 M628 M629 N632 V633 K634 D635 V636 Q637 D638 M641 A642 S643 Y644 N645 A646 K647 I648 S649 D654 Y657 E658 K662 E668

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.06Å 141.06Å 146.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.89 – 2.45 24.88 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.9 (24.89-2.45) 98.1 (24.88-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.44Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.270 , 0.324 0.269 , 0.322	Depositor DCC
R_{free} test set	3086 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.6	EDS
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 61038 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	10089	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CD

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	0.48	4/5086 (0.1%)	0.69	5/6812 (0.1%)
1	B	0.40	0/5122	0.65	0/6861
All	All	0.44	4/10208 (0.0%)	0.67	5/13673 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	GLU	CD-OE2	-10.92	1.13	1.25
1	A	145	GLU	CD-OE1	-7.97	1.16	1.25
1	A	145	GLU	CG-CD	7.46	1.63	1.51
1	A	145	GLU	CB-CG	6.55	1.64	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	145	GLU	OE1-CD-OE2	-13.63	106.94	123.30
1	A	145	GLU	CG-CD-OE1	6.66	131.63	118.30
1	A	454	ASP	CB-CG-OD2	6.48	124.13	118.30
1	A	454	ASP	CB-CG-OD1	-6.05	112.85	118.30
1	A	144	ILE	N-CA-C	-5.05	97.37	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	5019	0	5005	201	1
1	B	5054	0	5039	207	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	2	0	0	1	0
3	B	2	0	0	0	0
4	A	6	0	0	0	2
4	B	2	0	0	0	0
All	All	10089	0	10044	403	2

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 20.

All (403) 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:87:LYS:H	1:A:87:LYS:HD3	1.18	1.08
1:A:222:GLU:HA	1:A:225:SER:HB3	1.30	1.08
1:A:138:LYS:H	1:A:138:LYS:HD2	1.18	1.04
1:A:145:GLU:OE1	3:A:1207:CL:CL	2.12	1.04
1:B:611:GLY:HA3	1:B:635:ASP:OD1	1.59	1.02
1:A:419:LEU:HD11	1:A:455:LEU:HD22	1.40	1.01
1:A:381:ASN:HA	1:A:384:THR:HG22	1.43	1.00
1:B:87:LYS:HD3	1:B:87:LYS:H	1.30	0.93
1:A:143:HIS:HB3	1:A:145:GLU:HG3	1.50	0.92
1:A:576:GLN:HE21	1:A:593:ASN:HD21	1.16	0.90
1:A:112:VAL:HG11	1:A:134:PRO:HB3	1.54	0.89
1:B:219:LYS:NZ	1:B:219:LYS:H	1.74	0.85
1:A:138:LYS:N	1:A:138:LYS:HD2	1.90	0.85
1:B:87:LYS:HD3	1:B:87:LYS:N	1.91	0.85
1:B:510:ASN:HB3	1:B:513:LEU:HB2	1.58	0.84
1:B:27:ASP:HB2	1:B:30:ILE:HB	1.60	0.83
1:B:602:GLU:HG2	1:B:613:GLN:HE22	1.45	0.82
1:B:300:THR:HG22	1:B:312:THR:HA	1.62	0.82
1:A:265:LYS:HE3	1:A:265:LYS:HA	1.63	0.81
1:B:602:GLU:HG2	1:B:613:GLN:NE2	1.97	0.80
1:A:174:VAL:HB	1:A:177:ASN:HD22	1.47	0.80
1:A:87:LYS:N	1:A:87:LYS:HD3	1.96	0.79
1:A:562:ILE:HG13	1:A:563:ILE:HG22	1.65	0.79
1:B:506:LYS:HE2	1:B:507:ASN:ND2	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:LEU:HB3	1:A:575:MSE:HE3	1.64	0.78
1:B:230:LYS:HE3	1:B:231:PHE:HE2	1.49	0.77
1:A:51:TYR:HA	1:A:54:LYS:HE2	1.66	0.77
1:B:436:LYS:H	1:B:436:LYS:HD3	1.49	0.77
1:B:419:LEU:HD13	1:B:420:ASP:N	2.00	0.76
1:B:138:LYS:H	1:B:138:LYS:HD2	1.49	0.76
1:B:43:LYS:O	1:B:47:LYS:HG2	1.86	0.76
1:A:146:ASN:ND2	1:A:147:LEU:N	2.33	0.76
1:A:186:ILE:HD13	1:A:233:LEU:HD21	1.67	0.75
1:B:506:LYS:HE2	1:B:507:ASN:HD21	1.51	0.75
1:A:407:ILE:HD12	1:A:575:MSE:HE2	1.68	0.75
1:B:433:GLN:HB3	1:B:442:ASN:ND2	2.02	0.74
1:A:571:LEU:O	1:A:575:MSE:HG3	1.88	0.74
1:A:146:ASN:HD22	1:A:147:LEU:H	1.34	0.74
1:B:94:ARG:HE	1:B:113:GLN:HG3	1.53	0.73
1:A:620:TYR:CD2	1:A:628:MSE:HE3	2.24	0.73
1:B:627:MSE:HE3	1:B:629:MSE:HB2	1.70	0.72
1:B:219:LYS:HZ2	1:B:219:LYS:H	1.36	0.72
1:B:572:THR:HA	1:B:575:MSE:HE2	1.72	0.72
1:A:538:LEU:HD11	1:A:575:MSE:HE1	1.72	0.72
1:A:220:MSE:HA	1:A:220:MSE:HE2	1.71	0.72
1:B:74:GLY:HA3	1:B:104:ASN:ND2	2.04	0.71
1:A:576:GLN:NE2	1:A:593:ASN:HD21	1.87	0.70
1:A:471:ALA:HB1	1:A:514:LEU:CD2	2.22	0.70
1:A:381:ASN:HA	1:A:384:THR:CG2	2.21	0.70
1:B:476:SER:O	1:B:480:GLU:HG3	1.92	0.69
1:A:477:LYS:HB3	1:A:477:LYS:NZ	2.07	0.69
1:B:112:VAL:HG22	1:B:134:PRO:HB3	1.73	0.69
1:A:449:VAL:HG23	1:A:453:ILE:CD1	2.23	0.68
1:A:176:LYS:HG3	1:A:177:ASN:H	1.58	0.68
1:A:217:VAL:HG21	1:A:220:MSE:HE3	1.75	0.68
1:A:384:THR:HG23	1:A:385:GLU:HG3	1.74	0.68
1:A:516:ASP:HA	1:A:519:TYR:CE2	2.28	0.68
1:B:466:PHE:O	1:B:470:VAL:HG23	1.94	0.68
1:A:146:ASN:HD22	1:A:147:LEU:N	1.92	0.68
1:A:260:ASN:OD1	1:A:263:GLU:HG3	1.94	0.68
1:A:180:LYS:HA	1:A:180:LYS:NZ	2.10	0.67
1:A:138:LYS:CD	1:A:138:LYS:H	2.01	0.67
1:B:436:LYS:N	1:B:436:LYS:HD3	2.08	0.67
1:B:245:LEU:HD13	1:B:334:LYS:HG3	1.76	0.67
1:B:99:TYR:HB2	1:B:112:VAL:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ILE:HB	1:B:163:ALA:HB3	1.76	0.67
1:A:173:ILE:HG12	1:A:178:VAL:HG21	1.76	0.66
1:B:614:ILE:HD11	1:B:634:LYS:HG3	1.77	0.66
1:B:69:ILE:HG23	1:B:142:ILE:HD12	1.78	0.66
1:A:112:VAL:CG1	1:A:134:PRO:HB3	2.24	0.66
1:A:495:ASP:OD1	1:A:548:HIS:HB2	1.96	0.66
1:B:435:ASP:HB2	1:B:436:LYS:HD3	1.77	0.66
1:B:488:VAL:O	1:B:503:ILE:HD11	1.95	0.66
1:A:137:GLN:HB3	1:A:138:LYS:HD2	1.78	0.65
1:A:39:ASP:O	1:A:40:LYS:HB2	1.95	0.65
1:A:307:ASN:ND2	1:B:144:ILE:H	1.93	0.65
1:A:579:VAL:HG13	1:A:587:ILE:HG23	1.78	0.65
1:A:174:VAL:HB	1:A:177:ASN:ND2	2.11	0.65
1:A:407:ILE:O	1:A:411:MSE:HG3	1.97	0.65
1:B:112:VAL:CG2	1:B:134:PRO:HB3	2.27	0.64
1:A:449:VAL:HG23	1:A:453:ILE:HD11	1.77	0.64
1:A:333:GLN:HE22	1:A:360:LEU:H	1.45	0.64
1:A:273:LYS:NZ	1:A:294:GLU:HG3	2.13	0.64
1:B:306:SER:O	1:B:307:ASN:HB2	1.97	0.64
1:A:637:GLN:O	1:A:638:ASP:HB2	1.97	0.64
1:B:129:HIS:HB2	1:B:137:GLN:HA	1.79	0.64
1:A:79:ASN:HB3	1:A:81:GLN:NE2	2.13	0.64
1:A:28:LYS:HE2	1:A:32:ASN:OD1	1.97	0.64
1:A:392:LEU:HD22	1:A:397:ILE:HD13	1.80	0.63
1:B:538:LEU:HD13	1:B:575:MSE:HE1	1.80	0.63
1:B:488:VAL:HG12	1:B:503:ILE:HG12	1.80	0.63
1:A:143:HIS:ND1	1:A:145:GLU:OE2	2.32	0.63
1:A:383:LEU:HB3	1:A:391:LEU:CD1	2.29	0.62
1:B:87:LYS:CD	1:B:87:LYS:H	2.06	0.62
1:B:593:ASN:HB2	1:B:623:ASP:OD2	1.99	0.62
1:A:280:LYS:O	1:A:281:LYS:HG3	1.99	0.62
1:B:629:MSE:HE1	1:B:649:SER:HA	1.81	0.61
1:A:580:ASN:O	1:A:584:LYS:HB3	2.00	0.61
1:B:427:ILE:O	1:B:450:ASN:HA	2.00	0.61
1:B:164:ASN:HD21	1:B:242:ASN:HD22	1.46	0.61
1:B:430:LYS:O	1:B:444:THR:HA	2.00	0.61
1:B:502:GLN:NE2	1:B:525:LEU:HD12	2.16	0.61
1:A:620:TYR:CE2	1:A:628:MSE:HE3	2.36	0.60
1:B:521:GLN:NE2	1:B:602:GLU:O	2.34	0.60
1:B:138:LYS:H	1:B:138:LYS:CD	2.05	0.60
1:A:62:MSE:HE3	1:A:127:TRP:CG	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:LYS:NZ	1:A:511:GLU:OE1	2.30	0.60
1:A:408:LEU:HD12	1:A:483:MSE:HE1	1.84	0.60
1:B:138:LYS:HD2	1:B:138:LYS:N	2.16	0.60
1:B:207:GLN:H	1:B:210:THR:HB	1.67	0.60
1:B:329:ASP:OD1	1:B:331:LYS:HG3	2.02	0.60
1:B:27:ASP:OD2	1:B:27:ASP:N	2.34	0.59
1:B:595:ILE:HD11	1:B:620:TYR:CZ	2.37	0.59
1:A:119:GLU:O	1:A:120:ASP:HB2	2.03	0.59
1:A:146:ASN:ND2	1:A:147:LEU:H	1.95	0.59
1:A:477:LYS:HB3	1:A:477:LYS:HZ2	1.67	0.59
1:B:99:TYR:HB2	1:B:112:VAL:CG2	2.31	0.59
1:B:430:LYS:HG2	1:B:448:VAL:CG1	2.32	0.59
1:B:504:SER:O	1:B:506:LYS:N	2.36	0.59
1:B:230:LYS:HE3	1:B:231:PHE:CE2	2.35	0.59
1:A:369:TYR:HD2	1:A:372:MSE:HE2	1.67	0.58
1:A:381:ASN:CA	1:A:384:THR:HG22	2.27	0.58
1:A:185:ALA:O	1:A:188:LYS:HG2	2.02	0.58
1:B:184:LYS:HG2	1:B:194:GLU:OE2	2.03	0.58
1:B:407:ILE:O	1:B:411:MSE:HG3	2.04	0.58
1:A:300:THR:HG22	1:A:312:THR:HA	1.86	0.58
1:B:27:ASP:OD1	1:B:30:ILE:HD12	2.03	0.57
1:A:265:LYS:O	1:A:266:GLN:O	2.21	0.57
1:B:158:ASN:O	1:B:159:ASN:HB2	2.05	0.57
1:B:566:GLU:CD	1:B:566:GLU:H	2.07	0.57
1:A:221:ASP:OD2	1:A:223:TYR:HB2	2.04	0.57
1:B:164:ASN:HD22	1:B:164:ASN:C	2.09	0.56
1:B:289:LYS:HD3	1:B:289:LYS:H	1.69	0.56
1:B:94:ARG:NE	1:B:113:GLN:HG3	2.20	0.56
1:B:576:GLN:HA	1:B:595:ILE:HG22	1.88	0.56
1:B:346:SER:HB3	1:B:394:LYS:HB3	1.88	0.56
1:B:69:ILE:CG2	1:B:142:ILE:HD12	2.36	0.56
1:A:180:LYS:HA	1:A:180:LYS:HZ3	1.71	0.56
1:A:158:ASN:O	1:A:159:ASN:HB2	2.06	0.56
1:B:306:SER:O	1:B:307:ASN:CB	2.53	0.55
1:A:189:GLU:HG2	1:A:227:PHE:CE2	2.42	0.55
1:B:413:GLY:HA2	1:B:474:LEU:HD21	1.89	0.55
1:B:187:ALA:HB1	1:B:192:ILE:O	2.07	0.55
1:A:98:GLN:OE1	1:A:111:ASN:HA	2.06	0.55
1:B:614:ILE:HD13	1:B:634:LYS:HA	1.88	0.55
1:A:383:LEU:HB3	1:A:391:LEU:HD11	1.88	0.55
1:B:502:GLN:CG	1:B:525:LEU:HB2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:LYS:HG2	1:B:448:VAL:HG11	1.88	0.55
1:B:474:LEU:O	1:B:478:LYS:HD2	2.06	0.55
1:B:502:GLN:HE21	1:B:525:LEU:HD12	1.73	0.54
1:A:369:TYR:HB2	1:A:370:PRO:HD3	1.89	0.54
1:A:502:GLN:HG3	1:A:525:LEU:HB2	1.89	0.54
1:B:427:ILE:HD12	1:B:453:ILE:HG13	1.88	0.54
1:B:189:GLU:HG2	1:B:227:PHE:CZ	2.42	0.54
1:A:387:LYS:HE3	1:A:387:LYS:HA	1.89	0.54
1:B:657:TYR:O	1:B:658:GLU:HB2	2.08	0.54
1:B:389:GLU:N	1:B:390:PRO:HD3	2.23	0.54
1:B:145:GLU:HG3	1:B:298:ARG:NH2	2.23	0.54
1:B:658:GLU:OE2	1:B:662:LYS:HE3	2.08	0.54
1:A:185:ALA:HA	1:A:188:LYS:HG2	1.89	0.53
1:A:157:ARG:HD3	1:A:666:ILE:O	2.08	0.53
1:B:611:GLY:O	1:B:612:ARG:HB2	2.07	0.53
1:A:176:LYS:HG3	1:A:177:ASN:N	2.21	0.53
1:B:449:VAL:O	1:B:453:ILE:HD11	2.08	0.53
1:B:645:ASN:HD22	1:B:645:ASN:H	1.56	0.53
1:B:137:GLN:HG3	1:B:138:LYS:HD2	1.90	0.53
1:A:407:ILE:CD1	1:A:575:MSE:HE2	2.36	0.53
1:A:449:VAL:O	1:A:449:VAL:HG23	2.09	0.53
1:B:351:HIS:CE1	1:B:353:GLN:OE1	2.61	0.53
1:B:29:GLU:OE1	1:B:123:TRP:CD1	2.62	0.53
1:B:85:ILE:HG12	1:B:95:VAL:HG22	1.91	0.53
1:B:179:SER:HB2	1:B:181:LYS:HG2	1.91	0.53
1:B:643:SER:O	1:B:647:LYS:HG3	2.09	0.53
1:A:207:GLN:HB2	1:A:210:THR:OG1	2.08	0.53
1:B:480:GLU:HG2	1:B:508:LEU:HD12	1.91	0.52
1:B:504:SER:C	1:B:506:LYS:N	2.63	0.52
1:A:189:GLU:C	1:A:191:SER:H	2.12	0.52
1:A:392:LEU:CD2	1:A:397:ILE:HD13	2.39	0.52
1:A:403:SER:CB	1:A:599:GLY:HA3	2.40	0.52
1:B:436:LYS:H	1:B:436:LYS:CD	2.20	0.52
1:A:502:GLN:HG3	1:A:525:LEU:HD12	1.92	0.52
1:B:450:ASN:N	1:B:450:ASN:OD1	2.40	0.52
1:A:130:SER:HA	1:A:133:ILE:O	2.09	0.52
1:A:612:ARG:HH21	1:A:635:ASP:CG	2.12	0.52
1:A:43:LYS:O	1:A:47:LYS:HG2	2.10	0.52
1:A:95:VAL:O	1:A:113:GLN:HA	2.10	0.52
1:A:143:HIS:ND1	1:A:145:GLU:CD	2.63	0.52
1:B:364:PRO:HG2	1:B:388:LYS:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ASP:OD2	1:B:79:ASN:ND2	2.43	0.52
1:A:273:LYS:HZ1	1:A:294:GLU:HG3	1.74	0.51
1:A:200:GLN:OE1	1:A:200:GLN:HA	2.11	0.51
1:B:401:PRO:HB2	1:B:405:GLN:HB2	1.91	0.51
1:A:603:LEU:HD13	1:A:603:LEU:O	2.11	0.51
1:B:186:ILE:HA	1:B:227:PHE:HZ	1.75	0.51
1:B:363:THR:HA	1:B:364:PRO:C	2.31	0.51
1:A:589:ARG:HE	1:A:654:ASP:CG	2.14	0.51
1:A:76:LYS:HG3	1:A:77:ASP:H	1.76	0.51
1:B:460:GLU:O	1:B:582:THR:HG21	2.09	0.51
1:A:145:GLU:CD	1:B:145:GLU:OE1	2.49	0.51
1:B:425:TYR:OH	1:B:473:GLU:HG3	2.11	0.51
1:A:52:ILE:O	1:A:55:SER:HB3	2.11	0.51
1:B:176:LYS:NZ	1:B:176:LYS:HB3	2.26	0.51
1:A:50:SER:O	1:A:54:LYS:HG2	2.11	0.51
1:A:637:GLN:O	1:A:638:ASP:CB	2.58	0.51
1:B:423:THR:O	1:B:424:SER:HB3	2.11	0.50
1:B:432:TRP:CH2	1:B:434:LYS:HA	2.46	0.50
1:B:252:LEU:HD13	1:B:253:LEU:HD23	1.92	0.50
1:A:449:VAL:HG23	1:A:453:ILE:HD12	1.92	0.50
1:B:132:ILE:HG22	1:B:133:ILE:HG12	1.92	0.50
1:B:73:LEU:O	1:B:103:THR:HB	2.11	0.50
1:A:277:VAL:HG23	1:A:277:VAL:O	2.11	0.50
1:B:419:LEU:HD22	1:B:423:THR:HG21	1.93	0.50
1:A:135:GLY:HA2	1:B:209:ASP:OD2	2.12	0.50
1:A:146:ASN:ND2	1:A:296:GLY:O	2.44	0.50
1:B:433:GLN:NE2	1:B:442:ASN:HD21	2.10	0.49
1:A:269:TYR:OH	1:A:278:ILE:HD12	2.11	0.49
1:B:438:TRP:O	1:B:439:GLY:C	2.49	0.49
1:B:189:GLU:HG2	1:B:227:PHE:CE1	2.47	0.49
1:B:218:LYS:HE2	1:B:369:TYR:CZ	2.48	0.49
1:A:350:ILE:HG13	1:A:356:GLU:O	2.12	0.49
1:A:74:GLY:HA3	1:A:104:ASN:ND2	2.27	0.49
1:B:406:LYS:NZ	1:B:462:SER:OG	2.39	0.49
1:A:263:GLU:O	1:A:265:LYS:N	2.46	0.49
1:A:51:TYR:HA	1:A:54:LYS:CE	2.39	0.49
1:A:471:ALA:HB1	1:A:514:LEU:HD21	1.95	0.49
1:A:28:LYS:HA	1:A:28:LYS:HE3	1.95	0.49
1:B:428:ASP:HA	1:B:450:ASN:HB3	1.94	0.48
1:B:174:VAL:O	1:B:175:PRO:C	2.51	0.48
1:A:586:ASP:OD2	1:A:643:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:LEU:HD22	1:A:568:ILE:HG23	1.94	0.48
1:B:614:ILE:CD1	1:B:634:LYS:HA	2.43	0.48
1:A:383:LEU:HB3	1:A:391:LEU:HD13	1.94	0.48
1:A:595:ILE:HD11	1:A:620:TYR:CE2	2.48	0.48
1:B:289:LYS:HD3	1:B:289:LYS:N	2.26	0.48
1:A:125:LEU:HD13	1:A:127:TRP:N	2.29	0.48
1:A:344:TYR:CD2	1:A:344:TYR:C	2.87	0.48
1:A:54:LYS:HA	1:A:62:MSE:SE	2.64	0.48
1:B:364:PRO:CD	1:B:388:LYS:HB3	2.44	0.48
1:A:76:LYS:HE2	1:A:102:LYS:HB3	1.94	0.48
1:A:65:ARG:HB3	1:A:66:PRO:HD3	1.96	0.48
1:B:566:GLU:N	1:B:566:GLU:OE2	2.45	0.48
1:B:489:GLY:HA3	1:B:503:ILE:HD11	1.96	0.47
1:A:221:ASP:HB2	1:A:223:TYR:HD2	1.77	0.47
1:A:145:GLU:OE2	1:B:145:GLU:OE2	2.32	0.47
1:A:613:GLN:HG3	1:A:637:GLN:HB3	1.95	0.47
1:A:627:MSE:HE3	1:A:629:MSE:HB2	1.97	0.47
1:B:441:TYR:C	1:B:442:ASN:HD22	2.17	0.47
1:A:595:ILE:HD11	1:A:620:TYR:CZ	2.49	0.47
1:A:419:LEU:C	1:A:419:LEU:HD13	2.35	0.47
1:B:589:ARG:NH2	1:B:654:ASP:OD2	2.42	0.47
1:B:176:LYS:HZ3	1:B:176:LYS:HB3	1.79	0.47
1:A:226:ASP:O	1:A:230:LYS:HG3	2.15	0.47
1:A:333:GLN:NE2	1:A:360:LEU:H	2.10	0.47
1:B:406:LYS:HE2	1:B:519:TYR:HB2	1.97	0.47
1:A:600:THR:OG1	1:A:642:ALA:HB2	2.14	0.47
1:A:290:LYS:HE3	1:A:324:ILE:HG12	1.94	0.47
1:A:34:ILE:O	1:A:37:ILE:HB	2.15	0.47
1:A:154:ILE:HB	1:A:163:ALA:HB3	1.97	0.47
1:B:516:ASP:HA	1:B:519:TYR:CE2	2.49	0.47
1:B:472:LEU:HD23	1:B:514:LEU:HD13	1.97	0.47
1:A:471:ALA:HB1	1:A:514:LEU:HD22	1.96	0.47
1:B:645:ASN:H	1:B:645:ASN:ND2	2.12	0.47
1:B:259:ILE:HG13	1:B:263:GLU:OE2	2.15	0.47
1:A:403:SER:OG	1:A:599:GLY:HA3	2.15	0.47
1:B:504:SER:O	1:B:505:ASN:C	2.53	0.46
1:B:425:TYR:O	1:B:427:ILE:HG13	2.15	0.46
1:A:438:TRP:HZ3	1:A:443:VAL:HG23	1.81	0.46
1:B:114:PHE:CE2	1:B:131:VAL:HG22	2.50	0.46
1:A:217:VAL:CG2	1:A:220:MSE:HE3	2.42	0.46
1:B:578:VAL:HA	1:B:582:THR:OG1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:ILE:HD12	1:B:453:ILE:CG1	2.45	0.46
1:A:363:THR:HA	1:A:364:PRO:C	2.36	0.46
1:B:506:LYS:HG2	1:B:507:ASN:N	2.31	0.46
1:A:634:LYS:O	1:A:635:ASP:HB2	2.16	0.46
1:B:62:MSE:HE3	1:B:127:TRP:HB3	1.98	0.46
1:A:189:GLU:C	1:A:191:SER:N	2.68	0.46
1:B:502:GLN:NE2	1:B:525:LEU:CD1	2.79	0.46
1:B:544:ILE:HG13	1:B:562:ILE:HG13	1.97	0.46
1:A:346:SER:HB3	1:A:394:LYS:CB	2.46	0.46
1:B:358:LEU:HD12	1:B:627:MSE:HG3	1.97	0.46
1:B:436:LYS:N	1:B:436:LYS:CD	2.79	0.45
1:B:571:LEU:O	1:B:575:MSE:HG3	2.16	0.45
1:B:589:ARG:HH21	1:B:654:ASP:CG	2.19	0.45
1:A:215:LYS:NZ	1:A:373:TYR:O	2.50	0.45
1:B:371:PHE:CZ	1:B:375:MSE:HE1	2.51	0.45
1:A:87:LYS:H	1:A:87:LYS:CD	2.07	0.45
1:B:99:TYR:CB	1:B:112:VAL:HG21	2.46	0.45
1:B:465:ILE:O	1:B:469:ARG:HG2	2.15	0.45
1:B:371:PHE:CE2	1:B:375:MSE:HE1	2.52	0.45
1:A:307:ASN:HD21	1:B:143:HIS:HA	1.81	0.45
1:B:110:ARG:HH21	1:B:135:GLY:HA3	1.81	0.45
1:B:612:ARG:HG2	1:B:613:GLN:OE1	2.17	0.45
1:A:33:THR:O	1:A:36:ALA:HB3	2.17	0.45
1:B:345:GLY:HA3	1:B:632:ASN:O	2.17	0.45
1:B:133:ILE:HG13	1:B:142:ILE:HD11	1.99	0.45
1:B:654:ASP:O	1:B:658:GLU:N	2.49	0.45
1:B:446:TYR:CE1	1:B:641:MSE:HE2	2.52	0.44
1:B:173:ILE:HG23	1:B:178:VAL:HB	1.99	0.44
1:A:186:ILE:HA	1:A:227:PHE:HZ	1.83	0.44
1:A:112:VAL:CG1	1:A:134:PRO:CB	2.95	0.44
1:B:506:LYS:CE	1:B:507:ASN:ND2	2.77	0.44
1:B:277:VAL:HG23	1:B:277:VAL:O	2.17	0.44
1:B:402:GLY:O	1:B:520:GLY:HA3	2.18	0.44
1:A:182:ASP:O	1:A:186:ILE:HG13	2.17	0.44
1:B:179:SER:CB	1:B:181:LYS:HG2	2.48	0.44
1:A:255:TYR:HE2	1:A:281:LYS:HD3	1.83	0.44
1:B:583:HIS:O	1:B:587:ILE:HG22	2.18	0.44
1:A:215:LYS:CG	1:A:216:THR:N	2.80	0.44
1:B:544:ILE:HD12	1:B:559:LYS:HG3	2.00	0.44
1:A:598:SER:OG	1:A:599:GLY:N	2.50	0.43
1:A:543:ASN:OD1	1:A:560:LYS:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:ILE:CD1	1:B:634:LYS:HG3	2.46	0.43
1:A:619:SER:O	1:A:620:TYR:HB3	2.17	0.43
1:A:186:ILE:O	1:A:189:GLU:HB3	2.19	0.43
1:A:389:GLU:HB3	1:A:392:LEU:HB2	2.01	0.43
1:A:369:TYR:HD2	1:A:372:MSE:CE	2.31	0.43
1:B:414:LEU:HD22	1:B:567:ASN:OD1	2.18	0.43
1:B:174:VAL:HG22	1:B:211:PHE:HA	2.00	0.43
1:A:355:GLY:O	1:A:547:PRO:HA	2.19	0.43
1:B:612:ARG:HG3	1:B:612:ARG:NH1	2.32	0.43
1:B:263:GLU:O	1:B:269:TYR:HD1	2.00	0.43
1:B:197:ILE:HG12	1:B:214:LEU:HD22	2.00	0.43
1:A:173:ILE:HG23	1:A:178:VAL:CG2	2.49	0.43
1:B:364:PRO:CG	1:B:388:LYS:HB3	2.48	0.43
1:B:300:THR:HB	1:B:311:HIS:O	2.18	0.43
1:A:340:MSE:HE1	1:A:346:SER:C	2.39	0.43
1:B:403:SER:CB	1:B:599:GLY:HA3	2.49	0.43
1:A:503:ILE:HG12	1:A:524:ILE:HG12	1.99	0.43
1:A:255:TYR:CE2	1:A:281:LYS:HD3	2.54	0.43
1:B:588:TYR:O	1:B:589:ARG:HD2	2.19	0.42
1:A:102:LYS:HE3	1:A:107:ASN:ND2	2.33	0.42
1:B:138:LYS:O	1:B:140:GLN:HG3	2.18	0.42
1:B:446:TYR:HB3	1:B:447:GLU:H	1.63	0.42
1:B:175:PRO:O	1:B:176:LYS:C	2.58	0.42
1:B:636:VAL:O	1:B:638:ASP:N	2.53	0.42
1:B:128:ASP:OD2	1:B:130:SER:HB3	2.20	0.42
1:A:441:TYR:CE2	1:A:512:ILE:HG23	2.55	0.42
1:A:346:SER:HB3	1:A:394:LYS:HB3	2.02	0.42
1:B:193:SER:OG	1:B:195:ASP:HB3	2.19	0.42
1:B:219:LYS:N	1:B:219:LYS:HD3	2.34	0.42
1:A:263:GLU:O	1:A:266:GLN:HB2	2.20	0.42
1:A:538:LEU:CD2	1:A:568:ILE:HG23	2.49	0.42
1:A:34:ILE:HA	1:A:37:ILE:HD12	2.01	0.42
1:B:618:ILE:HA	1:B:629:MSE:O	2.20	0.42
1:A:386:ASP:HB3	1:A:390:PRO:CD	2.50	0.42
1:A:122:MSE:H	1:A:122:MSE:HG2	1.60	0.42
1:A:174:VAL:O	1:A:175:PRO:C	2.59	0.41
1:A:411:MSE:HE1	1:A:562:ILE:HD11	2.02	0.41
1:B:205:TRP:HZ3	1:B:210:THR:CG2	2.32	0.41
1:B:446:TYR:OH	1:B:641:MSE:HG3	2.20	0.41
1:A:572:THR:HG22	1:A:595:ILE:CD1	2.50	0.41
1:B:175:PRO:O	1:B:177:ASN:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ILE:HA	1:A:98:GLN:O	2.19	0.41
1:A:175:PRO:O	1:A:176:LYS:C	2.58	0.41
1:A:189:GLU:O	1:A:191:SER:N	2.53	0.41
1:B:614:ILE:HD13	1:B:614:ILE:HA	1.93	0.41
1:B:430:LYS:O	1:B:445:ARG:N	2.52	0.41
1:B:118:LYS:HD3	1:B:123:TRP:CH2	2.55	0.41
1:A:129:HIS:C	1:A:131:VAL:H	2.22	0.41
1:A:111:ASN:HD22	1:A:112:VAL:N	2.19	0.41
1:A:255:TYR:CE1	1:A:280:LYS:HB2	2.54	0.41
1:A:367:ASP:O	1:A:370:PRO:HD2	2.19	0.41
1:B:128:ASP:C	1:B:128:ASP:OD2	2.59	0.41
1:A:474:LEU:O	1:A:478:LYS:HD2	2.21	0.41
1:B:291:LEU:O	1:B:321:GLY:HA3	2.20	0.41
1:B:290:LYS:HE2	1:B:290:LYS:HB2	1.68	0.41
1:A:502:GLN:CG	1:A:525:LEU:HB2	2.50	0.41
1:B:173:ILE:CG2	1:B:178:VAL:HB	2.50	0.41
1:A:551:LYS:HD3	1:A:551:LYS:HA	1.89	0.41
1:B:197:ILE:O	1:B:201:MSE:HG2	2.20	0.41
1:B:180:LYS:HA	1:B:183:TYR:CE1	2.55	0.41
1:B:563:ILE:HG12	1:B:564:SER:N	2.36	0.41
1:A:263:GLU:C	1:A:265:LYS:N	2.74	0.41
1:B:587:ILE:O	1:B:587:ILE:HG12	2.20	0.41
1:A:29:GLU:OE2	1:A:122:MSE:HB3	2.21	0.41
1:A:186:ILE:HG12	1:A:231:PHE:CD1	2.56	0.41
1:A:408:LEU:HD22	1:A:534:ILE:HG21	2.02	0.41
1:A:221:ASP:O	1:A:223:TYR:N	2.44	0.41
1:B:579:VAL:HG13	1:B:587:ILE:HG23	2.02	0.41
1:A:193:SER:C	1:A:195:ASP:N	2.71	0.41
1:B:569:ASN:HA	1:B:572:THR:OG1	2.21	0.41
1:B:488:VAL:O	1:B:503:ILE:CD1	2.67	0.41
1:A:43:LYS:O	1:A:47:LYS:HE2	2.20	0.41
1:B:183:TYR:N	1:B:183:TYR:CD1	2.88	0.41
1:A:192:ILE:O	1:A:193:SER:C	2.59	0.41
1:B:65:ARG:N	1:B:66:PRO:CD	2.84	0.41
1:A:435:ASP:OD1	1:A:437:SER:N	2.48	0.41
1:A:456:LYS:HB2	1:A:456:LYS:HE3	1.86	0.41
1:B:197:ILE:HG23	1:B:214:LEU:HD21	2.02	0.41
1:B:290:LYS:HB3	1:B:324:ILE:HD11	2.03	0.41
1:B:183:TYR:N	1:B:183:TYR:HD1	2.19	0.41
1:A:570:LEU:HA	1:A:570:LEU:HD12	1.92	0.41
1:B:506:LYS:HG2	1:B:507:ASN:ND2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:SER:HA	1:A:628:MSE:SE	2.71	0.40
1:B:502:GLN:HG3	1:B:525:LEU:HB2	2.03	0.40
1:A:600:THR:HA	1:A:614:ILE:O	2.21	0.40
1:B:50:SER:HA	1:B:124:LYS:HB3	2.03	0.40
1:A:142:ILE:CD1	1:A:301:ILE:HG12	2.51	0.40
1:A:277:VAL:CG2	1:A:277:VAL:O	2.70	0.40
1:A:99:TYR:HB3	1:A:134:PRO:HG3	2.03	0.40
1:A:495:ASP:OD2	1:A:549:LEU:HD12	2.22	0.40
1:A:612:ARG:NH2	1:A:635:ASP:OD2	2.52	0.40
1:B:544:ILE:HB	1:B:559:LYS:HB2	2.04	0.40

All (2) 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)
4:A:7:HOH:O	4:A:7:HOH:O[5_555]	0.88	1.32
1:A:509:ASP:OD1	4:A:7:HOH:O[5_555]	2.18	0.02

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	614/646 (95%)	548 (89%)	56 (9%)	10 (2%)	12 11
1	B	621/646 (96%)	569 (92%)	39 (6%)	13 (2%)	9 6
All	All	1235/1292 (96%)	1117 (90%)	95 (8%)	23 (2%)	10 8

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	GLN
1	B	307	ASN

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Mol	Chain	Res	Type
1	B	341	LYS
1	A	175	PRO
1	A	264	LEU
1	A	265	LYS
1	A	269	TYR
1	A	435	ASP
1	B	176	LYS
1	B	437	SER
1	B	446	TYR
1	B	504	SER
1	B	505	ASN
1	B	612	ARG
1	B	637	GLN
1	A	182	ASP
1	A	222	GLU
1	B	424	SER
1	B	204	ASN
1	A	190	LEU
1	A	624	ASN
1	B	439	GLY
1	B	175	PRO

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	557/559 (100%)	523 (94%)	34 (6%)	23	32
1	B	561/559 (100%)	524 (93%)	37 (7%)	21	28
All	All	1118/1118 (100%)	1047 (94%)	71 (6%)	22	29

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	87	LYS

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Mol	Chain	Res	Type
1	A	99	TYR
1	A	111	ASN
1	A	138	LYS
1	A	156	ASP
1	A	175	PRO
1	A	180	LYS
1	A	202	ASP
1	A	222	GLU
1	A	231	PHE
1	A	252	LEU
1	A	262	GLU
1	A	265	LYS
1	A	266	GLN
1	A	269	TYR
1	A	273	LYS
1	A	303	ASP
1	A	333	GLN
1	A	344	TYR
1	A	367	ASP
1	A	387	LYS
1	A	391	LEU
1	A	392	LEU
1	A	446	TYR
1	A	502	GLN
1	A	513	LEU
1	A	514	LEU
1	A	532	LEU
1	A	549	LEU
1	A	551	LYS
1	A	560	LYS
1	A	593	ASN
1	A	662	LYS
1	B	27	ASP
1	B	87	LYS
1	B	99	TYR
1	B	125	LEU
1	B	137	GLN
1	B	138	LYS
1	B	141	SER
1	B	148	LYS
1	B	156	ASP
1	B	164	ASN

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Mol	Chain	Res	Type
1	B	175	PRO
1	B	176	LYS
1	B	208	ASP
1	B	219	LYS
1	B	221	ASP
1	B	223	TYR
1	B	262	GLU
1	B	289	LYS
1	B	307	ASN
1	B	331	LYS
1	B	391	LEU
1	B	408	LEU
1	B	436	LYS
1	B	448	VAL
1	B	450	ASN
1	B	502	GLN
1	B	503	ILE
1	B	514	LEU
1	B	532	LEU
1	B	549	LEU
1	B	552	ASP
1	B	566	GLU
1	B	593	ASN
1	B	612	ARG
1	B	613	GLN
1	B	624	ASN
1	B	636	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	111	ASN
1	A	113	GLN
1	A	146	ASN
1	A	177	ASN
1	A	203	GLN
1	A	207	GLN
1	A	251	HIS
1	A	266	GLN
1	A	307	ASN
1	A	333	GLN

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Mol	Chain	Res	Type
1	A	396	GLN
1	A	433	GLN
1	A	502	GLN
1	A	540	ASN
1	A	545	ASN
1	A	577	GLN
1	A	593	ASN
1	A	661	ASN
1	B	41	ASN
1	B	98	GLN
1	B	104	ASN
1	B	137	GLN
1	B	164	ASN
1	B	207	GLN
1	B	266	GLN
1	B	351	HIS
1	B	433	GLN
1	B	442	ASN
1	B	502	GLN
1	B	507	ASN
1	B	540	ASN
1	B	593	ASN
1	B	624	ASN
1	B	645	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	609/646 (94%)	0.43	39 (6%)	23	24	7, 27, 47, 57	0
1	B	614/646 (95%)	0.41	45 (7%)	18	19	5, 26, 47, 56	0
All	All	1223/1292 (94%)	0.42	84 (6%)	20	21	5, 27, 47, 57	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	505	ASN	7.4
1	A	223	TYR	6.7
1	B	603	LEU	6.0
1	B	611	GLY	5.5
1	A	503	ILE	5.0
1	A	51	TYR	4.8
1	B	604	LYS	4.4
1	A	603	LEU	4.3
1	A	224	LEU	4.3
1	B	504	SER	3.9
1	A	261	SER	3.8
1	B	502	GLN	3.8
1	B	506	LYS	3.7
1	B	381	ASN	3.6
1	B	384	THR	3.6
1	B	222	GLU	3.6
1	B	436	LYS	3.6
1	B	503	ILE	3.5
1	A	121	GLY	3.4
1	B	426	LYS	3.3
1	B	51	TYR	3.3
1	A	268	GLU	3.2
1	A	630	ALA	3.2
1	A	267	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	437	SER	3.1
1	A	85	ILE	3.0
1	B	446	TYR	3.0
1	A	145	GLU	3.0
1	A	222	GLU	3.0
1	A	612	ARG	3.0
1	B	638	ASP	3.0
1	B	267	LYS	2.9
1	B	266	GLN	2.9
1	B	448	VAL	2.9
1	B	223	TYR	2.9
1	A	120	ASP	2.9
1	A	232	HIS	2.8
1	A	378	GLU	2.8
1	B	427	ILE	2.8
1	B	188	LYS	2.7
1	A	188	LYS	2.7
1	A	500	ASN	2.7
1	B	265	LYS	2.7
1	A	231	PHE	2.7
1	A	178	VAL	2.7
1	B	447	GLU	2.6
1	A	87	LYS	2.6
1	B	224	LEU	2.6
1	A	193	SER	2.6
1	B	226	ASP	2.6
1	B	452	ASN	2.6
1	B	636	VAL	2.6
1	A	264	LEU	2.6
1	A	349	ALA	2.5
1	A	438	TRP	2.5
1	B	449	VAL	2.5
1	A	198	LYS	2.5
1	B	612	ARG	2.5
1	A	86	LYS	2.4
1	A	508	LEU	2.4
1	B	377	ASN	2.4
1	A	454	ASP	2.4
1	B	268	GLU	2.3
1	B	385	GLU	2.3
1	B	133	ILE	2.3
1	A	123	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	230	LYS	2.2
1	B	440	GLY	2.2
1	A	618	ILE	2.2
1	A	179	SER	2.2
1	A	205	TRP	2.2
1	B	378	GLU	2.2
1	A	613	GLN	2.2
1	B	428	ASP	2.1
1	B	407	ILE	2.1
1	A	502	GLN	2.1
1	A	440	GLY	2.1
1	B	507	ASN	2.1
1	B	422	LYS	2.1
1	B	198	LYS	2.1
1	B	221	ASP	2.1
1	B	86	LYS	2.1
1	A	199	GLN	2.0
1	A	221	ASP	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CL	A	1207	1/1	0.94	0.12	-0.68	15,15,15,15	0
2	CD	B	1201	1/1	0.99	0.12	-0.85	19,19,19,19	0
3	CL	B	1206	1/1	0.99	0.10	-1.55	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CL	B	1208	1/1	0.99	0.06	-1.57	10,10,10,10	0
2	CD	A	1202	1/1	1.00	0.07	-2.38	17,17,17,17	0
2	CD	B	1204	1/1	0.99	0.08	-3.63	21,21,21,21	0
3	CL	A	1205	1/1	0.99	0.06	-4.64	16,16,16,16	0
2	CD	A	1203	1/1	1.00	0.07	-	21,21,21,21	0

6.5 Other polymers

There are no such residues in this entry.