Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 11:35 am BST

PDB ID	:	1ORD
Title	:	CRYSTALLOGRAPHIC STRUCTURE OF A PLP-DEPENDENT ORNITHINE DECARBOXYLASE FROM LACTOBACILLUS 30A TO 3.1 ANGSTROMS RESOLUTION
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Deposited on	:	1995-02-08
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

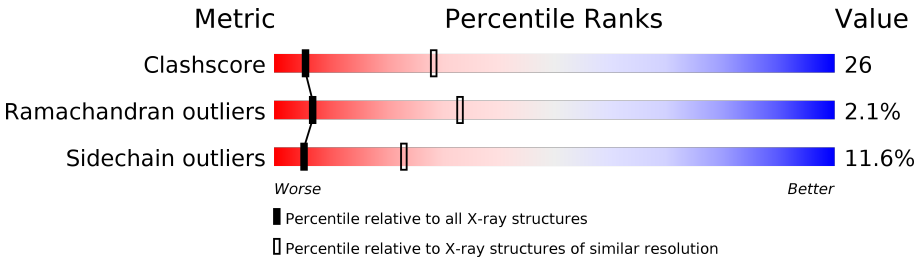
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	730	55% 36% 8%
1	B	730	55% 36% 8%

2 Entry composition

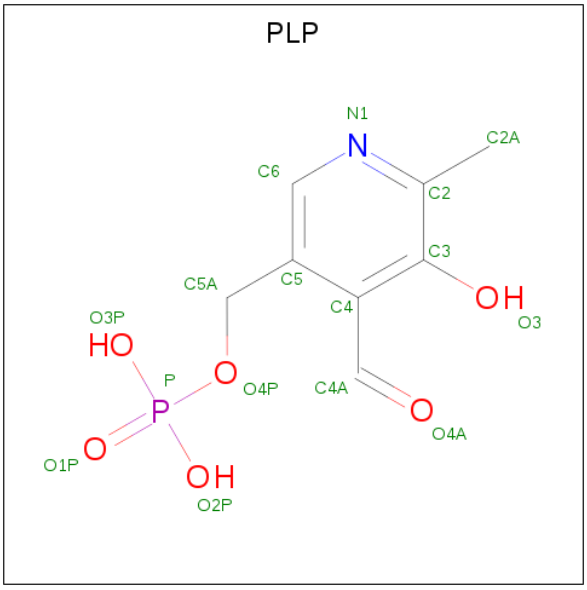
There are 3 unique types of molecules in this entry. The entry contains 14561 atoms, of which 2752 are hydrogens and 0 are deuteriums.

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 ORNITHINE DECARBOXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	730	Total	C	H	N	O	S	0	0	0
			7105	3726	1269	982	1109	19			
1	B	730	Total	C	H	N	O	S	0	0	0
			7105	3726	1269	982	1109	19			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	47	Total H O 141 94 47	0	0
3	B	60	Total H O 180 120 60	0	0

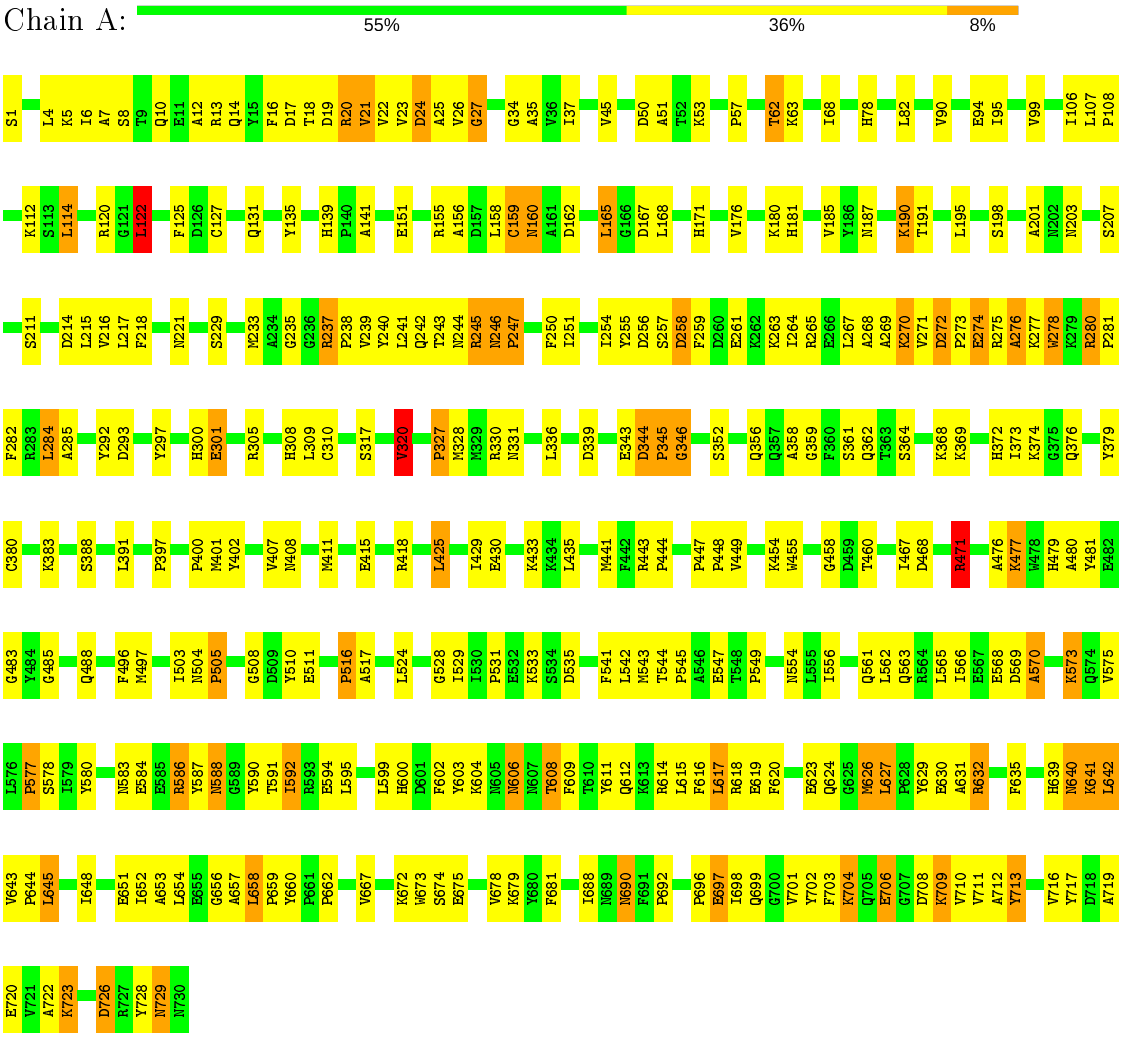
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

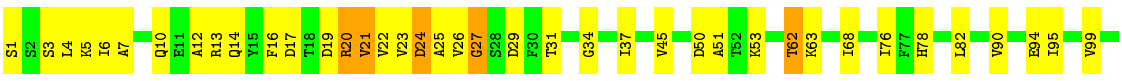
- Molecule 1: ORNITHINE DECARBOXYLASE

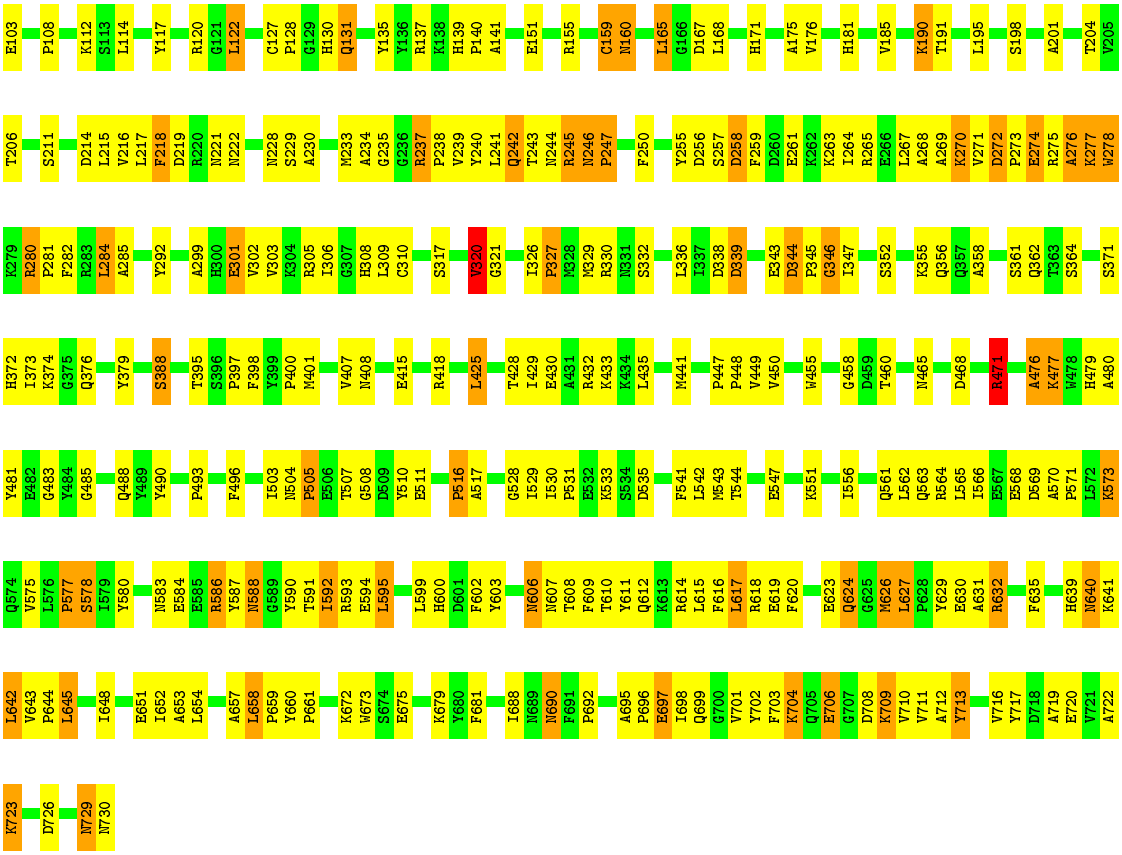
Chain A:



- Molecule 1: ORNITHINE DECARBOXYLASE

Chain B:




E103 P108 K112 S113 L114 Y117 R120 G121 L122 C127 P128 G129 H130 Q131 Y135 Y136 R137 K138 H139 P140 A141 E151 R155 C159 N160 L165 G166 D167 L168 H171 A175 V176 H181 V185 K190 T191 L195 S198 A201 T204 V205
T206 S211 D214 L215 V216 L217 F218 D219 R220 N221 N222 N228 S229 A230 M233 A234 G235 G236 R237 P238 V239 Y240 L241 Q242 T243 N244 R245 N246 P247 F250 Y255 D256 S257 D258 F259 D260 E261 K262 K263 I264 R265 E266 L267 A268 A269 K270 V271 D272 P273 E274 R275 A276 K277 W278
K279 R280 P281 F282 R283 L284 A285 Y292 A299 H300 E301 V302 V303 K304 R305 I306 G307 H308 L309 C310 S317 V320 G321 I326 P327 M328 M329 R330 N331 S332 L336 I337 D338 D339 E343 D344 P345 G346 I347 S352 K355 Q356 Q357 A358 S361 Q362 T363 S364 S371
H372 I373 K374 G375 Q376 Y379 S388 T395 S396 P397 F398 Y399 P400 M401 V407 N408 E415 R418 L425 T428 I429 E430 A431 R432 K433 K434 L435 M441 P447 P448 V449 V450 W455 G458 D459 T460 N465 D468 R471 A476 K477 W478 H479 A480
Y481 E482 G483 Y484 G485 Q488 Y489 Y490 P493 F496 I503 N504 P505 E506 T507 G508 D509 Y510 E511 P516 A517 G528 I529 I530 P531 E532 K533 S534 D535 F541 L542 M543 T544 E547 K551 I556 Q561 L562 Q563 R564 L565 I566 E567 E568 D569 A570 P571 L572 K573
Q574 V575 L576 P577 S578 I579 Y580 N583 E584 E585 R586 Y587 N588 G589 Y590 T591 I592 R593 E594 L595 L599 H600 D601 F602 Y603 N606 N607 T608 F609 T610 Y611 Q612 K613 R614 L615 F616 L617 R618 E619 F620 E623 Q624 G625 M626 L627 P628 Y629 E630 A631 R632 F635 H639 N640 K641
L642 V643 P644 L645 I648 E651 I652 A653 L654 A657 L658 P659 Y660 P661 K672 W673 S674 E675 K679 Y680 F681 I688 N689 N690 F691 P692 A695 P696 E697 I698 Q699 G700 V701 Y702 F703 K704 Q705 E706 G707 D708 K709 V710 V711 A712 Y713 V716 Y717 D718 A719 E720 V721 A722
K723 D726 N729 N730

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α, β, γ	195.60Å 195.60Å 97.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.219 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14561	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.75	0/5985	0.88	7/8118 (0.1%)
1	B	0.78	0/5985	0.89	9/8118 (0.1%)
All	All	0.77	0/11970	0.88	16/16236 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	27	GLY	N-CA-C	-7.66	93.96	113.10
1	B	27	GLY	N-CA-C	-7.24	95.01	113.10
1	B	239	VAL	N-CA-C	-6.45	93.60	111.00
1	A	122	LEU	CA-CB-CG	6.11	129.36	115.30
1	B	471	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	122	LEU	CA-CB-CG	5.84	128.74	115.30
1	B	284	LEU	CA-CB-CG	5.84	128.72	115.30
1	A	284	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	471	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	239	VAL	N-CA-C	-5.23	96.89	111.00
1	A	391	LEU	CA-CB-CG	5.13	127.10	115.30
1	B	218	PHE	N-CA-C	5.12	124.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	346	GLY	N-CA-C	-5.12	100.30	113.10
1	B	471	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	476	ALA	N-CA-C	5.02	124.56	111.00
1	A	346	GLY	N-CA-C	-5.01	100.58	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	402	TYR	Sidechain
1	A	713	TYR	Sidechain
1	B	713	TYR	Sidechain

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	5836	1269	5623	295	0
1	B	5836	1269	5623	307	0
2	A	15	0	7	0	0
2	B	15	0	7	0	0
3	A	47	94	0	5	0
3	B	60	120	0	3	0
All	All	11809	2752	11260	589	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 26.

All (589) 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:B:269:ALA:HA	1:B:275:ARG:NH2	1.83	0.92
1:B:612:GLN:HA	1:B:615:LEU:HD12	1.57	0.86
1:B:273:PRO:O	1:B:277:LYS:HB2	1.74	0.86
1:B:20:ARG:HA	1:B:20:ARG:HE	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ALA:HA	1:B:275:ARG:CZ	2.06	0.84
1:A:269:ALA:HA	1:A:275:ARG:NH2	1.92	0.84
1:A:273:PRO:O	1:A:277:LYS:HB2	1.77	0.83
1:A:26:VAL:HG11	1:A:45:VAL:HG13	1.60	0.83
1:B:719:ALA:O	1:B:723:LYS:HB2	1.77	0.82
1:A:20:ARG:HA	1:A:20:ARG:HE	1.44	0.81
1:A:477:LYS:HD2	1:A:477:LYS:H	1.46	0.80
1:B:623:GLU:O	1:B:672:LYS:HG2	1.82	0.79
1:A:612:GLN:HA	1:A:615:LEU:HD12	1.66	0.78
1:A:269:ALA:HA	1:A:275:ARG:CZ	2.13	0.78
1:A:623:GLU:O	1:A:672:LYS:HG2	1.84	0.78
1:A:645:LEU:O	1:A:648:ILE:HG22	1.84	0.78
1:A:719:ALA:O	1:A:723:LYS:HB2	1.83	0.78
1:A:271:VAL:HG12	1:A:274:GLU:HB2	1.65	0.77
1:A:723:LYS:HB3	1:A:723:LYS:NZ	1.98	0.77
1:B:271:VAL:HG12	1:B:274:GLU:HB2	1.66	0.77
1:B:565:LEU:HD13	1:B:575:VAL:HG22	1.68	0.76
1:B:120:ARG:HB2	1:B:122:LEU:HD22	1.68	0.76
1:B:704:LYS:HB2	1:B:713:TYR:CE1	2.22	0.75
1:B:726:ASP:HA	1:B:729:ASN:ND2	2.03	0.74
1:B:703:PHE:HB3	1:B:710:VAL:HG22	1.71	0.73
1:A:703:PHE:HB3	1:A:710:VAL:HG22	1.71	0.73
1:A:604:LYS:HD2	3:A:763:HOH:O	1.87	0.73
1:A:704:LYS:HB2	1:A:713:TYR:CE1	2.23	0.73
1:B:301:GLU:O	1:B:305:ARG:HG3	1.89	0.72
1:B:697:GLU:CD	1:B:697:GLU:H	1.92	0.72
1:A:122:LEU:HD12	1:B:528:GLY:HA2	1.71	0.72
1:A:569:ASP:OD1	1:A:591:THR:HB	1.90	0.72
1:A:1:SER:HB2	1:A:21:VAL:HG11	1.70	0.72
1:B:1:SER:HB2	1:B:21:VAL:HG11	1.69	0.72
1:B:26:VAL:HG11	1:B:45:VAL:HG13	1.71	0.71
1:B:263:LYS:HD2	1:B:267:LEU:HD22	1.72	0.71
1:B:657:ALA:HB1	1:B:681:PHE:CZ	2.25	0.71
1:B:477:LYS:H	1:B:477:LYS:HD2	1.55	0.71
1:B:76:ILE:HG21	3:B:742:HOH:O	1.91	0.71
1:A:565:LEU:HD13	1:A:575:VAL:HG22	1.71	0.71
1:B:504:ASN:OD1	1:B:505:PRO:HD2	1.92	0.70
1:A:479:HIS:CD2	1:A:481:TYR:HB2	2.27	0.70
1:A:51:ALA:O	1:A:53:LYS:HG2	1.90	0.70
1:A:697:GLU:H	1:A:697:GLU:CD	1.96	0.69
1:A:703:PHE:HB3	1:A:710:VAL:CG2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:ASP:HA	1:A:729:ASN:ND2	2.08	0.68
1:A:237:ARG:HG2	1:A:270:LYS:HE2	1.76	0.68
1:A:374:LYS:HE3	3:A:773:HOH:O	1.93	0.68
1:A:660:TYR:HD1	1:A:697:GLU:O	1.76	0.68
1:A:471:ARG:NH1	1:A:471:ARG:HB3	2.08	0.68
1:B:275:ARG:HG3	1:B:276:ALA:H	1.59	0.68
1:A:271:VAL:CG1	1:A:274:GLU:HB2	2.24	0.68
1:B:471:ARG:NH1	1:B:471:ARG:HB3	2.09	0.67
1:B:723:LYS:NZ	1:B:723:LYS:HB3	2.09	0.67
1:A:20:ARG:NE	1:A:20:ARG:HA	2.09	0.67
1:A:602:PHE:O	1:A:606:ASN:HB2	1.93	0.67
1:A:344:ASP:HB2	1:A:345:PRO:HD2	1.77	0.67
1:A:528:GLY:HA2	1:B:122:LEU:HD12	1.76	0.67
1:B:660:TYR:HD1	1:B:697:GLU:O	1.77	0.67
1:B:476:ALA:HB2	1:B:479:HIS:CE1	2.30	0.66
1:B:20:ARG:HA	1:B:20:ARG:NE	2.08	0.66
1:B:476:ALA:CB	1:B:479:HIS:CE1	2.79	0.66
1:A:468:ASP:HA	1:A:471:ARG:NH2	2.11	0.66
1:B:344:ASP:HB2	1:B:345:PRO:HD2	1.78	0.66
1:A:301:GLU:O	1:A:305:ARG:HG3	1.95	0.66
1:B:271:VAL:CG1	1:B:274:GLU:HB2	2.26	0.65
1:B:479:HIS:CD2	1:B:481:TYR:HB2	2.31	0.65
1:B:51:ALA:O	1:B:53:LYS:HG2	1.95	0.65
1:B:640:ASN:HB3	1:B:654:LEU:CD1	2.26	0.65
1:B:703:PHE:HB3	1:B:710:VAL:CG2	2.26	0.65
1:A:516:PRO:HG2	1:A:599:LEU:HB3	1.79	0.64
1:B:235:GLY:HA2	1:B:629:TYR:HB2	1.77	0.64
1:B:90:VAL:O	1:B:94:GLU:HG3	1.97	0.64
1:A:278:TRP:CD1	1:A:278:TRP:N	2.61	0.64
1:A:8:SER:HG	1:A:16:PHE:HE1	1.44	0.64
1:A:235:GLY:HA2	1:A:629:TYR:HB2	1.79	0.63
1:B:645:LEU:O	1:B:648:ILE:HG22	1.98	0.63
1:B:602:PHE:O	1:B:606:ASN:HB2	1.98	0.63
1:A:723:LYS:HZ2	1:A:723:LYS:HB3	1.61	0.63
1:B:697:GLU:O	1:B:698:ILE:HD13	1.98	0.63
1:B:278:TRP:CD1	1:B:278:TRP:N	2.62	0.63
1:A:62:THR:HG21	1:A:68:ILE:HD11	1.81	0.62
1:A:476:ALA:CB	1:A:479:HIS:CE1	2.82	0.62
1:B:569:ASP:OD1	1:B:591:THR:HB	1.98	0.62
1:B:697:GLU:C	1:B:698:ILE:HD13	2.19	0.62
1:A:479:HIS:HD2	1:A:481:TYR:HB2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:PRO:HG2	1:B:599:LEU:HB3	1.80	0.62
1:B:517:ALA:HB3	1:B:535:ASP:O	1.99	0.62
1:B:595:LEU:O	1:B:595:LEU:HD12	1.99	0.62
1:A:263:LYS:HD2	1:A:267:LEU:HD22	1.81	0.62
1:A:640:ASN:HB3	1:A:654:LEU:CD1	2.29	0.62
1:B:217:LEU:HD11	1:B:241:LEU:HD21	1.82	0.62
1:B:648:ILE:HD11	1:B:716:VAL:HG23	1.81	0.62
1:B:639:HIS:HB3	1:B:722:ALA:HB2	1.82	0.61
1:B:529:ILE:O	1:B:531:PRO:HD3	2.00	0.61
1:A:361:SER:O	1:A:362:GLN:HB2	2.01	0.61
1:A:247:PRO:HD2	1:A:480:ALA:HB1	1.82	0.61
1:A:63:LYS:HG3	1:A:82:LEU:HD11	1.82	0.61
1:B:247:PRO:HD2	1:B:480:ALA:HB1	1.81	0.61
1:A:517:ALA:HB3	1:A:535:ASP:O	2.01	0.61
1:B:479:HIS:HD2	1:B:481:TYR:HB2	1.65	0.61
1:B:76:ILE:HD13	3:B:742:HOH:O	2.00	0.61
1:A:504:ASN:OD1	1:A:505:PRO:HD2	2.01	0.61
1:B:1:SER:HB3	1:B:99:VAL:HG11	1.83	0.60
1:B:358:ALA:O	1:B:408:ASN:HB2	2.01	0.60
1:A:468:ASP:HA	1:A:471:ARG:HH22	1.67	0.60
1:A:1:SER:HB2	1:A:4:LEU:O	2.02	0.60
1:A:476:ALA:HB2	1:A:479:HIS:CE1	2.37	0.60
1:A:587:TYR:HA	1:A:590:TYR:CD1	2.37	0.60
1:B:151:GLU:O	1:B:155:ARG:HG2	2.01	0.60
1:B:701:VAL:CG1	1:B:712:ALA:HB1	2.32	0.60
1:A:639:HIS:HB3	1:A:722:ALA:HB2	1.84	0.60
1:A:706:GLU:HB2	1:A:711:VAL:HG23	1.84	0.60
1:B:569:ASP:HA	1:B:592:ILE:CD1	2.32	0.59
1:A:1:SER:OG	1:A:21:VAL:HG21	2.02	0.59
1:B:243:THR:HG21	1:B:245:ARG:NH2	2.18	0.59
1:B:243:THR:HG21	1:B:245:ARG:HH21	1.67	0.59
1:A:528:GLY:HA2	1:B:122:LEU:CD1	2.33	0.59
1:A:272:ASP:HA	1:A:275:ARG:NE	2.18	0.58
1:A:614:ARG:HA	1:A:617:LEU:HB2	1.83	0.58
1:B:640:ASN:HB3	1:B:654:LEU:HD12	1.85	0.58
1:A:703:PHE:HA	1:A:711:VAL:O	2.03	0.58
1:A:627:LEU:HB2	1:A:630:GLU:OE2	2.04	0.58
1:A:433:LYS:HZ1	1:A:460:THR:HG22	1.68	0.58
1:B:274:GLU:HG3	1:B:278:TRP:CZ3	2.38	0.58
1:B:569:ASP:HA	1:B:592:ILE:HD11	1.85	0.58
1:A:1:SER:HB3	1:A:99:VAL:HG11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:ILE:HD11	1:B:716:VAL:CG2	2.34	0.58
1:A:471:ARG:HH11	1:A:471:ARG:CG	2.16	0.57
1:A:653:ALA:HB2	1:A:673:TRP:NE1	2.18	0.57
1:B:274:GLU:HG3	1:B:278:TRP:CH2	2.38	0.57
1:B:562:LEU:O	1:B:566:ILE:HG13	2.04	0.57
1:B:619:GLU:HG3	1:B:620:PHE:CD1	2.38	0.57
1:A:216:VAL:O	1:A:238:PRO:HA	2.05	0.57
1:B:34:GLY:HA3	1:B:99:VAL:HG13	1.86	0.57
1:B:361:SER:O	1:B:362:GLN:HB2	2.04	0.57
1:A:471:ARG:HH11	1:A:471:ARG:HG2	1.69	0.57
1:B:6:ILE:O	1:B:23:VAL:HA	2.05	0.57
1:A:120:ARG:HB2	1:A:122:LEU:HD22	1.86	0.57
1:A:7:ALA:HA	1:A:24:ASP:O	2.04	0.57
1:A:328:MET:HE3	1:A:467:ILE:HD12	1.85	0.57
1:B:7:ALA:HA	1:B:24:ASP:O	2.04	0.57
1:B:706:GLU:HB2	1:B:711:VAL:HG23	1.85	0.57
1:A:122:LEU:CD1	1:B:528:GLY:HA2	2.35	0.57
1:A:660:TYR:CD1	1:A:697:GLU:O	2.57	0.57
1:B:590:TYR:HA	1:B:594:GLU:OE1	2.04	0.57
1:A:247:PRO:HD2	1:A:480:ALA:CB	2.35	0.56
1:A:441:MET:CE	1:A:563:GLN:HG3	2.35	0.56
1:B:441:MET:CE	1:B:563:GLN:HG3	2.35	0.56
1:A:181:HIS:O	1:A:185:VAL:HG23	2.06	0.56
1:B:726:ASP:HA	1:B:729:ASN:HD21	1.69	0.56
1:A:657:ALA:HB1	1:A:681:PHE:CZ	2.40	0.56
1:A:590:TYR:HA	1:A:594:GLU:OE1	2.06	0.56
1:A:12:ALA:HB1	1:A:37:ILE:HG22	1.87	0.56
1:A:704:LYS:HB2	1:A:713:TYR:HE1	1.68	0.56
1:B:255:TYR:CD1	1:B:483:GLY:HA3	2.39	0.56
1:B:37:ILE:HD11	1:B:95:ILE:HD13	1.88	0.56
1:A:272:ASP:HA	1:A:275:ARG:HE	1.69	0.56
1:A:569:ASP:HA	1:A:592:ILE:CD1	2.36	0.56
1:B:211:SER:HB3	1:B:214:ASP:OD2	2.05	0.56
1:A:271:VAL:HG12	1:A:274:GLU:H	1.71	0.55
1:A:6:ILE:O	1:A:23:VAL:HA	2.06	0.55
1:B:195:LEU:HB3	1:B:401:MET:CE	2.36	0.55
1:A:640:ASN:HB3	1:A:654:LEU:HD11	1.87	0.55
1:A:264:ILE:HG21	1:A:309:LEU:HD13	1.88	0.55
1:A:374:LYS:HG3	1:A:379:TYR:CZ	2.42	0.55
1:B:240:TYR:O	1:B:618:ARG:NH1	2.39	0.55
1:B:624:GLN:OE1	1:B:627:LEU:HD12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ARG:HD2	1:A:336:LEU:HD12	1.89	0.55
1:B:237:ARG:HG2	1:B:270:LYS:HE2	1.87	0.55
1:B:471:ARG:HH11	1:B:471:ARG:CG	2.18	0.55
1:A:645:LEU:HG	1:A:712:ALA:HB3	1.87	0.55
1:B:12:ALA:HB1	1:B:37:ILE:HG22	1.88	0.55
1:A:195:LEU:HB3	1:A:401:MET:CE	2.36	0.55
1:B:643:VAL:HG11	1:B:648:ILE:HA	1.87	0.55
1:A:477:LYS:CD	1:A:477:LYS:H	2.19	0.55
1:A:643:VAL:HB	1:A:648:ILE:HG13	1.89	0.55
1:A:697:GLU:C	1:A:698:ILE:HD13	2.27	0.55
1:B:62:THR:HG21	1:B:68:ILE:HD11	1.89	0.55
1:B:504:ASN:O	1:B:508:GLY:N	2.39	0.55
1:A:34:GLY:HA3	1:A:99:VAL:HG13	1.89	0.54
1:B:471:ARG:HH11	1:B:471:ARG:HG2	1.73	0.54
1:A:237:ARG:HG2	1:A:270:LYS:CE	2.37	0.54
1:A:282:PHE:O	1:A:310:CYS:HA	2.07	0.54
1:A:358:ALA:O	1:A:408:ASN:HB2	2.06	0.54
1:A:256:ASP:HA	1:A:488:GLN:HE22	1.73	0.54
1:A:611:TYR:CZ	1:A:679:LYS:HD2	2.43	0.54
1:B:1:SER:HB2	1:B:4:LEU:O	2.08	0.54
1:B:471:ARG:HH11	1:B:471:ARG:HB3	1.71	0.54
1:B:468:ASP:HA	1:B:471:ARG:NH2	2.23	0.54
1:A:726:ASP:HA	1:A:729:ASN:HD21	1.72	0.54
1:B:275:ARG:HA	1:B:281:PRO:HB3	1.88	0.54
1:A:383:LYS:HB2	3:A:746:HOH:O	2.06	0.54
1:B:338:ASP:O	1:B:339:ASP:HB3	2.08	0.54
1:B:645:LEU:HG	1:B:712:ALA:HB3	1.90	0.54
1:A:151:GLU:O	1:A:155:ARG:HG2	2.08	0.53
1:A:277:LYS:HB3	1:A:278:TRP:HD1	1.73	0.53
1:A:229:SER:HA	1:A:233:MET:HB2	1.90	0.53
1:B:243:THR:HG22	1:B:244:ASN:N	2.23	0.53
1:B:344:ASP:CB	1:B:345:PRO:HD2	2.38	0.53
1:B:255:TYR:CE1	1:B:483:GLY:HA3	2.43	0.53
1:B:374:LYS:HG3	1:B:379:TYR:CE2	2.44	0.53
1:B:271:VAL:HG12	1:B:274:GLU:H	1.73	0.53
1:B:587:TYR:HA	1:B:590:TYR:CD1	2.43	0.53
1:A:372:HIS:CD2	1:A:373:ILE:HG23	2.43	0.53
1:A:640:ASN:O	1:A:641:LYS:HE3	2.09	0.53
1:A:717:TYR:CZ	1:A:719:ALA:HA	2.44	0.53
1:A:90:VAL:O	1:A:94:GLU:HG3	2.08	0.53
1:B:704:LYS:HB2	1:B:713:TYR:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ARG:NH1	1:A:690:ASN:O	2.41	0.53
1:B:374:LYS:HG3	1:B:379:TYR:CZ	2.44	0.53
1:A:708:ASP:C	1:A:709:LYS:HZ3	2.12	0.52
1:A:702:TYR:O	1:A:712:ALA:HA	2.09	0.52
1:B:607:ASN:ND2	1:B:610:THR:OG1	2.43	0.52
1:A:246:ASN:HD22	1:A:246:ASN:N	2.07	0.52
1:B:614:ARG:HA	1:B:617:LEU:HB2	1.90	0.52
1:A:648:ILE:HD11	1:A:716:VAL:HG23	1.91	0.52
1:B:1:SER:OG	1:B:21:VAL:HG21	2.09	0.52
1:B:221:ASN:OD1	1:B:245:ARG:NH2	2.43	0.52
1:B:433:LYS:NZ	1:B:458:GLY:O	2.43	0.52
1:B:653:ALA:HB2	1:B:673:TRP:NE1	2.24	0.52
1:A:246:ASN:HD21	1:A:250:PHE:HB2	1.75	0.52
1:A:468:ASP:OD1	1:A:471:ARG:NH2	2.43	0.52
1:A:587:TYR:HA	1:A:590:TYR:CE1	2.44	0.52
1:A:697:GLU:O	1:A:698:ILE:HD13	2.09	0.52
1:A:429:ILE:O	1:A:433:LYS:HG3	2.10	0.52
1:B:660:TYR:CD1	1:B:697:GLU:O	2.61	0.52
1:A:242:GLN:HB3	1:A:618:ARG:H	1.75	0.52
1:B:247:PRO:HD2	1:B:480:ALA:CB	2.40	0.52
1:B:330:ARG:HD2	1:B:336:LEU:HD12	1.92	0.52
1:B:580:TYR:HE1	1:B:587:TYR:O	1.92	0.52
1:A:255:TYR:CD1	1:A:483:GLY:HA3	2.45	0.51
1:A:471:ARG:HH11	1:A:471:ARG:HB3	1.74	0.51
1:A:698:ILE:HG22	1:A:699:GLN:N	2.26	0.51
1:B:448:PRO:HG2	1:B:449:VAL:H	1.74	0.51
1:B:717:TYR:CZ	1:B:719:ALA:HA	2.46	0.51
1:A:1:SER:CB	1:A:21:VAL:HG11	2.38	0.51
1:A:237:ARG:HH22	1:A:271:VAL:HG21	1.75	0.51
1:A:275:ARG:HA	1:A:281:PRO:HB3	1.91	0.51
1:A:619:GLU:HG3	1:A:620:PHE:CD2	2.45	0.51
1:B:590:TYR:CD2	1:B:594:GLU:HB3	2.45	0.51
1:B:237:ARG:HH22	1:B:271:VAL:HG21	1.74	0.51
1:B:702:TYR:O	1:B:712:ALA:HA	2.10	0.51
1:B:216:VAL:O	1:B:238:PRO:HA	2.11	0.51
1:B:447:PRO:O	1:B:455:TRP:HB2	2.11	0.51
1:B:708:ASP:C	1:B:709:LYS:HZ3	2.14	0.51
1:A:511:GLU:O	1:A:600:HIS:HE1	1.94	0.51
1:A:397:PRO:HA	1:B:362:GLN:OE1	2.11	0.51
1:A:562:LEU:O	1:A:566:ILE:HG13	2.12	0.50
1:B:1:SER:CB	1:B:21:VAL:HG11	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ALA:HB1	1:B:26:VAL:HG22	1.93	0.50
1:A:5:LYS:HG2	1:A:22:VAL:HB	1.93	0.50
1:A:660:TYR:HB2	1:A:697:GLU:HG2	1.93	0.50
1:B:372:HIS:CD2	1:B:373:ILE:HG23	2.46	0.50
1:B:583:ASN:ND2	1:B:692:PRO:HB2	2.26	0.50
1:B:221:ASN:OD1	1:B:243:THR:HG21	2.10	0.50
1:A:211:SER:HB3	1:A:214:ASP:OD2	2.11	0.50
1:A:476:ALA:HB3	1:A:479:HIS:CE1	2.46	0.50
1:B:246:ASN:HD22	1:B:246:ASN:N	2.09	0.50
1:A:274:GLU:HG3	1:A:278:TRP:CZ3	2.46	0.50
1:A:243:THR:HG21	1:A:245:ARG:NH2	2.27	0.50
1:A:644:PRO:HG3	1:A:713:TYR:CE2	2.47	0.50
1:A:327:PRO:O	1:A:330:ARG:HG2	2.12	0.50
1:B:274:GLU:HA	1:B:278:TRP:CZ2	2.47	0.50
1:A:274:GLU:HA	1:A:278:TRP:CE2	2.47	0.49
1:B:511:GLU:O	1:B:600:HIS:HE1	1.95	0.49
1:A:254:ILE:HG13	1:A:297:TYR:OH	2.12	0.49
1:A:656:GLY:HA2	1:A:667:VAL:O	2.11	0.49
1:B:181:HIS:O	1:B:185:VAL:HG23	2.12	0.49
1:A:62:THR:CG2	1:A:68:ILE:HD11	2.42	0.49
1:B:246:ASN:HD21	1:B:250:PHE:HB2	1.77	0.49
1:A:245:ARG:NH2	1:A:251:ILE:HG23	2.27	0.49
1:B:468:ASP:OD1	1:B:471:ARG:NH2	2.46	0.49
1:B:619:GLU:HG3	1:B:620:PHE:HD1	1.77	0.49
1:A:344:ASP:CB	1:A:345:PRO:HD2	2.40	0.49
1:A:648:ILE:HD11	1:A:716:VAL:CG2	2.43	0.49
1:B:701:VAL:HG11	1:B:712:ALA:HB1	1.95	0.49
1:A:257:SER:O	1:A:259:PHE:N	2.46	0.49
1:A:448:PRO:HG2	1:A:449:VAL:H	1.78	0.49
1:B:590:TYR:HA	1:B:594:GLU:CD	2.33	0.49
1:A:374:LYS:HG3	1:A:379:TYR:CE2	2.48	0.49
1:B:257:SER:O	1:B:259:PHE:N	2.46	0.49
1:B:5:LYS:HG2	1:B:22:VAL:HB	1.95	0.49
1:B:229:SER:HA	1:B:233:MET:HB2	1.95	0.48
1:B:243:THR:CG2	1:B:245:ARG:HH21	2.26	0.48
1:B:510:TYR:CE1	1:B:609:PHE:CD2	3.01	0.48
1:A:1:SER:OG	1:A:21:VAL:CG2	2.60	0.48
1:A:243:THR:HG22	1:A:244:ASN:N	2.28	0.48
1:A:626:MET:HE3	1:A:652:ILE:HG21	1.94	0.48
1:B:167:ASP:O	1:B:171:HIS:HA	2.12	0.48
1:A:267:LEU:HD11	1:A:618:ARG:CZ	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ARG:O	1:A:635:PHE:HB3	2.13	0.48
1:A:660:TYR:CG	1:A:697:GLU:HG2	2.48	0.48
1:A:95:ILE:O	1:A:99:VAL:HG23	2.13	0.48
1:B:274:GLU:HA	1:B:278:TRP:CE2	2.48	0.48
1:B:242:GLN:HB3	1:B:618:ARG:H	1.79	0.48
1:B:723:LYS:HB3	1:B:723:LYS:HZ2	1.77	0.48
1:A:529:ILE:O	1:A:531:PRO:HD3	2.13	0.48
1:B:264:ILE:HG21	1:B:309:LEU:HD13	1.96	0.48
1:B:640:ASN:HB3	1:B:654:LEU:HD11	1.95	0.48
1:A:644:PRO:O	1:A:648:ILE:HB	2.14	0.48
1:A:383:LYS:NZ	1:B:642:LEU:HD21	2.29	0.48
1:A:37:ILE:HD11	1:A:95:ILE:HD13	1.95	0.48
1:A:243:THR:HG21	1:A:245:ARG:HH21	1.77	0.48
1:A:267:LEU:HD11	1:A:618:ARG:NE	2.28	0.48
1:A:653:ALA:HB2	1:A:673:TRP:HE1	1.76	0.48
1:B:247:PRO:O	1:B:503:ILE:HD13	2.14	0.48
1:A:569:ASP:HA	1:A:592:ILE:HD11	1.95	0.48
1:A:243:THR:HB	1:A:616:PHE:HB3	1.95	0.48
1:A:122:LEU:HG	1:B:530:ILE:HD11	1.96	0.48
1:A:168:LEU:N	1:A:168:LEU:HD12	2.29	0.48
1:A:603:TYR:HB3	1:A:608:THR:OG1	2.14	0.48
1:B:471:ARG:HA	1:B:490:TYR:HA	1.96	0.48
1:B:580:TYR:CE1	1:B:587:TYR:O	2.67	0.48
1:A:471:ARG:NH1	1:A:471:ARG:CB	2.77	0.47
1:A:504:ASN:O	1:A:508:GLY:N	2.47	0.47
1:B:128:PRO:O	1:B:131:GLN:HG3	2.14	0.47
1:B:698:ILE:HG22	1:B:699:GLN:N	2.29	0.47
1:A:720:GLU:HA	1:A:723:LYS:HB2	1.96	0.47
1:B:429:ILE:O	1:B:433:LYS:HG3	2.14	0.47
1:B:611:TYR:CZ	1:B:679:LYS:HD2	2.49	0.47
1:B:688:ILE:HG23	1:B:695:ALA:CB	2.44	0.47
1:A:510:TYR:CE1	1:A:609:PHE:CD2	3.02	0.47
1:B:317:SER:HB2	1:B:320:VAL:HG23	1.96	0.47
1:B:477:LYS:CD	1:B:477:LYS:H	2.22	0.47
1:B:326:ILE:HD12	1:B:329:MET:SD	2.55	0.47
1:B:603:TYR:HB3	1:B:608:THR:OG1	2.14	0.47
1:B:706:GLU:HB2	1:B:711:VAL:CG2	2.44	0.47
1:B:435:LEU:HD23	1:B:556:ILE:HG23	1.96	0.47
1:A:221:ASN:OD1	1:A:243:THR:HG21	2.14	0.47
1:A:626:MET:CE	1:A:652:ILE:HG21	2.45	0.47
1:B:504:ASN:OD1	1:B:505:PRO:CD	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLY:HA2	1:A:372:HIS:CE1	2.50	0.47
1:A:701:VAL:CG1	1:A:712:ALA:HB1	2.45	0.47
1:A:623:GLU:OE1	1:A:672:LYS:HD2	2.15	0.47
1:B:272:ASP:O	1:B:276:ALA:HB3	2.15	0.47
1:A:583:ASN:ND2	1:A:692:PRO:HB2	2.29	0.47
1:A:635:PHE:HA	1:A:654:LEU:HD13	1.97	0.47
1:B:256:ASP:HA	1:B:488:GLN:HE22	1.79	0.47
1:B:272:ASP:HA	1:B:275:ARG:NE	2.30	0.47
1:B:580:TYR:OH	1:B:588:ASN:HA	2.15	0.47
1:B:623:GLU:OE1	1:B:672:LYS:HD2	2.15	0.47
1:A:542:LEU:HD12	1:B:127:CYS:HB3	1.95	0.46
1:B:29:ASP:O	1:B:31:THR:HG23	2.14	0.46
1:B:626:MET:CE	1:B:652:ILE:HG21	2.45	0.46
1:A:255:TYR:CE1	1:A:483:GLY:HA3	2.49	0.46
1:B:117:TYR:HB2	1:B:165:LEU:HD11	1.98	0.46
1:A:281:PRO:HG2	1:A:282:PHE:CD2	2.50	0.46
1:B:195:LEU:HB3	1:B:401:MET:HE2	1.96	0.46
1:B:476:ALA:CB	1:B:479:HIS:ND1	2.79	0.46
1:A:415:GLU:HA	1:A:418:ARG:CG	2.46	0.46
1:A:443:ARG:HG3	1:A:444:PRO:HD2	1.97	0.46
1:A:706:GLU:HB2	1:A:711:VAL:CG2	2.44	0.46
1:B:17:ASP:O	1:B:19:ASP:N	2.41	0.46
1:B:247:PRO:HG3	1:B:609:PHE:CE1	2.50	0.46
1:B:614:ARG:HB3	1:B:620:PHE:CG	2.50	0.46
1:B:631:ALA:O	1:B:654:LEU:HD22	2.15	0.46
1:A:108:PRO:HG2	1:A:407:VAL:HA	1.96	0.46
1:A:274:GLU:HG3	1:A:278:TRP:CH2	2.50	0.46
1:A:407:VAL:O	1:A:411:MET:HG3	2.15	0.46
1:A:476:ALA:CB	1:A:479:HIS:ND1	2.79	0.46
1:A:544:THR:O	1:A:547:GLU:HG2	2.15	0.46
1:A:719:ALA:O	1:A:723:LYS:N	2.42	0.46
1:B:264:ILE:O	1:B:267:LEU:HB3	2.16	0.46
1:B:346:GLY:HA2	1:B:372:HIS:CE1	2.51	0.46
1:A:125:PHE:CZ	1:B:551:LYS:HG2	2.51	0.46
1:A:274:GLU:HA	1:A:278:TRP:CZ2	2.51	0.46
1:A:280:ARG:HB3	1:A:280:ARG:HE	1.53	0.46
1:A:524:LEU:HD13	1:A:531:PRO:HG3	1.98	0.46
1:B:276:ALA:O	1:B:277:LYS:HG2	2.16	0.46
1:B:63:LYS:HG3	1:B:82:LEU:HD11	1.98	0.46
1:B:282:PHE:O	1:B:310:CYS:HA	2.15	0.46
1:B:485:GLY:N	1:B:488:GLN:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:TYR:HB2	1:B:697:GLU:HG2	1.98	0.46
1:A:187:ASN:O	1:A:369:LYS:HE3	2.16	0.46
1:A:5:LYS:HB3	1:A:22:VAL:O	2.16	0.46
1:B:468:ASP:HA	1:B:471:ARG:HH22	1.79	0.46
1:B:703:PHE:HA	1:B:711:VAL:O	2.15	0.46
1:A:195:LEU:HB3	1:A:401:MET:HE2	1.98	0.45
1:A:619:GLU:HG3	1:A:620:PHE:HD2	1.80	0.45
1:A:631:ALA:O	1:A:654:LEU:HD22	2.15	0.45
1:B:479:HIS:O	1:B:480:ALA:HB3	2.15	0.45
1:B:159:CYS:SG	1:B:160:ASN:N	2.88	0.45
1:B:198:SER:HA	1:B:201:ALA:HB3	1.98	0.45
1:B:635:PHE:HA	1:B:654:LEU:HD13	1.98	0.45
1:B:586:ARG:NH1	1:B:690:ASN:O	2.47	0.45
1:B:272:ASP:HA	1:B:275:ARG:HE	1.80	0.45
1:B:441:MET:HE3	1:B:563:GLN:HG3	1.98	0.45
1:A:277:LYS:HB3	1:A:278:TRP:CD1	2.51	0.45
1:B:573:LYS:O	1:B:577:PRO:HA	2.17	0.45
1:B:644:PRO:O	1:B:648:ILE:HB	2.17	0.45
1:A:271:VAL:HG11	1:A:274:GLU:OE1	2.15	0.45
1:B:327:PRO:HB2	1:B:465:ASN:HD21	1.81	0.45
1:B:267:LEU:HD11	1:B:618:ARG:CZ	2.47	0.45
1:B:627:LEU:HB2	1:B:630:GLU:OE2	2.16	0.45
1:A:158:LEU:HB3	1:A:162:ASP:OD2	2.16	0.45
1:A:198:SER:HA	1:A:201:ALA:HB3	1.99	0.45
1:A:221:ASN:OD1	1:A:245:ARG:NH2	2.49	0.45
1:A:570:ALA:N	1:A:592:ILE:HD11	2.31	0.45
1:B:570:ALA:HB1	1:B:571:PRO:CD	2.47	0.45
1:B:643:VAL:HB	1:B:648:ILE:HG13	1.98	0.45
1:A:7:ALA:HB1	1:A:26:VAL:HG22	1.98	0.45
1:B:595:LEU:C	1:B:595:LEU:HD12	2.37	0.45
1:B:4:LEU:CD1	1:B:103:GLU:HB2	2.47	0.45
1:B:230:ALA:O	1:B:234:ALA:HB3	2.16	0.45
1:B:471:ARG:HH11	1:B:471:ARG:CB	2.29	0.45
1:B:476:ALA:HB3	1:B:479:HIS:CE1	2.51	0.45
1:B:701:VAL:HG13	1:B:712:ALA:HB1	1.98	0.45
1:A:237:ARG:NH2	1:A:271:VAL:HG21	2.31	0.45
1:B:308:HIS:HE1	1:B:343:GLU:HB3	1.82	0.45
1:B:352:SER:HA	1:B:364:SER:HB3	1.99	0.45
1:B:430:GLU:OE2	1:B:460:THR:HG21	2.16	0.45
1:A:167:ASP:O	1:A:171:HIS:HA	2.16	0.45
1:A:293:ASP:OD1	1:A:533:LYS:NZ	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ARG:HG2	1:B:270:LYS:CE	2.47	0.45
1:A:165:LEU:N	1:A:165:LEU:HD22	2.32	0.44
1:A:246:ASN:HD21	1:A:250:PHE:H	1.64	0.44
1:A:139:HIS:CD2	1:A:141:ALA:H	2.35	0.44
1:A:246:ASN:ND2	1:A:250:PHE:HB2	2.32	0.44
1:B:280:ARG:HB3	1:B:280:ARG:HE	1.57	0.44
1:A:247:PRO:O	1:A:503:ILE:HD13	2.17	0.44
1:A:308:HIS:HE1	1:A:343:GLU:HB3	1.82	0.44
1:B:269:ALA:CA	1:B:275:ARG:CZ	2.87	0.44
1:B:271:VAL:O	1:B:275:ARG:HG2	2.18	0.44
1:A:127:CYS:HB3	1:B:542:LEU:HD12	1.99	0.44
1:A:17:ASP:O	1:A:19:ASP:N	2.45	0.44
1:B:228:ASN:O	1:B:233:MET:HG3	2.17	0.44
1:B:139:HIS:CD2	1:B:141:ALA:H	2.36	0.44
1:B:303:VAL:HG11	1:B:347:ILE:HD11	1.98	0.44
1:B:730:ASN:HB3	3:B:791:HOH:O	2.16	0.44
1:A:496:PHE:HB3	1:A:541:PHE:HB2	1.99	0.44
1:A:672:LYS:HB3	1:A:672:LYS:HE2	1.72	0.44
1:B:285:ALA:HB2	1:B:310:CYS:SG	2.57	0.44
1:B:496:PHE:HB3	1:B:541:PHE:HB2	1.99	0.44
1:A:471:ARG:HH11	1:A:471:ARG:CB	2.31	0.44
1:A:642:LEU:O	1:A:713:TYR:HD2	2.01	0.44
1:B:577:PRO:HG2	1:B:578:SER:H	1.82	0.44
1:B:471:ARG:NH1	1:B:471:ARG:CB	2.79	0.44
1:B:533:LYS:HB3	1:B:533:LYS:HE2	1.75	0.44
1:A:352:SER:HA	1:A:364:SER:HB3	1.99	0.43
1:A:433:LYS:NZ	1:A:460:THR:HG22	2.33	0.43
1:A:590:TYR:CD2	1:A:594:GLU:HB3	2.53	0.43
1:B:108:PRO:HG2	1:B:407:VAL:HA	1.99	0.43
1:A:265:ARG:O	1:A:268:ALA:HB3	2.18	0.43
3:A:732:HOH:O	1:B:140:PRO:HB3	2.18	0.43
1:B:171:HIS:C	1:B:176:VAL:HB	2.38	0.43
1:A:573:LYS:O	1:A:577:PRO:HA	2.18	0.43
1:B:206:THR:HG21	1:B:230:ALA:HB2	2.00	0.43
1:B:425:LEU:HD11	1:B:493:PRO:HB2	2.00	0.43
1:A:203:ASN:O	1:A:207:SER:HB2	2.18	0.43
1:A:635:PHE:HB2	1:A:654:LEU:HB3	2.01	0.43
1:A:447:PRO:O	1:A:455:TRP:HB2	2.18	0.43
1:A:580:TYR:OH	1:A:588:ASN:HA	2.18	0.43
1:A:704:LYS:O	1:A:711:VAL:N	2.48	0.43
1:B:632:ARG:O	1:B:635:PHE:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:TYR:CE2	1:B:719:ALA:HB2	2.53	0.43
1:B:246:ASN:HD22	1:B:246:ASN:H	1.67	0.43
1:B:246:ASN:HD21	1:B:250:PHE:H	1.65	0.43
1:B:265:ARG:O	1:B:268:ALA:HB3	2.18	0.43
1:B:327:PRO:O	1:B:330:ARG:HG2	2.18	0.43
1:B:356:GLN:NE2	1:B:543:MET:O	2.51	0.43
1:A:275:ARG:HG3	1:A:276:ALA:H	1.84	0.43
1:B:587:TYR:HA	1:B:590:TYR:CE1	2.53	0.43
1:B:660:TYR:CG	1:B:697:GLU:HG2	2.54	0.43
1:A:211:SER:O	1:A:214:ASP:HB2	2.18	0.43
1:B:247:PRO:HA	1:B:609:PHE:CD1	2.54	0.43
1:B:618:ARG:C	1:B:620:PHE:H	2.22	0.43
1:B:476:ALA:HB3	1:B:479:HIS:CD2	2.53	0.43
1:B:704:LYS:O	1:B:711:VAL:N	2.51	0.43
1:A:159:CYS:SG	1:A:160:ASN:N	2.92	0.43
1:A:688:ILE:HG12	1:A:696:PRO:HD2	2.00	0.43
1:A:640:ASN:HB3	1:A:654:LEU:HD12	2.00	0.42
1:A:717:TYR:CE2	1:A:719:ALA:HB2	2.54	0.42
1:B:215:LEU:HD23	1:B:237:ARG:HE	1.84	0.42
1:B:632:ARG:O	1:B:635:PHE:N	2.51	0.42
1:B:643:VAL:HB	1:B:648:ILE:CG1	2.49	0.42
1:B:720:GLU:HA	1:B:723:LYS:HB2	2.00	0.42
1:B:246:ASN:HB2	1:B:480:ALA:HB3	2.01	0.42
1:B:544:THR:O	1:B:547:GLU:HG2	2.19	0.42
1:B:719:ALA:O	1:B:723:LYS:CB	2.59	0.42
1:A:425:LEU:HD13	1:A:425:LEU:HA	1.68	0.42
1:A:587:TYR:C	1:A:590:TYR:HD1	2.22	0.42
1:B:719:ALA:O	1:B:723:LYS:N	2.47	0.42
1:A:433:LYS:NZ	1:A:458:GLY:O	2.52	0.42
1:A:435:LEU:HD21	1:A:556:ILE:HG12	2.00	0.42
1:A:702:TYR:N	1:A:702:TYR:CD1	2.88	0.42
1:B:168:LEU:HD12	1:B:168:LEU:N	2.34	0.42
1:B:195:LEU:HD12	1:B:397:PRO:HB3	2.00	0.42
1:B:570:ALA:N	1:B:592:ILE:HD11	2.34	0.42
1:B:62:THR:CG2	1:B:68:ILE:HD11	2.49	0.42
1:A:237:ARG:HG3	1:A:627:LEU:HD21	2.02	0.42
1:B:415:GLU:HA	1:B:418:ARG:CG	2.49	0.42
1:A:180:LYS:NZ	1:A:180:LYS:HB3	2.34	0.42
1:A:190:LYS:HE2	1:A:191:THR:O	2.20	0.42
1:A:217:LEU:HB3	1:A:285:ALA:HA	2.01	0.42
1:B:617:LEU:HD23	1:B:619:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:ARG:HG3	1:B:618:ARG:O	2.18	0.42
1:B:635:PHE:HB2	1:B:654:LEU:HB3	2.01	0.42
1:A:35:ALA:HA	1:A:57:PRO:HG2	2.02	0.42
1:B:642:LEU:O	1:B:713:TYR:HD2	2.02	0.42
1:A:618:ARG:C	1:A:620:PHE:H	2.23	0.42
1:A:359:GLY:O	1:B:130:HIS:HD2	2.03	0.42
1:B:660:TYR:HA	1:B:661:PRO:HA	1.92	0.42
1:A:246:ASN:H	1:A:246:ASN:HD22	1.67	0.42
1:A:485:GLY:N	1:A:488:GLN:OE1	2.51	0.42
1:B:299:ALA:HB2	1:B:332:SER:O	2.19	0.42
1:A:256:ASP:HA	1:A:488:GLN:NE2	2.34	0.42
1:A:264:ILE:O	1:A:267:LEU:HB3	2.20	0.42
1:B:190:LYS:HE2	1:B:191:THR:O	2.20	0.42
1:B:243:THR:HB	1:B:616:PHE:HB3	2.01	0.42
1:B:242:GLN:HB3	1:B:618:ARG:N	2.35	0.42
1:A:139:HIS:HD2	1:A:141:ALA:H	1.68	0.41
1:A:285:ALA:HB2	1:A:310:CYS:SG	2.60	0.41
1:A:703:PHE:HB3	1:A:710:VAL:HG21	2.00	0.41
1:B:271:VAL:HG11	1:B:274:GLU:OE1	2.20	0.41
1:B:371:SER:HA	1:B:374:LYS:NZ	2.34	0.41
1:A:454:LYS:HB3	1:A:454:LYS:HE2	1.90	0.41
1:A:588:ASN:ND2	3:A:762:HOH:O	2.52	0.41
1:A:645:LEU:HA	1:A:645:LEU:HD22	1.89	0.41
1:A:651:GLU:OE1	1:A:716:VAL:HG11	2.20	0.41
1:B:217:LEU:HB3	1:B:285:ALA:HA	2.01	0.41
1:A:361:SER:HB2	1:B:398:PHE:HA	2.02	0.41
1:B:658:LEU:HB3	1:B:699:GLN:HB2	2.02	0.41
1:A:242:GLN:HB3	1:A:618:ARG:N	2.35	0.41
1:B:255:TYR:O	1:B:256:ASP:C	2.59	0.41
1:B:237:ARG:NH2	1:B:271:VAL:HG21	2.34	0.41
1:A:240:TYR:O	1:A:241:LEU:HD23	2.20	0.41
1:A:504:ASN:HA	1:A:505:PRO:HD3	1.68	0.41
1:B:435:LEU:HD21	1:B:556:ILE:HG12	2.01	0.41
1:A:18:THR:HG22	1:A:18:THR:O	2.20	0.41
1:A:300:HIS:CD2	1:A:331:ASN:O	2.74	0.41
1:B:168:LEU:HA	1:B:175:ALA:HB1	2.03	0.41
1:B:237:ARG:HB2	1:B:237:ARG:HE	1.76	0.41
1:B:586:ARG:NH2	1:B:590:TYR:OH	2.53	0.41
1:B:643:VAL:HB	1:B:648:ILE:HD12	2.01	0.41
1:A:106:ILE:HD13	1:B:140:PRO:HB2	2.01	0.41
1:B:449:VAL:O	1:B:450:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:ILE:HD12	1:B:593:ARG:H	1.85	0.41
1:A:356:GLN:NE2	1:A:543:MET:O	2.53	0.41
1:B:20:ARG:CA	1:B:20:ARG:NE	2.79	0.41
1:B:591:THR:O	1:B:594:GLU:HB2	2.20	0.41
1:A:368:LYS:NZ	1:A:380:CYS:O	2.49	0.41
1:A:504:ASN:OD1	1:A:505:PRO:CD	2.69	0.41
1:A:590:TYR:HA	1:A:594:GLU:CD	2.40	0.41
1:A:626:MET:HG2	1:A:630:GLU:HB2	2.03	0.41
1:A:648:ILE:HG12	1:A:648:ILE:O	2.20	0.41
1:A:719:ALA:O	1:A:723:LYS:CB	2.63	0.41
1:B:246:ASN:ND2	1:B:250:PHE:HB2	2.36	0.41
1:B:435:LEU:CD2	1:B:556:ILE:HG23	2.51	0.41
1:A:215:LEU:HD23	1:A:237:ARG:HE	1.86	0.41
1:A:708:ASP:OD1	1:A:709:LYS:HG2	2.21	0.41
1:B:1:SER:OG	1:B:21:VAL:CG2	2.69	0.41
1:B:320:VAL:HB	1:B:321:GLY:H	1.58	0.41
1:B:16:PHE:CD1	1:B:37:ILE:HG21	2.56	0.41
1:B:302:VAL:O	1:B:306:ILE:HG13	2.20	0.41
1:B:428:THR:CG2	1:B:432:ARG:HH21	2.34	0.41
1:B:688:ILE:HG12	1:B:696:PRO:HD2	2.02	0.41
1:A:476:ALA:HB3	1:A:479:HIS:CG	2.56	0.41
1:A:573:LYS:HG3	1:A:580:TYR:CE1	2.56	0.41
1:A:107:LEU:HA	1:A:108:PRO:HD3	1.95	0.40
1:A:114:LEU:HD21	1:A:156:ALA:HB1	2.03	0.40
1:A:171:HIS:C	1:A:176:VAL:HB	2.42	0.40
1:A:471:ARG:NH1	1:A:471:ARG:CG	2.80	0.40
1:A:573:LYS:HZ3	1:A:573:LYS:H	1.69	0.40
1:B:137:ARG:C	1:B:137:ARG:HD2	2.42	0.40
1:B:651:GLU:O	1:B:672:LYS:HA	2.20	0.40
1:A:20:ARG:CA	1:A:20:ARG:NE	2.83	0.40
1:A:247:PRO:HA	1:A:609:PHE:CD1	2.56	0.40
1:A:276:ALA:O	1:A:277:LYS:HG2	2.20	0.40
1:A:63:LYS:HE3	1:A:63:LYS:HB3	1.92	0.40
1:B:219:ASP:HB3	1:B:222:ASN:ND2	2.36	0.40
1:B:504:ASN:HA	1:B:505:PRO:HD3	1.62	0.40
1:B:204:THR:HG23	1:B:388:SER:HB3	2.02	0.40
1:B:5:LYS:HB3	1:B:22:VAL:O	2.21	0.40
1:B:618:ARG:HD3	1:B:618:ARG:HH11	1.78	0.40
1:B:679:LYS:HE3	1:B:679:LYS:HB2	1.81	0.40
1:A:317:SER:HB2	1:A:320:VAL:HG23	2.03	0.40
1:A:444:PRO:HA	1:A:497:MET:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ARG:O	1:A:635:PHE:N	2.55	0.40
1:A:643:VAL:HB	1:A:648:ILE:CG1	2.51	0.40
1:A:658:LEU:HB3	1:A:699:GLN:HB2	2.03	0.40
1:A:674:SER:O	1:A:678:VAL:HG23	2.22	0.40
1:A:660:TYR:CB	1:A:697:GLU:HG2	2.51	0.40
1:B:277:LYS:HB3	1:B:278:TRP:HD1	1.86	0.40
1:A:430:GLU:OE2	1:A:460:THR:HG21	2.21	0.40
1:A:618:ARG:O	1:A:618:ARG:HG3	2.22	0.40
1:B:504:ASN:HB3	1:B:507:THR:OG1	2.21	0.40
1:B:356:GLN:OE1	1:B:542:LEU:HD22	2.20	0.40
1:B:651:GLU:OE1	1:B:716:VAL:HG11	2.22	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	728/730 (100%)	642 (88%)	70 (10%)	16 (2%)	6 31
1	B	728/730 (100%)	643 (88%)	70 (10%)	15 (2%)	7 33
All	All	1456/1460 (100%)	1285 (88%)	140 (10%)	31 (2%)	7 33

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ALA
1	A	339	ASP
1	A	376	GLN
1	B	339	ASP
1	B	376	GLN
1	A	131	GLN
1	A	258	ASP

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Mol	Chain	Res	Type
1	A	270	LYS
1	A	690	ASN
1	A	729	ASN
1	B	25	ALA
1	B	131	GLN
1	B	270	LYS
1	B	276	ALA
1	B	690	ASN
1	B	729	ASN
1	A	276	ALA
1	A	505	PRO
1	B	258	ASP
1	A	726	ASP
1	B	505	PRO
1	A	570	ALA
1	A	608	THR
1	B	277	LYS
1	B	320	VAL
1	B	355	LYS
1	A	320	VAL
1	A	27	GLY
1	A	577	PRO
1	B	27	GLY
1	B	577	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	617/617 (100%)	544 (88%)	73 (12%)	5 22
1	B	617/617 (100%)	547 (89%)	70 (11%)	6 24
All	All	1234/1234 (100%)	1091 (88%)	143 (12%)	5 23

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	13	ARG
1	A	14	GLN
1	A	20	ARG
1	A	21	VAL
1	A	24	ASP
1	A	50	ASP
1	A	62	THR
1	A	78	HIS
1	A	112	LYS
1	A	114	LEU
1	A	122	LEU
1	A	135	TYR
1	A	159	CYS
1	A	160	ASN
1	A	165	LEU
1	A	190	LYS
1	A	218	PHE
1	A	237	ARG
1	A	245	ARG
1	A	246	ASN
1	A	247	PRO
1	A	258	ASP
1	A	261	GLU
1	A	272	ASP
1	A	274	GLU
1	A	278	TRP
1	A	280	ARG
1	A	284	LEU
1	A	292	TYR
1	A	301	GLU
1	A	320	VAL
1	A	327	PRO
1	A	344	ASP
1	A	345	PRO
1	A	388	SER
1	A	400	PRO
1	A	425	LEU
1	A	471	ARG
1	A	477	LYS
1	A	516	PRO
1	A	545	PRO
1	A	549	PRO

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Mol	Chain	Res	Type
1	A	554	ASN
1	A	561	GLN
1	A	568	GLU
1	A	573	LYS
1	A	578	SER
1	A	584	GLU
1	A	586	ARG
1	A	588	ASN
1	A	592	ILE
1	A	595	LEU
1	A	606	ASN
1	A	617	LEU
1	A	624	GLN
1	A	626	MET
1	A	627	LEU
1	A	632	ARG
1	A	640	ASN
1	A	641	LYS
1	A	642	LEU
1	A	645	LEU
1	A	658	LEU
1	A	659	PRO
1	A	662	PRO
1	A	675	GLU
1	A	697	GLU
1	A	704	LYS
1	A	706	GLU
1	A	709	LYS
1	A	723	LYS
1	A	728	TYR
1	B	3	SER
1	B	10	GLN
1	B	13	ARG
1	B	14	GLN
1	B	20	ARG
1	B	21	VAL
1	B	24	ASP
1	B	50	ASP
1	B	62	THR
1	B	78	HIS
1	B	112	LYS
1	B	114	LEU

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Mol	Chain	Res	Type
1	B	135	TYR
1	B	159	CYS
1	B	160	ASN
1	B	165	LEU
1	B	190	LYS
1	B	218	PHE
1	B	237	ARG
1	B	242	GLN
1	B	245	ARG
1	B	246	ASN
1	B	247	PRO
1	B	258	ASP
1	B	261	GLU
1	B	272	ASP
1	B	274	GLU
1	B	278	TRP
1	B	280	ARG
1	B	284	LEU
1	B	292	TYR
1	B	301	GLU
1	B	320	VAL
1	B	327	PRO
1	B	344	ASP
1	B	388	SER
1	B	395	THR
1	B	400	PRO
1	B	425	LEU
1	B	471	ARG
1	B	477	LYS
1	B	516	PRO
1	B	561	GLN
1	B	564	ARG
1	B	568	GLU
1	B	573	LYS
1	B	578	SER
1	B	584	GLU
1	B	586	ARG
1	B	588	ASN
1	B	592	ILE
1	B	595	LEU
1	B	606	ASN
1	B	617	LEU

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Mol	Chain	Res	Type
1	B	624	GLN
1	B	626	MET
1	B	627	LEU
1	B	632	ARG
1	B	640	ASN
1	B	641	LYS
1	B	642	LEU
1	B	645	LEU
1	B	658	LEU
1	B	659	PRO
1	B	675	GLU
1	B	697	GLU
1	B	704	LYS
1	B	706	GLU
1	B	709	LYS
1	B	723	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	139	HIS
1	A	187	ASN
1	A	202	ASN
1	A	222	ASN
1	A	246	ASN
1	A	308	HIS
1	A	465	ASN
1	A	479	HIS
1	A	494	ASN
1	A	583	ASN
1	A	600	HIS
1	A	607	ASN
1	A	624	GLN
1	B	10	GLN
1	B	101	ASN
1	B	139	HIS
1	B	187	ASN
1	B	202	ASN
1	B	222	ASN
1	B	246	ASN
1	B	300	HIS

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Mol	Chain	Res	Type
1	B	308	HIS
1	B	351	GLN
1	B	465	ASN
1	B	479	HIS
1	B	583	ASN
1	B	600	HIS
1	B	607	ASN
1	B	624	GLN
1	B	640	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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PLP	A	731	1	15,15,16	2.00	3 (20%)	20,22,23	1.74	6 (30%)
2	PLP	B	731	1	15,15,16	2.21	5 (33%)	20,22,23	1.45	2 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	731	1	-	4/6/6/8	0/1/1/1
2	PLP	B	731	1	-	4/6/6/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	731	PLP	C2A-C2	4.65	1.58	1.50
2	B	731	PLP	C6-N1	3.95	1.42	1.34
2	B	731	PLP	C2-N1	3.83	1.41	1.33
2	A	731	PLP	C2-N1	3.59	1.40	1.33
2	B	731	PLP	C4A-C4	3.41	1.58	1.51
2	B	731	PLP	P-O4P	2.91	1.69	1.60
2	B	731	PLP	O3-C3	2.50	1.42	1.37
2	A	731	PLP	P-O2P	-2.13	1.46	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	731	PLP	O3P-P-O4P	3.35	115.64	106.73
2	A	731	PLP	C6-C5-C4	3.01	120.53	118.16
2	B	731	PLP	C2A-C2-N1	2.82	123.18	117.67
2	B	731	PLP	C2A-C2-C3	-2.58	117.70	120.89
2	A	731	PLP	C2A-C2-C3	-2.58	117.70	120.89
2	A	731	PLP	O4P-P-O1P	-2.45	99.60	106.47
2	A	731	PLP	C2A-C2-N1	2.24	122.05	117.67
2	A	731	PLP	C4A-C4-C5	-2.08	118.79	120.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	731	PLP	C5A-O4P-P-O3P
2	B	731	PLP	C5A-O4P-P-O3P
2	A	731	PLP	C5A-O4P-P-O1P
2	B	731	PLP	C5A-O4P-P-O1P
2	A	731	PLP	C4-C5-C5A-O4P
2	B	731	PLP	C4-C5-C5A-O4P
2	A	731	PLP	C5A-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
2	B	731	PLP	C5A-O4P-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.