Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 12:14 pm BST

PDB ID	:	1WA9
Title	:	Crystal Structure of the PAS repeat region of the Drosophila clock protein PERIOD
Authors	:	Yildiz, O.; Doi, M.; Yujnovsky, I.; Cardone, L.; Berndt, A.; Hennig, S.; Schulze, S.; Urbanke, C.; Sassone-Corsi, P.; Wolf, E.
Deposited on	:	2004-10-25
Resolution	:	3.15 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:

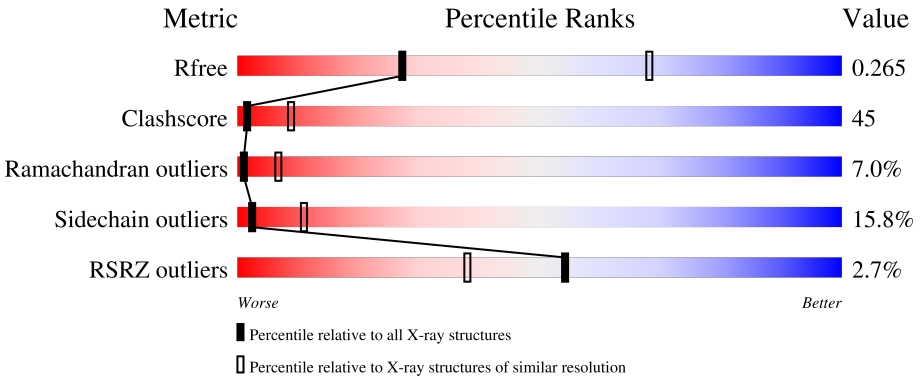
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	368	3% 35% 40% 11% • 14%
1	B	368	% 31% 44% 11% • 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5039 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 PERIOD CIRCADIAN PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	1
			2504	1585	437	464	18			
1	B	319	Total	C	N	O	S	0	0	1
			2529	1605	437	468	19			

- Molecule 2 is water.

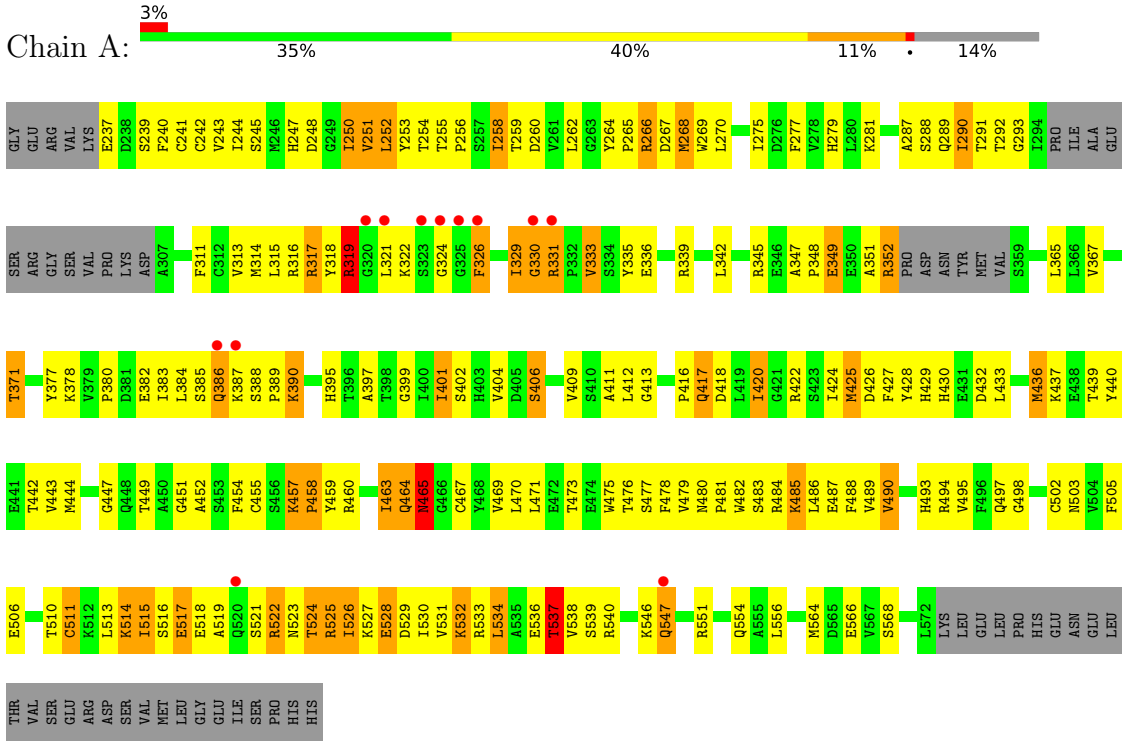
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	O	0	0
			5	5		
2	B	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

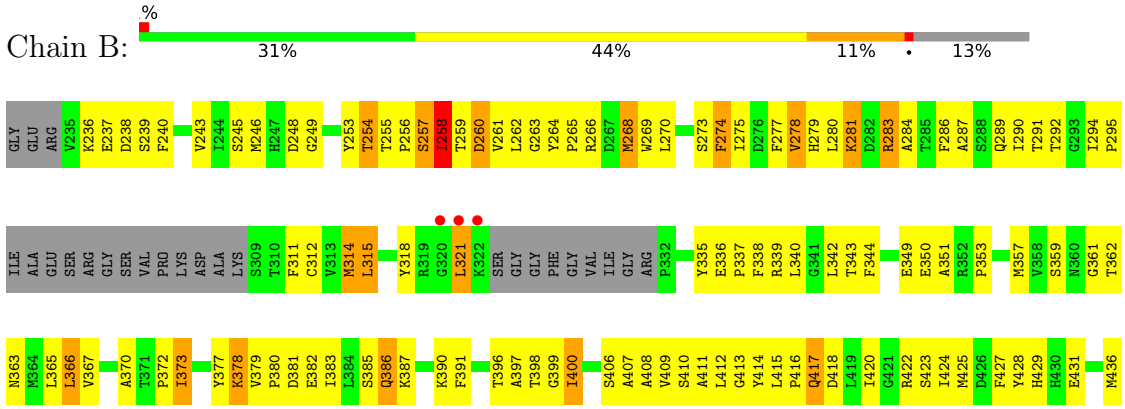
• Molecule 1: PERIOD CIRCADIAN PROTEIN

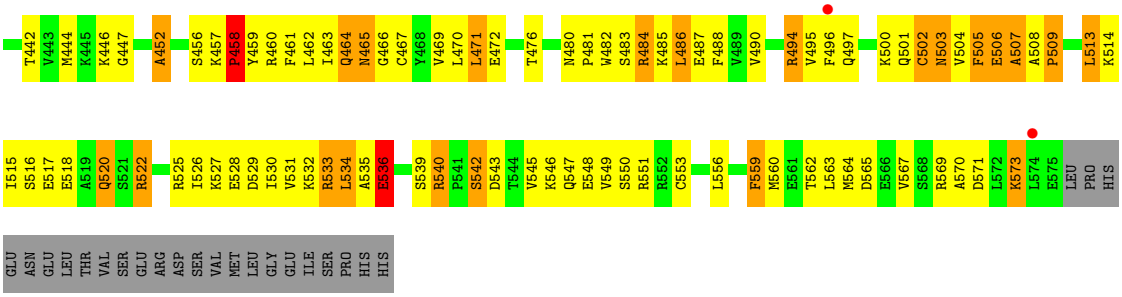
Chain A:



• Molecule 1: PERIOD CIRCADIAN PROTEIN

Chain B:




T442 V443 M444 K445 K446 G447 A452 S456 K457 P458 Y459 R460 F461 L462 I463 Q464 N465 G466 C467 Y468 V469 L470 L471 E472 T476 N480 P481 W482 S483 R484 K485 L486 E487 F488 V489 V490 R494 V495 F496 Q497 K500 Q501 C502 N503 V504 F505 E506 A507 A508 P509 L513 K514
I515 S516 E517 E518 A519 Q520 S521 R522 R525 I526 K527 E528 D529 I530 V531 K532 R533 L534 A535 E536 S539 R540 P541 S542 D543 T544 V545 K546 Q547 E548 V549 S550 R551 H552 C553 L556 F559 M560 E561 T562 L563 M564 D565 E566 V567 S568 R569 A570 D571 L572 K573 L574 E575 LEU PRO HIS
GLU ASN GLU LEU THR VAL SER GLU ARG ASP SER VAL MET LEU GLY GLU ILE SER PRO HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	140.44Å 140.44Å 61.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.15 29.35 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.00-3.15) 99.5 (29.35-3.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.277 0.219 , 0.265	Depositor DCC
R_{free} test set	1207 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	97.4	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 99.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5039	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.49	0/2556	0.71	0/3450
1	B	0.46	0/2583	0.70	1/3490 (0.0%)
All	All	0.48	0/5139	0.70	1/6940 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	494	ARG	N-CA-C	-6.07	94.63	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	2504	0	2500	244	0
1	B	2529	0	2532	237	0
2	A	5	0	0	0	0
2	B	1	0	0	0	0
All	All	5039	0	5032	457	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 45.

All (457) 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:470:LEU:HB2	1:B:497:GLN:HB3	1.21	1.20
1:A:317:ARG:HB3	1:A:317:ARG:HH21	1.11	1.05
1:B:476:THR:HG23	1:B:490:VAL:HG13	1.40	1.04
1:B:465:ASN:HD22	1:B:466:GLY:N	1.57	1.01
1:B:533:ARG:NH2	1:B:533:ARG:HB2	1.72	1.01
1:A:522:ARG:CZ	1:A:522:ARG:HA	1.91	1.01
1:B:417:GLN:HE21	1:B:417:GLN:H	1.11	0.98
1:A:523:ASN:HA	1:A:526:ILE:HG22	1.47	0.95
1:A:319:ARG:HA	1:A:319:ARG:HH11	1.31	0.95
1:A:275:ILE:HD13	1:B:482:TRP:HB3	1.49	0.94
1:A:417:GLN:H	1:A:417:GLN:NE2	1.64	0.94
1:A:417:GLN:HE21	1:A:417:GLN:N	1.65	0.94
1:B:417:GLN:H	1:B:417:GLN:NE2	1.65	0.93
1:B:390:LYS:HG2	1:B:494:ARG:HG2	1.53	0.91
1:B:465:ASN:HD22	1:B:466:GLY:H	1.17	0.91
1:A:433:LEU:HD12	1:A:523:ASN:HD22	1.36	0.91
1:A:463:ILE:HD11	1:A:465:ASN:ND2	1.86	0.90
1:A:255:THR:HG22	1:B:564:MET:HG2	1.52	0.89
1:A:521:SER:HA	1:A:524:THR:HG22	1.51	0.89
1:A:317:ARG:HB3	1:A:317:ARG:NH2	1.90	0.87
1:B:429:HIS:HB2	1:B:460:ARG:HB2	1.56	0.87
1:A:401:ILE:HD13	1:A:402:SER:N	1.89	0.87
1:A:514:LYS:HD2	1:A:515:ILE:N	1.89	0.87
1:A:329:ILE:H	1:A:329:ILE:HD13	1.41	0.86
1:A:479:VAL:HG11	1:A:538:VAL:HG11	1.56	0.85
1:B:527:LYS:HA	1:B:530:ILE:HD12	1.58	0.85
1:B:533:ARG:O	1:B:535:ALA:N	2.09	0.85
1:A:523:ASN:HA	1:A:526:ILE:CG2	2.07	0.84
1:B:444:MET:CE	1:B:533:ARG:HG2	2.08	0.83
1:A:486:LEU:HD21	1:A:489:VAL:HG23	1.61	0.83
1:A:416:PRO:O	1:A:420:ILE:HG22	1.79	0.82
1:A:390:LYS:H	1:A:390:LYS:HD3	1.44	0.82
1:A:390:LYS:HD3	1:A:390:LYS:N	1.94	0.81
1:A:465:ASN:HD22	1:A:465:ASN:C	1.83	0.81
1:A:503:ASN:HB3	1:A:506:GLU:HB2	1.65	0.77
1:A:517:GLU:HG2	1:A:518:GLU:HG3	1.66	0.77
1:A:347:ALA:HB2	1:A:365:LEU:HD13	1.64	0.77
1:A:451:GLY:HA3	1:B:362:THR:HG22	1.66	0.77
1:B:533:ARG:HB2	1:B:533:ARG:CZ	2.12	0.77
1:B:417:GLN:HE21	1:B:417:GLN:N	1.82	0.76
1:A:411:ALA:C	1:A:412:LEU:HD23	2.06	0.76
1:A:321:LEU:HD13	1:A:322:LYS:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:ASN:ND2	1:B:467:CYS:H	1.84	0.76
1:B:383:ILE:HG13	1:B:496:PHE:O	1.87	0.75
1:B:470:LEU:CB	1:B:497:GLN:HB3	2.11	0.75
1:A:485:LYS:HE2	1:A:537:THR:HB	1.67	0.74
1:A:319:ARG:HA	1:A:319:ARG:NH1	2.02	0.74
1:B:546:LYS:HA	1:B:549:VAL:HG12	1.69	0.74
1:B:380:PRO:HB3	1:B:500:LYS:O	1.88	0.74
1:B:396:THR:HG22	1:B:400:ILE:O	1.88	0.73
1:B:239:SER:HB2	1:B:370:ALA:O	1.90	0.72
1:A:436:MET:HE3	1:A:436:MET:HA	1.72	0.72
1:B:240:PHE:HB2	1:B:255:THR:CG2	2.20	0.71
1:A:265:PRO:HD2	1:A:268:MET:HG3	1.72	0.71
1:B:514:LYS:HG2	1:B:518:GLU:OE2	1.90	0.71
1:A:248:ASP:OD1	1:A:250:ILE:HG12	1.91	0.71
1:B:486:LEU:HD23	1:B:487:GLU:N	2.05	0.71
1:B:513:LEU:HD23	1:B:513:LEU:H	1.55	0.71
1:A:417:GLN:H	1:A:417:GLN:HE21	0.83	0.71
1:A:460:ARG:HA	1:A:469:VAL:O	1.90	0.70
1:B:514:LYS:HG3	1:B:515:ILE:H	1.56	0.70
1:A:477:SER:HB2	1:A:486:LEU:HD11	1.72	0.70
1:B:379:VAL:HG23	1:B:382:GLU:HB3	1.72	0.70
1:B:378:LYS:NZ	1:B:378:LYS:HB3	2.08	0.69
1:B:343:THR:HB	1:B:367:VAL:HB	1.75	0.69
1:A:321:LEU:HD22	1:A:322:LYS:H	1.57	0.69
1:A:266:ARG:HG3	1:A:267:ASP:OD2	1.93	0.68
1:A:321:LEU:HD13	1:A:322:LYS:H	1.56	0.68
1:A:254:THR:HG22	1:A:255:THR:O	1.94	0.68
1:A:485:LYS:CE	1:A:537:THR:HB	2.22	0.68
1:B:470:LEU:HB2	1:B:497:GLN:CB	2.13	0.67
1:B:483:SER:O	1:B:485:LYS:N	2.23	0.67
1:B:258:ILE:HD13	1:B:264:TYR:HB2	1.77	0.67
1:A:449:THR:HB	1:A:452:ALA:HB2	1.77	0.67
1:B:311:PHE:HE1	1:B:342:LEU:HD13	1.59	0.67
1:B:423:SER:O	1:B:425:MET:N	2.28	0.67
1:A:377:TYR:OH	1:A:495:VAL:HG21	1.95	0.67
1:B:526:ILE:HG13	1:B:527:LYS:N	2.10	0.67
1:B:549:VAL:HG13	1:B:550:SER:N	2.10	0.67
1:A:275:ILE:CD1	1:B:482:TRP:HB3	2.24	0.66
1:A:484:ARG:HH12	1:B:248:ASP:HA	1.59	0.66
1:A:239:SER:HB3	1:A:371:THR:HB	1.76	0.66
1:A:425:MET:O	1:A:427:PHE:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:HIS:CD2	1:B:460:ARG:HE	2.14	0.65
1:A:436:MET:HA	1:A:436:MET:CE	2.25	0.65
1:B:464:GLN:HE21	1:B:464:GLN:HA	1.61	0.65
1:B:533:ARG:O	1:B:536:GLU:N	2.28	0.65
1:A:425:MET:HE1	1:A:428:TYR:CD1	2.31	0.65
1:B:559:PHE:C	1:B:559:PHE:CD2	2.70	0.65
1:A:247:HIS:CE1	1:B:540:ARG:HD2	2.32	0.65
1:A:317:ARG:HH21	1:A:317:ARG:CB	2.00	0.65
1:A:287:ALA:HA	1:A:290:ILE:CD1	2.27	0.65
1:A:440:TYR:O	1:A:443:VAL:HG12	1.97	0.65
1:B:506:GLU:O	1:B:507:ALA:HB2	1.97	0.64
1:A:401:ILE:HG23	1:A:420:ILE:HA	1.78	0.64
1:B:542:SER:HB2	1:B:547:GLN:OE1	1.96	0.64
1:A:290:ILE:HG22	1:A:342:LEU:CD1	2.28	0.63
1:A:287:ALA:O	1:A:290:ILE:HD13	1.99	0.63
1:A:457:LYS:O	1:A:457:LYS:HG2	1.99	0.63
1:A:449:THR:HG21	1:B:359:SER:OG	1.99	0.63
1:A:479:VAL:HG11	1:A:538:VAL:CG1	2.28	0.63
1:B:416:PRO:HG2	1:B:417:GLN:NE2	2.14	0.63
1:B:464:GLN:HE21	1:B:464:GLN:CA	2.12	0.62
1:A:275:ILE:HG12	1:B:482:TRP:CD1	2.35	0.62
1:A:533:ARG:HH21	1:A:536:GLU:HG3	1.64	0.62
1:A:258:ILE:CG2	1:A:259:THR:N	2.63	0.62
1:B:527:LYS:O	1:B:531:VAL:HG23	2.00	0.62
1:A:290:ILE:HG22	1:A:342:LEU:HD11	1.81	0.62
1:A:401:ILE:HG22	1:A:422:ARG:O	2.00	0.62
1:B:546:LYS:O	1:B:549:VAL:HG12	1.99	0.62
1:A:531:VAL:HG13	1:A:532:LYS:N	2.15	0.62
1:B:428:TYR:HE2	1:B:459:TYR:CE2	2.18	0.62
1:B:533:ARG:HB2	1:B:533:ARG:HH21	1.62	0.62
1:A:270:LEU:CD1	1:B:551:ARG:HH11	2.13	0.61
1:A:551:ARG:HA	1:A:554:GLN:HG2	1.82	0.61
1:A:351:ALA:CB	1:A:352:ARG:HE	2.13	0.61
1:A:482:TRP:NE1	1:B:249:GLY:HA3	2.16	0.61
1:A:319:ARG:HB3	1:A:331:ARG:HB2	1.82	0.61
1:A:523:ASN:CA	1:A:526:ILE:HG22	2.27	0.61
1:A:316:ARG:HB3	1:A:335:TYR:CE1	2.36	0.61
1:B:549:VAL:HG13	1:B:550:SER:H	1.65	0.61
1:A:465:ASN:ND2	1:A:465:ASN:C	2.54	0.61
1:A:351:ALA:HB1	1:A:352:ARG:HH11	1.66	0.60
1:B:465:ASN:ND2	1:B:466:GLY:N	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:PHE:O	1:B:461:PHE:HA	2.01	0.60
1:A:485:LYS:HE2	1:A:537:THR:CB	2.32	0.59
1:B:269:TRP:CD1	1:B:277:PHE:CE1	2.91	0.59
1:B:533:ARG:CZ	1:B:533:ARG:CB	2.80	0.59
1:A:482:TRP:CZ3	1:B:286:PHE:HE1	2.21	0.59
1:B:255:THR:OG1	1:B:256:PRO:HD2	2.03	0.59
1:A:528:GLU:O	1:A:531:VAL:HG12	2.02	0.58
1:B:427:PHE:N	1:B:427:PHE:CD1	2.71	0.58
1:B:525:ARG:O	1:B:528:GLU:HB3	2.03	0.58
1:A:331:ARG:O	1:A:331:ARG:HG2	2.02	0.58
1:B:429:HIS:CG	1:B:460:ARG:HD2	2.39	0.58
1:B:444:MET:HE3	1:B:533:ARG:HG2	1.85	0.58
1:B:447:GLY:O	1:B:540:ARG:NH2	2.37	0.58
1:B:287:ALA:O	1:B:290:ILE:HB	2.03	0.58
1:B:337:PRO:O	1:B:373:ILE:HG12	2.04	0.58
1:A:420:ILE:C	1:A:420:ILE:HD13	2.25	0.57
1:B:412:LEU:C	1:B:414:TYR:H	2.07	0.57
1:B:559:PHE:C	1:B:559:PHE:HD2	2.07	0.57
1:A:339:ARG:NH2	1:A:406:SER:HB3	2.18	0.57
1:A:433:LEU:CD1	1:A:523:ASN:HB3	2.35	0.57
1:A:486:LEU:HD21	1:A:489:VAL:CG2	2.34	0.57
1:A:527:LYS:HA	1:A:530:ILE:HD12	1.87	0.56
1:B:442:THR:O	1:B:446:LYS:HB2	2.05	0.56
1:B:508:ALA:N	1:B:509:PRO:HD3	2.18	0.56
1:A:333:VAL:HG13	1:A:333:VAL:O	2.04	0.56
1:A:566:GLU:O	1:A:566:GLU:HG2	2.05	0.56
1:B:283:ARG:HG2	1:B:283:ARG:HH11	1.70	0.56
1:B:315:LEU:O	1:B:335:TYR:HA	2.05	0.56
1:A:521:SER:HA	1:A:524:THR:CG2	2.30	0.56
1:A:546:LYS:HD3	1:A:547:GLN:N	2.20	0.56
1:A:254:THR:CG2	1:A:258:ILE:HB	2.35	0.56
1:A:399:GLY:O	1:A:424:ILE:HG22	2.06	0.56
1:B:481:PRO:HG2	1:B:482:TRP:CE3	2.41	0.56
1:B:527:LYS:HA	1:B:530:ILE:CD1	2.34	0.56
1:B:379:VAL:O	1:B:382:GLU:HB3	2.06	0.56
1:B:546:LYS:HA	1:B:549:VAL:CG1	2.35	0.56
1:A:425:MET:HE1	1:A:428:TYR:HD1	1.69	0.55
1:A:386:GLN:HE21	1:A:494:ARG:HH12	1.52	0.55
1:B:545:VAL:HG13	1:B:546:LYS:N	2.22	0.55
1:A:464:GLN:HG3	1:A:465:ASN:N	2.22	0.55
1:B:398:THR:HG22	1:B:534:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:VAL:HG23	1:B:382:GLU:CB	2.37	0.55
1:A:386:GLN:HE21	1:A:494:ARG:NH1	2.04	0.55
1:B:456:SER:O	1:B:458:PRO:HD3	2.06	0.55
1:B:531:VAL:O	1:B:533:ARG:N	2.40	0.55
1:B:444:MET:SD	1:B:533:ARG:HG2	2.46	0.55
1:A:256:PRO:HA	1:A:266:ARG:HH21	1.72	0.55
1:A:258:ILE:HG22	1:A:259:THR:N	2.22	0.54
1:A:420:ILE:HD13	1:A:420:ILE:O	2.07	0.54
1:A:463:ILE:HD11	1:A:465:ASN:HD21	1.70	0.54
1:A:339:ARG:HH22	1:A:406:SER:HB3	1.72	0.54
1:B:411:ALA:C	1:B:412:LEU:HD12	2.28	0.54
1:B:422:ARG:HG2	1:B:422:ARG:HH11	1.73	0.54
1:A:463:ILE:HG12	1:A:464:GLN:N	2.22	0.54
1:B:420:ILE:HD12	1:B:420:ILE:O	2.07	0.54
1:A:432:ASP:OD2	1:A:460:ARG:HD2	2.07	0.54
1:A:425:MET:HA	1:A:425:MET:HE2	1.89	0.53
1:B:236:LYS:O	1:B:238:ASP:N	2.38	0.53
1:A:564:MET:O	1:A:568:SER:N	2.31	0.53
1:B:546:LYS:CA	1:B:549:VAL:HG12	2.36	0.53
1:B:465:ASN:OD1	1:B:503:ASN:HB2	2.08	0.53
1:B:377:TYR:OH	1:B:495:VAL:HG11	2.08	0.53
1:B:280:LEU:HA	1:B:283:ARG:HD3	1.91	0.53
1:A:270:LEU:HD13	1:B:551:ARG:HH11	1.73	0.53
1:A:538:VAL:HG22	1:A:539:SER:N	2.24	0.53
1:A:288:SER:O	1:A:292:THR:HG23	2.09	0.52
1:A:317:ARG:HD2	1:A:336:GLU:OE2	2.09	0.52
1:A:348:PRO:HG3	1:B:559:PHE:CE1	2.43	0.52
1:B:261:VAL:HG23	1:B:262:LEU:N	2.24	0.52
1:B:415:LEU:O	1:B:418:ASP:HB2	2.10	0.52
1:A:444:MET:HE1	1:A:486:LEU:HB2	1.90	0.52
1:A:519:ALA:C	1:A:521:SER:H	2.13	0.52
1:B:279:HIS:HB2	1:B:314:MET:HB3	1.91	0.52
1:B:337:PRO:HB2	1:B:373:ILE:HG13	1.92	0.52
1:A:321:LEU:CD1	1:A:322:LYS:H	2.23	0.52
1:A:522:ARG:HA	1:A:522:ARG:NE	2.24	0.52
1:B:338:PHE:CE2	1:B:372:PRO:HG3	2.44	0.52
1:A:433:LEU:HB3	1:A:526:ILE:HD12	1.91	0.52
1:B:406:SER:C	1:B:408:ALA:H	2.13	0.52
1:B:506:GLU:O	1:B:507:ALA:CB	2.58	0.52
1:A:411:ALA:O	1:A:412:LEU:HD23	2.09	0.52
1:A:319:ARG:HD3	1:A:331:ARG:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:LEU:HD23	1:B:340:LEU:N	2.24	0.52
1:A:321:LEU:CD2	1:A:322:LYS:H	2.23	0.51
1:B:513:LEU:HD23	1:B:513:LEU:N	2.24	0.51
1:A:241:CYS:HB2	1:A:255:THR:CG2	2.39	0.51
1:A:515:ILE:HG12	1:A:517:GLU:OE2	2.10	0.51
1:B:429:HIS:CD2	1:B:431:GLU:HB2	2.46	0.51
1:A:425:MET:CE	1:A:428:TYR:CE1	2.94	0.51
1:A:515:ILE:HG23	1:A:515:ILE:O	2.11	0.51
1:A:351:ALA:HB1	1:A:352:ARG:HE	1.76	0.51
1:B:275:ILE:O	1:B:278:VAL:HG13	2.11	0.51
1:A:377:TYR:O	1:A:502:CYS:HB3	2.10	0.51
1:B:428:TYR:HE2	1:B:459:TYR:HE2	1.58	0.51
1:A:318:TYR:O	1:A:319:ARG:HG2	2.11	0.51
1:A:429:HIS:ND1	1:A:460:ARG:HD2	2.26	0.51
1:B:400:ILE:HA	1:B:423:SER:HA	1.92	0.51
1:A:290:ILE:HG12	1:A:290:ILE:O	2.10	0.51
1:A:470:LEU:HB2	1:A:497:GLN:H	1.75	0.51
1:B:342:LEU:N	1:B:342:LEU:CD1	2.74	0.51
1:A:527:LYS:HA	1:A:530:ILE:CD1	2.42	0.50
1:B:381:ASP:OD2	1:B:500:LYS:HA	2.11	0.50
1:B:427:PHE:HB3	1:B:461:PHE:CE1	2.46	0.50
1:A:522:ARG:HA	1:A:522:ARG:NH1	2.25	0.50
1:B:562:THR:O	1:B:565:ASP:N	2.44	0.50
1:A:551:ARG:NH2	1:A:551:ARG:HB2	2.27	0.50
1:B:353:PRO:O	1:B:357:MET:HG2	2.12	0.50
1:A:253:TYR:CE2	1:B:560:MET:HG3	2.46	0.50
1:B:257:SER:O	1:B:260:ASP:N	2.45	0.49
1:B:545:VAL:HG13	1:B:546:LYS:H	1.75	0.49
1:A:531:VAL:HG13	1:A:532:LYS:H	1.76	0.49
1:B:397:ALA:C	1:B:399:GLY:H	2.15	0.49
1:A:429:HIS:CE1	1:A:460:ARG:HH21	2.30	0.49
1:A:440:TYR:HA	1:A:443:VAL:HG12	1.93	0.49
1:B:258:ILE:CD1	1:B:264:TYR:HB2	2.42	0.49
1:B:383:ILE:O	1:B:383:ILE:HG23	2.11	0.49
1:B:429:HIS:HB2	1:B:460:ARG:CB	2.35	0.49
1:B:549:VAL:CG1	1:B:550:SER:H	2.25	0.49
1:B:446:LYS:HD2	1:B:452:ALA:HB1	1.95	0.49
1:A:513:LEU:HD12	1:A:513:LEU:C	2.32	0.49
1:A:255:THR:CG2	1:B:564:MET:HG2	2.34	0.49
1:B:378:LYS:HB3	1:B:378:LYS:HZ3	1.77	0.49
1:A:316:ARG:HH11	1:A:333:VAL:HG21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:PRO:HG2	1:B:268:MET:HB2	1.94	0.49
1:B:290:ILE:O	1:B:292:THR:N	2.46	0.49
1:A:315:LEU:O	1:A:335:TYR:HA	2.13	0.49
1:B:391:PHE:CD1	1:B:408:ALA:HB2	2.48	0.49
1:A:289:GLN:HG3	1:A:311:PHE:CE2	2.47	0.48
1:A:384:LEU:C	1:A:384:LEU:HD23	2.34	0.48
1:B:398:THR:HG22	1:B:534:LEU:CD1	2.43	0.48
1:B:464:GLN:HG3	1:B:465:ASN:N	2.28	0.48
1:A:289:GLN:HG3	1:A:311:PHE:CD2	2.47	0.48
1:B:253:TYR:CG	1:B:254:THR:N	2.81	0.48
1:B:273:SER:O	1:B:275:ILE:N	2.47	0.48
1:B:412:LEU:O	1:B:414:TYR:N	2.46	0.48
1:B:502:CYS:O	1:B:503:ASN:C	2.52	0.48
1:A:265:PRO:O	1:A:268:MET:HB2	2.13	0.48
1:B:549:VAL:CG1	1:B:550:SER:N	2.75	0.48
1:B:337:PRO:HB2	1:B:373:ILE:HD11	1.94	0.48
1:B:464:GLN:CA	1:B:464:GLN:NE2	2.75	0.48
1:B:259:THR:HA	1:B:264:TYR:O	2.13	0.48
1:B:283:ARG:HG2	1:B:283:ARG:NH1	2.27	0.48
1:A:386:GLN:NE2	1:A:494:ARG:NH1	2.62	0.48
1:A:429:HIS:HB3	1:A:432:ASP:OD2	2.12	0.48
1:B:486:LEU:CD2	1:B:488:PHE:N	2.76	0.48
1:A:319:ARG:HD3	1:A:331:ARG:CB	2.44	0.48
1:B:254:THR:HG22	1:B:270:LEU:HD21	1.95	0.48
1:A:532:LYS:HD3	1:A:532:LYS:C	2.33	0.48
1:A:386:GLN:NE2	1:A:494:ARG:HH12	2.11	0.48
1:A:319:ARG:CD	1:A:331:ARG:HB2	2.44	0.48
1:A:463:ILE:HD11	1:A:465:ASN:HD22	1.75	0.47
1:A:547:GLN:O	1:A:551:ARG:NH2	2.48	0.47
1:A:454:PHE:HD2	1:A:455:CYS:O	1.98	0.47
1:A:251:VAL:HG21	1:A:269:TRP:HB3	1.96	0.47
1:B:315:LEU:C	1:B:335:TYR:HD1	2.18	0.47
1:A:384:LEU:HD21	1:A:494:ARG:NH1	2.29	0.47
1:A:454:PHE:CD2	1:A:455:CYS:O	2.68	0.47
1:A:378:LYS:HD2	1:A:378:LYS:N	2.30	0.47
1:A:241:CYS:HB2	1:B:564:MET:HG3	1.97	0.47
1:A:321:LEU:HD22	1:A:322:LYS:N	2.26	0.47
1:A:409:VAL:CG2	1:A:416:PRO:HD3	2.45	0.47
1:A:523:ASN:C	1:A:525:ARG:H	2.18	0.47
1:B:383:ILE:O	1:B:383:ILE:HG12	2.15	0.47
1:B:423:SER:C	1:B:425:MET:N	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:PHE:HB2	1:B:255:THR:HG22	1.96	0.46
1:B:337:PRO:HB2	1:B:373:ILE:CD1	2.45	0.46
1:A:329:ILE:H	1:A:329:ILE:CD1	2.17	0.46
1:A:351:ALA:HB3	1:A:352:ARG:HE	1.79	0.46
1:A:425:MET:C	1:A:427:PHE:N	2.69	0.46
1:A:481:PRO:HG3	1:B:246:MET:HE3	1.98	0.46
1:A:523:ASN:C	1:A:525:ARG:N	2.69	0.46
1:A:531:VAL:CG1	1:A:532:LYS:N	2.79	0.46
1:B:548:GLU:OE2	1:B:548:GLU:HA	2.15	0.46
1:A:385:SER:C	1:A:387:LYS:H	2.19	0.46
1:A:425:MET:C	1:A:427:PHE:H	2.19	0.46
1:A:258:ILE:HD12	1:A:264:TYR:HB2	1.98	0.46
1:B:312:CYS:CB	1:B:415:LEU:HD22	2.46	0.46
1:B:417:GLN:NE2	1:B:417:GLN:N	2.47	0.46
1:B:465:ASN:HD22	1:B:465:ASN:C	2.12	0.46
1:B:311:PHE:CE1	1:B:342:LEU:HD13	2.46	0.46
1:B:531:VAL:C	1:B:533:ARG:H	2.18	0.46
1:A:401:ILE:HD13	1:A:401:ILE:C	2.36	0.45
1:A:241:CYS:HB2	1:A:255:THR:HG23	1.98	0.45
1:A:351:ALA:HB1	1:A:352:ARG:NH1	2.31	0.45
1:B:257:SER:O	1:B:260:ASP:HB2	2.16	0.45
1:A:349:GLU:OE1	1:A:349:GLU:N	2.49	0.45
1:A:444:MET:CE	1:A:486:LEU:HD22	2.46	0.45
1:A:526:ILE:O	1:A:530:ILE:HG13	2.15	0.45
1:B:289:GLN:HG3	1:B:311:PHE:CG	2.51	0.45
1:B:339:ARG:NH2	1:B:406:SER:HB2	2.31	0.45
1:B:378:LYS:HB3	1:B:378:LYS:HZ2	1.82	0.45
1:A:324:GLY:HA3	1:A:331:ARG:NH2	2.32	0.45
1:B:396:THR:OG1	1:B:397:ALA:N	2.50	0.45
1:B:406:SER:O	1:B:409:VAL:HG12	2.17	0.45
1:B:556:LEU:O	1:B:560:MET:HG2	2.17	0.45
1:B:338:PHE:CZ	1:B:372:PRO:HG3	2.51	0.45
1:B:480:ASN:OD1	1:B:480:ASN:C	2.55	0.45
1:B:535:ALA:O	1:B:536:GLU:C	2.55	0.45
1:A:425:MET:CE	1:A:428:TYR:CD1	2.99	0.45
1:B:269:TRP:O	1:B:270:LEU:C	2.54	0.45
1:B:423:SER:C	1:B:425:MET:H	2.20	0.45
1:B:504:VAL:C	1:B:505:PHE:HD2	2.19	0.45
1:A:279:HIS:HB2	1:A:314:MET:HB2	1.99	0.45
1:A:484:ARG:HG2	1:A:484:ARG:HH11	1.82	0.45
1:B:257:SER:O	1:B:258:ILE:C	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:PRO:HB2	1:B:373:ILE:CG1	2.46	0.45
1:B:412:LEU:C	1:B:414:TYR:N	2.71	0.45
1:B:465:ASN:HD21	1:B:467:CYS:H	1.61	0.45
1:B:501:GLN:O	1:B:503:ASN:N	2.47	0.45
1:A:538:VAL:HG22	1:A:539:SER:H	1.81	0.44
1:B:274:PHE:C	1:B:274:PHE:CD1	2.90	0.44
1:A:367:VAL:HG11	1:B:567:VAL:HG21	2.00	0.44
1:A:478:PHE:HB3	1:A:488:PHE:CE1	2.52	0.44
1:A:481:PRO:HB3	1:B:246:MET:O	2.17	0.44
1:A:522:ARG:CZ	1:A:522:ARG:CA	2.81	0.44
1:B:444:MET:HE1	1:B:533:ARG:HG2	1.97	0.44
1:A:333:VAL:O	1:A:333:VAL:CG1	2.65	0.44
1:B:312:CYS:HB3	1:B:415:LEU:HD22	2.00	0.44
1:B:486:LEU:HD23	1:B:487:GLU:H	1.79	0.44
1:B:569:ARG:O	1:B:573:LYS:HG3	2.17	0.44
1:A:256:PRO:HA	1:A:266:ARG:NH2	2.32	0.44
1:A:395:HIS:HA	1:A:401:ILE:HA	1.99	0.44
1:A:429:HIS:ND1	1:A:460:ARG:CD	2.80	0.44
1:A:475:TRP:CD1	1:A:475:TRP:N	2.85	0.44
1:B:315:LEU:HD12	1:B:315:LEU:HA	1.64	0.44
1:A:248:ASP:O	1:B:484:ARG:NH2	2.50	0.44
1:B:336:GLU:O	1:B:338:PHE:HD1	2.01	0.44
1:B:505:PHE:N	1:B:505:PHE:CD2	2.86	0.44
1:A:473:THR:HG22	1:A:475:TRP:CD1	2.53	0.44
1:A:281:LYS:HE3	1:A:418:ASP:OD1	2.17	0.44
1:A:523:ASN:O	1:A:525:ARG:N	2.51	0.44
1:A:290:ILE:HG22	1:A:342:LEU:HD13	1.97	0.43
1:A:514:LYS:HD2	1:A:515:ILE:CA	2.47	0.43
1:B:533:ARG:O	1:B:534:LEU:C	2.55	0.43
1:A:264:TYR:HH	1:A:277:PHE:HD2	1.65	0.43
1:A:412:LEU:HD23	1:A:412:LEU:N	2.33	0.43
1:B:526:ILE:HG13	1:B:527:LYS:H	1.81	0.43
1:A:243:VAL:HG23	1:B:564:MET:SD	2.59	0.43
1:A:425:MET:HE2	1:A:425:MET:CA	2.49	0.43
1:A:465:ASN:ND2	1:A:467:CYS:H	2.16	0.43
1:B:471:LEU:HD12	1:B:471:LEU:HA	1.84	0.43
1:B:484:ARG:H	1:B:484:ARG:HG2	1.59	0.43
1:A:447:GLY:O	1:A:540:ARG:NH2	2.52	0.43
1:B:294:ILE:HA	1:B:295:PRO:HD3	1.81	0.43
1:B:556:LEU:HD12	1:B:556:LEU:HA	1.69	0.43
1:B:472:GLU:HB3	1:B:494:ARG:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:ASP:C	1:B:531:VAL:N	2.70	0.43
1:B:543:ASP:OD2	1:B:546:LYS:HB2	2.18	0.43
1:B:515:ILE:C	1:B:515:ILE:HD12	2.38	0.43
1:B:533:ARG:NH2	1:B:533:ARG:CB	2.63	0.43
1:B:480:ASN:HB2	1:B:487:GLU:OE1	2.18	0.43
1:B:531:VAL:C	1:B:533:ARG:N	2.72	0.43
1:B:342:LEU:N	1:B:342:LEU:HD12	2.33	0.43
1:B:514:LYS:HD2	1:B:514:LYS:HA	1.77	0.43
1:A:287:ALA:HA	1:A:290:ILE:HD12	1.98	0.43
1:A:395:HIS:CD2	1:A:399:GLY:HA2	2.54	0.43
1:A:329:ILE:O	1:A:330:GLY:O	2.36	0.43
1:A:457:LYS:N	1:A:457:LYS:HE2	2.33	0.43
1:B:462:LEU:HD13	1:B:463:ILE:O	2.19	0.42
1:B:526:ILE:CG1	1:B:527:LYS:N	2.81	0.42
1:A:252:LEU:HD12	1:A:252:LEU:HA	1.62	0.42
1:A:457:LYS:HE2	1:A:457:LYS:H	1.85	0.42
1:B:414:TYR:OH	1:B:462:LEU:HD12	2.19	0.42
1:B:530:ILE:HG22	1:B:534:LEU:HD22	2.01	0.42
1:B:416:PRO:HG2	1:B:417:GLN:HE22	1.84	0.42
1:A:317:ARG:NH2	1:A:317:ARG:CB	2.73	0.42
1:A:493:HIS:O	1:A:494:ARG:HG2	2.18	0.42
1:A:397:ALA:O	1:A:534:LEU:HD23	2.18	0.42
1:A:527:LYS:O	1:A:530:ILE:N	2.45	0.42
1:B:543:ASP:O	1:B:547:GLN:HG3	2.19	0.42
1:A:326:PHE:HD2	1:A:326:PHE:O	2.03	0.42
1:A:484:ARG:HH22	1:B:248:ASP:HB2	1.84	0.42
1:B:436:MET:HE1	1:B:459:TYR:CE2	2.54	0.42
1:A:242:CYS:SG	1:A:244:ILE:HD11	2.59	0.42
1:A:242:CYS:HA	1:A:253:TYR:O	2.20	0.42
1:A:326:PHE:O	1:A:326:PHE:CD2	2.73	0.42
1:B:263:GLY:O	1:B:318:TYR:CB	2.68	0.42
1:B:280:LEU:HA	1:B:283:ARG:CD	2.50	0.42
1:A:339:ARG:HE	1:A:339:ARG:HB2	1.63	0.41
1:A:385:SER:O	1:A:387:LYS:N	2.53	0.41
1:A:388:SER:HA	1:A:389:PRO:HD3	1.85	0.41
1:B:530:ILE:H	1:B:530:ILE:HG13	1.60	0.41
1:A:290:ILE:HG13	1:B:482:TRP:HZ3	1.85	0.41
1:A:463:ILE:HD13	1:A:463:ILE:C	2.40	0.41
1:A:531:VAL:CG1	1:A:532:LYS:H	2.33	0.41
1:B:321:LEU:HD23	1:B:321:LEU:N	2.34	0.41
1:B:486:LEU:CD2	1:B:487:GLU:N	2.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.86	0.41
1:B:409:VAL:HG23	1:B:414:TYR:O	2.21	0.41
1:A:480:ASN:HB3	1:A:483:SER:OG	2.20	0.41
1:B:522:ARG:HA	1:B:522:ARG:HD2	1.85	0.41
1:B:416:PRO:C	1:B:418:ASP:H	2.24	0.41
1:B:516:SER:O	1:B:520:GLN:HB3	2.21	0.41
1:A:401:ILE:HD11	1:A:404:VAL:HG23	2.01	0.41
1:A:432:ASP:O	1:A:433:LEU:C	2.59	0.41
1:A:481:PRO:HG3	1:B:246:MET:CE	2.51	0.41
1:B:337:PRO:HG3	1:B:505:PHE:CZ	2.55	0.41
1:A:383:ILE:HG12	1:A:384:LEU:H	1.86	0.41
1:A:440:TYR:C	1:A:442:THR:N	2.74	0.41
1:B:245:SER:OG	1:B:248:ASP:OD2	2.39	0.41
1:B:344:PHE:CD1	1:B:344:PHE:N	2.89	0.41
1:B:377:TYR:OH	1:B:411:ALA:HB1	2.21	0.41
1:A:240:PHE:CD1	1:A:240:PHE:C	2.94	0.41
1:A:265:PRO:HD2	1:A:268:MET:CG	2.48	0.41
1:A:383:ILE:HG12	1:A:384:LEU:N	2.36	0.41
1:A:513:LEU:O	1:A:514:LYS:HB3	2.20	0.41
1:B:444:MET:CE	1:B:444:MET:CA	2.98	0.41
1:B:486:LEU:CD2	1:B:486:LEU:C	2.89	0.41
1:A:250:ILE:HG12	1:A:250:ILE:H	1.74	0.41
1:A:254:THR:HG21	1:A:258:ILE:HB	2.03	0.41
1:A:425:MET:CE	1:A:428:TYR:HE1	2.34	0.41
1:A:444:MET:CE	1:A:444:MET:HA	2.50	0.41
1:A:476:THR:OG1	1:A:490:VAL:HG13	2.21	0.41
1:B:236:LYS:O	1:B:236:LYS:HG2	2.21	0.41
1:B:243:VAL:HA	1:B:366:LEU:O	2.20	0.41
1:A:425:MET:HA	1:A:425:MET:CE	2.51	0.41
1:B:385:SER:O	1:B:387:LYS:N	2.54	0.41
1:A:377:TYR:HA	1:A:382:GLU:OE1	2.21	0.40
1:A:413:GLY:HA2	1:A:505:PHE:CE1	2.56	0.40
1:B:406:SER:C	1:B:408:ALA:N	2.75	0.40
1:B:406:SER:O	1:B:408:ALA:N	2.54	0.40
1:A:321:LEU:CG	1:A:322:LYS:H	2.34	0.40
1:A:459:TYR:HE1	1:A:473:THR:HG1	1.67	0.40
1:A:485:LYS:HE2	1:A:537:THR:CA	2.51	0.40
1:A:510:THR:O	1:A:511:CYS:HB2	2.20	0.40
1:B:257:SER:O	1:B:259:THR:N	2.55	0.40
1:B:349:GLU:O	1:B:351:ALA:N	2.54	0.40
1:A:384:LEU:HD21	1:A:494:ARG:HH11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ALA:C	1:A:521:SER:N	2.75	0.40
1:B:528:GLU:O	1:B:531:VAL:HB	2.21	0.40
1:B:502:CYS:O	1:B:503:ASN:O	2.38	0.40
1:B:548:GLU:O	1:B:551:ARG:N	2.51	0.40
1:B:562:THR:O	1:B:563:LEU:C	2.59	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	312/368 (85%)	255 (82%)	41 (13%)	16 (5%)	2 13
1	B	313/368 (85%)	233 (74%)	52 (17%)	28 (9%)	1 3
All	All	625/736 (85%)	488 (78%)	93 (15%)	44 (7%)	1 7

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	GLY
1	A	380	PRO
1	A	426	ASP
1	B	237	GLU
1	B	266	ARG
1	B	484	ARG
1	B	502	CYS
1	B	507	ALA
1	B	534	LEU
1	A	498	GLY
1	A	516	SER
1	B	274	PHE
1	B	281	LYS

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Mol	Chain	Res	Type
1	B	291	THR
1	B	361	GLY
1	B	386	GLN
1	B	407	ALA
1	B	413	GLY
1	B	424	ILE
1	B	452	ALA
1	B	503	ASN
1	B	532	LYS
1	B	553	CYS
1	A	266	ARG
1	A	386	GLN
1	A	458	PRO
1	A	465	ASN
1	A	511	CYS
1	A	537	THR
1	B	260	ASP
1	B	517	GLU
1	B	570	ALA
1	B	571	ASP
1	A	319	ARG
1	B	536	GLU
1	B	284	ALA
1	B	350	GLU
1	A	430	HIS
1	B	258	ILE
1	A	293	GLY
1	B	509	PRO
1	A	333	VAL
1	A	515	ILE
1	B	458	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	278/325 (86%)	227 (82%)	51 (18%)	1 8
1	B	284/325 (87%)	246 (87%)	38 (13%)	4 17
All	All	562/650 (86%)	473 (84%)	89 (16%)	2 11

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	GLU
1	A	245	SER
1	A	250	ILE
1	A	251	VAL
1	A	252	LEU
1	A	258	ILE
1	A	260	ASP
1	A	268	MET
1	A	290	ILE
1	A	291	THR
1	A	313	VAL
1	A	317	ARG
1	A	319	ARG
1	A	326	PHE
1	A	329	ILE
1	A	331	ARG
1	A	345	ARG
1	A	349	GLU
1	A	352	ARG
1	A	371	THR
1	A	390	LYS
1	A	401	ILE
1	A	406	SER
1	A	417	GLN
1	A	420	ILE
1	A	425	MET
1	A	436	MET
1	A	437	LYS
1	A	439	THR
1	A	457	LYS
1	A	458	PRO
1	A	463	ILE

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Mol	Chain	Res	Type
1	A	464	GLN
1	A	465	ASN
1	A	471	LEU
1	A	485	LYS
1	A	487	GLU
1	A	490	VAL
1	A	514	LYS
1	A	517	GLU
1	A	522	ARG
1	A	524	THR
1	A	525	ARG
1	A	526	ILE
1	A	528	GLU
1	A	529	ASP
1	A	532	LYS
1	A	534	LEU
1	A	537	THR
1	A	547	GLN
1	A	556	LEU
1	B	254	THR
1	B	257	SER
1	B	258	ILE
1	B	268	MET
1	B	278	VAL
1	B	281	LYS
1	B	283	ARG
1	B	314	MET
1	B	315	LEU
1	B	321	LEU
1	B	363	ASN
1	B	365	LEU
1	B	366	LEU
1	B	373	ILE
1	B	378	LYS
1	B	386	GLN
1	B	400	ILE
1	B	410	SER
1	B	417	GLN
1	B	457	LYS
1	B	458	PRO
1	B	464	GLN
1	B	465	ASN

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Mol	Chain	Res	Type
1	B	469	VAL
1	B	471	LEU
1	B	486	LEU
1	B	505	PHE
1	B	506	GLU
1	B	513	LEU
1	B	520	GLN
1	B	522	ARG
1	B	533	ARG
1	B	536	GLU
1	B	539	SER
1	B	540	ARG
1	B	542	SER
1	B	559	PHE
1	B	573	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	HIS
1	A	360	ASN
1	A	386	GLN
1	A	395	HIS
1	A	417	GLN
1	A	465	ASN
1	A	493	HIS
1	A	503	ASN
1	A	523	ASN
1	B	279	HIS
1	B	363	ASN
1	B	395	HIS
1	B	417	GLN
1	B	429	HIS
1	B	464	GLN
1	B	465	ASN
1	B	501	GLN
1	B	520	GLN
1	B	523	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	318/368 (86%)	-0.43	12 (3%) 40 25	30, 87, 193, 201	0
1	B	319/368 (86%)	-0.37	5 (1%) 72 59	27, 89, 188, 201	0
All	All	637/736 (86%)	-0.40	17 (2%) 54 38	27, 89, 189, 201	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	GLY	4.5
1	A	321	LEU	4.4
1	A	323	SER	4.0
1	A	520	GLN	3.8
1	B	322	LYS	3.3
1	A	320	GLY	3.2
1	A	326	PHE	3.0
1	A	547	GLN	2.8
1	A	325	GLY	2.6
1	B	496	PHE	2.6
1	B	320	GLY	2.3
1	A	386	GLN	2.3
1	B	321	LEU	2.2
1	B	574	LEU	2.1
1	A	324	GLY	2.1
1	A	331	ARG	2.1
1	A	387	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.