Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2021 – 02:03 pm BST

PDB ID	:	6YRA
Title	:	Crystal structure of ATP-dependent caprolactamase from Pseudomonas jessenii
Authors	:	Rozeboom, H.J.; Janssen, D.B.
Deposited on	:	2020-04-20
Resolution	:	4.00 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 ①) were used in the production of this report:

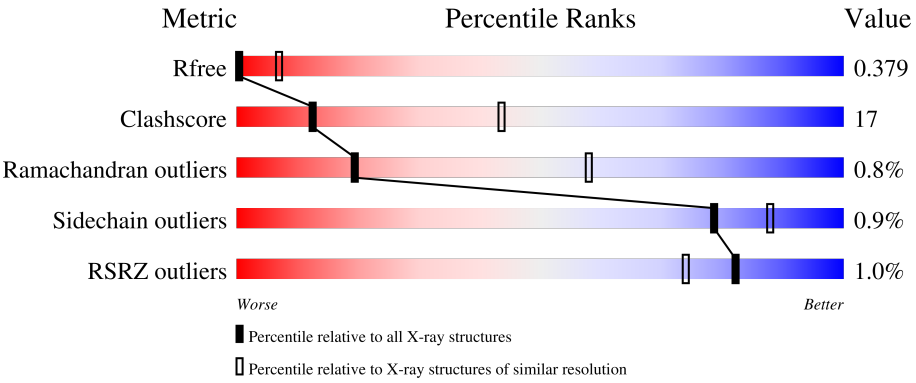
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 4.00 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))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	B	581	60% 37%
1	D	581	62% 36%
2	A	696	68% 31%
2	C	696	66% 33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19265 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 Hydantoinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	579	Total	C	N	O	S	0	0	0
			4385	2750	769	838	28			
1	D	579	Total	C	N	O	S	0	0	0
			4378	2744	769	837	28			

- Molecule 2 is a protein called 5-oxoprolinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	691	Total	C	N	O	S	0	0	0
			5250	3285	940	998	27			
2	C	691	Total	C	N	O	S	0	0	0
			5250	3285	940	998	27			

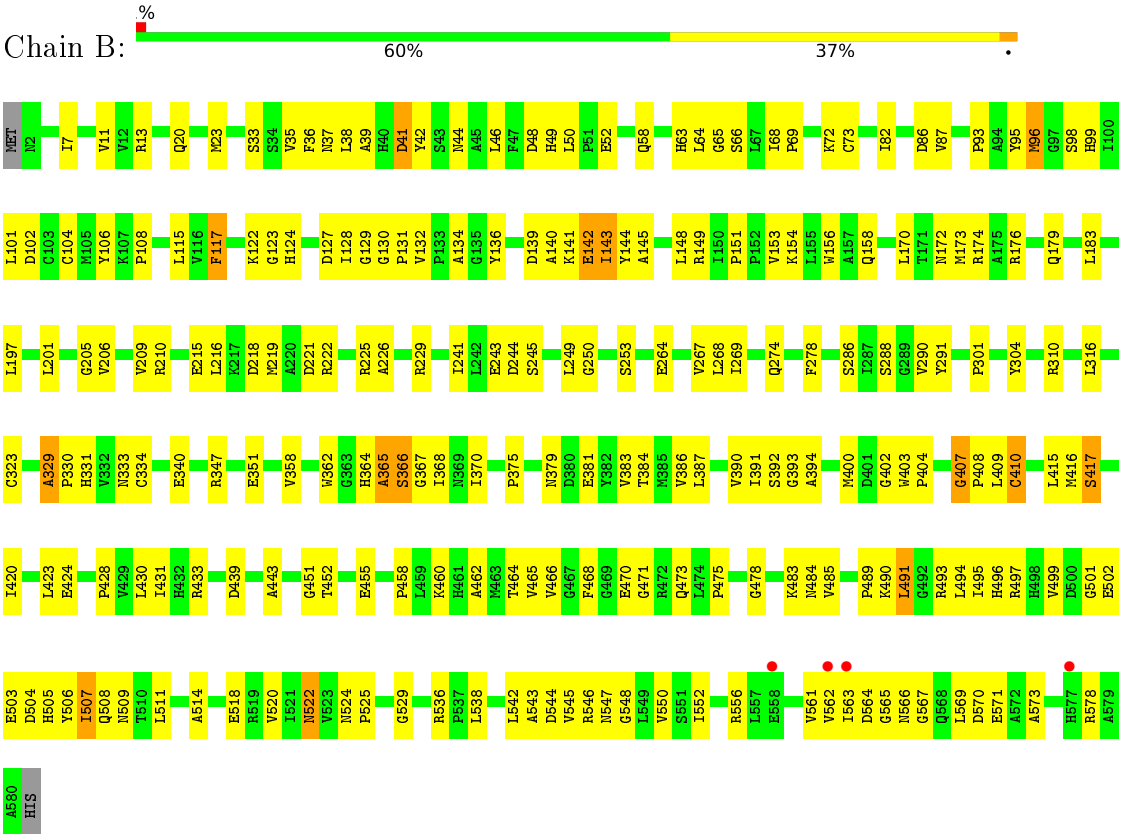
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

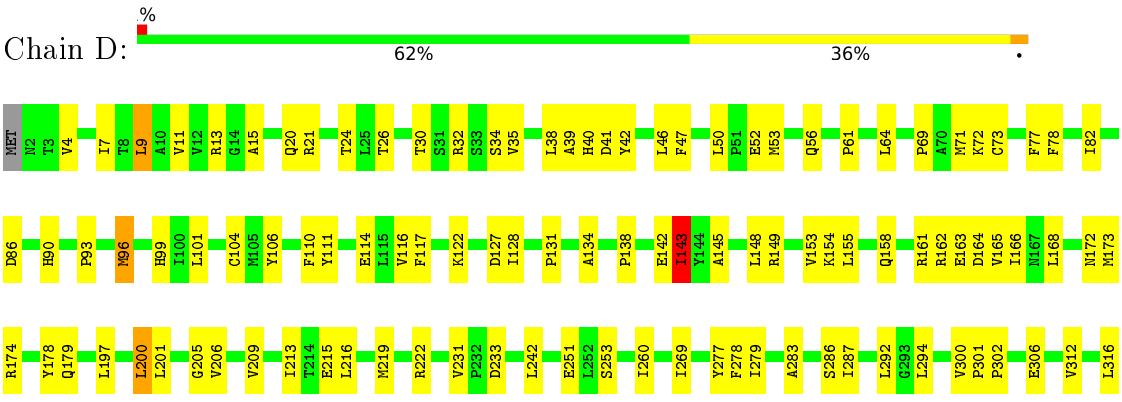
3 Residue-property plots (i)

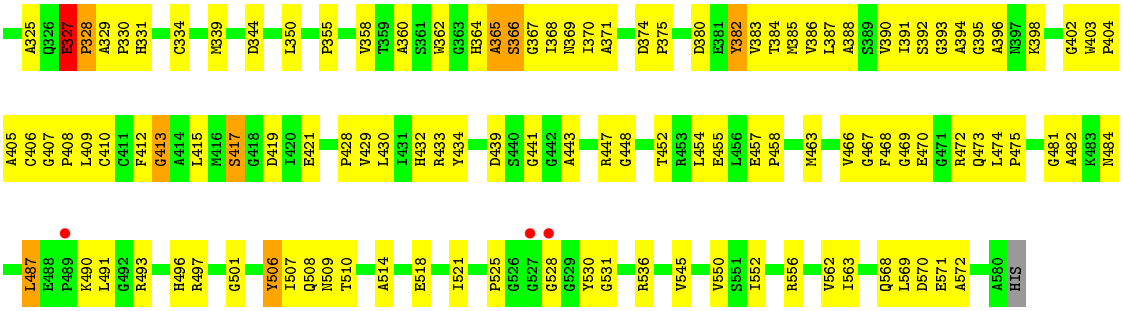
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

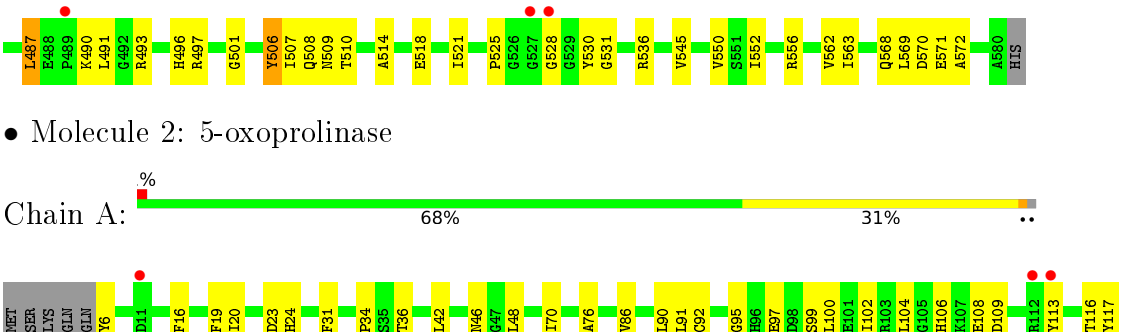
- Molecule 1: Hydantoinase



- Molecule 1: Hydantoinase





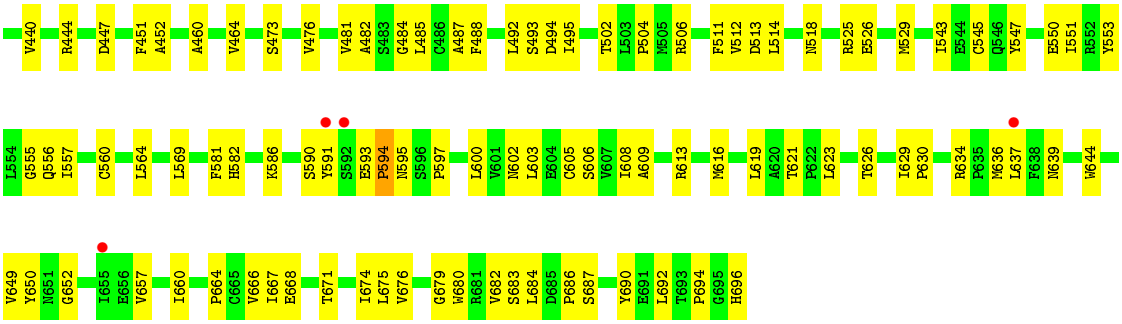


- Molecule 2: 5-oxoprolinase

Chain A:

- Molecule 2: 5-oxoprolinase

Chain C:


V440 R444 D447 F451 A452 A460 V464 S473 V476 V481 A482 S483 G484 L485 C486 A487 F488 L492 S493 D494 I495 T502 L503 P504 M505 R506 F511 V512 D513 L514 N518 R525 E526 M529 I543 E544 C545 Q546 Y547 E550 I551 R552 Y553
L554 G555 Q556 I557 C560 L564 L569 F581 H582 K586 S590 Y591 S592 E593 P594 N595 S596 P597 L600 V601 N602 L603 E604 C605 S606 V607 I608 A609 R613 M616 L619 A620 T621 P622 L623 T626 I629 P630 R634 P635 M636 L637 F638 N639 W644
V649 Y650 M651 G652 I655 E656 V657 I660 P664 C665 V666 I667 E668 T671 I674 L675 V676 G679 W680 R681 V682 S683 L684 D685 P686 S687 Y690 E691 L692 T693 P694 G695 H696

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	195.38Å 167.37Å 87.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.84 – 4.00 47.11 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.84-4.00) 98.5 (47.11-4.00)	Depositor EDS
R_{merge}	0.63	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.239 , 0.381 0.240 , 0.379	Depositor DCC
R_{free} test set	1156 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å^2)	65.2	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 131.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	19265	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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

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

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	B	0.33	0/4481	0.65	4/6096 (0.1%)
1	D	0.32	0/4473	0.67	6/6085 (0.1%)
2	A	0.31	0/5352	0.62	1/7269 (0.0%)
2	C	0.30	0/5352	0.60	1/7269 (0.0%)
All	All	0.32	0/19658	0.63	12/26719 (0.0%)

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	B	0	6
1	D	0	4
2	A	0	1
2	C	0	1
All	All	0	12

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	41	ASP	CB-CG-OD1	7.44	125.00	118.30
1	B	41	ASP	CB-CG-OD1	7.41	124.97	118.30
1	B	64	LEU	CA-CB-CG	7.32	132.15	115.30
1	B	41	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	D	143	ILE	CG1-CB-CG2	6.37	125.42	111.40
1	D	514	ALA	C-N-CA	5.91	136.47	121.70
2	C	428	LEU	CA-CB-CG	-5.70	102.18	115.30
1	D	487	LEU	C-N-CA	5.60	135.70	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	334	LEU	CA-CB-CG	5.57	128.11	115.30
1	B	491	LEU	CA-CB-CG	5.42	127.77	115.30
1	D	200	LEU	CA-CB-CG	-5.35	103.00	115.30
1	D	143	ILE	N-CA-C	5.27	125.24	111.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	255	ALA	Peptide
1	B	142	GLU	Peptide
1	B	301	PRO	Peptide
1	B	329	ALA	Peptide
1	B	365	ALA	Peptide
1	B	407	GLY	Peptide
1	B	410	CYS	Peptide
2	C	613	ARG	Peptide
1	D	142	GLU	Peptide
1	D	327	GLU	Peptide
1	D	366	SER	Peptide
1	D	410	CYS	Peptide

5.2 Too-close contacts (i)

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	B	4385	0	4276	177	0
1	D	4378	0	4269	180	0
2	A	5250	0	5201	162	0
2	C	5250	0	5201	154	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
All	All	19265	0	18947	641	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 17.

All (641) 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:390:VAL:HG12	1:B:391:ILE:HG13	1.51	0.93
1:B:490:LYS:HE3	1:B:522:ASN:HB2	1.50	0.91
1:D:13:ARG:HE	1:D:216:LEU:HD22	1.35	0.90
2:A:547:TYR:HB2	2:A:564:LEU:HB3	1.58	0.86
1:D:484:ASN:HB3	1:D:487:LEU:HD12	1.59	0.85
1:B:226:ALA:HA	1:B:229:ARG:HD2	1.58	0.84
1:B:142:GLU:O	1:B:144:TYR:N	2.11	0.84
2:A:352:VAL:HG11	2:A:425:ILE:HG23	1.60	0.84
2:C:547:TYR:HB2	2:C:564:LEU:HB3	1.59	0.83
2:A:100:LEU:HD23	2:A:129:ARG:HH12	1.44	0.82
1:D:552:ILE:HG12	1:D:563:ILE:HD11	1.62	0.81
2:C:55:LEU:HD22	2:C:62:ILE:HB	1.61	0.80
1:D:408:PRO:HD3	1:D:415:LEU:H	1.45	0.80
1:D:34:SER:HB3	2:C:557:ILE:HG13	1.65	0.79
2:C:88:VAL:HG22	2:C:165:ALA:HB3	1.65	0.79
1:D:371:ALA:HA	1:D:463:MET:O	1.83	0.78
1:B:390:VAL:HG21	1:B:417:SER:HB2	1.66	0.77
1:D:143:ILE:HD12	1:D:331:HIS:HB3	1.66	0.77
2:C:244:PRO:O	2:C:246:ARG:NH1	2.19	0.76
1:B:99:HIS:CE1	1:B:124:HIS:CE1	2.72	0.76
2:A:342:ALA:HB3	2:A:373:PRO:HG2	1.69	0.75
2:A:330:GLN:OE1	2:A:444:ARG:NH1	2.18	0.75
1:B:49:HIS:ND1	1:B:115:LEU:O	2.20	0.74
2:C:387:ASP:HA	2:C:397:LEU:HB2	1.68	0.74
1:B:206:VAL:HG13	1:B:210:ARG:HD3	1.70	0.73
1:D:215:GLU:OE2	1:D:222:ARG:NH2	2.21	0.73
2:A:437:ILE:HD12	2:A:471:ILE:HG13	1.72	0.72
1:B:536:ARG:NH2	1:B:544:ASP:OD2	2.21	0.72
1:B:400:MET:HG3	1:B:402:GLY:H	1.55	0.72
1:D:430:LEU:N	1:D:457:GLU:O	2.17	0.72
1:D:69:PRO:HA	1:D:72:LYS:HB3	1.72	0.71
1:D:393:GLY:HA2	1:D:404:PRO:HA	1.72	0.71
1:D:15:ALA:HB1	1:D:200:LEU:HD13	1.71	0.71
2:A:407:ARG:HA	2:A:411:ALA:HB3	1.72	0.71
1:D:35:VAL:HG22	2:C:557:ILE:HD11	1.73	0.70
1:D:327:GLU:O	1:D:329:ALA:N	2.22	0.70
1:D:392:SER:HB3	1:D:409:LEU:HD13	1.74	0.70
2:C:634:ARG:NH2	2:C:668:GLU:OE2	2.24	0.70
2:A:552:ARG:NH1	2:A:556:GLN:O	2.25	0.70
2:C:582:HIS:NE2	2:C:597:PRO:HG3	2.06	0.70
1:D:369:ASN:O	1:D:385:MET:HB2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:504:PRO:HA	2:C:600:LEU:O	1.92	0.70
1:D:368:ILE:HB	1:D:468:PHE:CD2	2.28	0.69
2:C:130:ARG:HD2	2:C:131:PRO:HD2	1.73	0.68
1:D:355:PRO:HA	1:D:358:VAL:HG23	1.75	0.68
2:C:679:GLY:HA2	2:C:696:HIS:HB2	1.75	0.68
2:C:293:THR:O	2:C:303:ILE:HA	1.93	0.68
1:D:366:SER:O	1:D:368:ILE:N	2.23	0.67
2:C:73:THR:HG21	2:C:228:TYR:HE2	1.59	0.67
1:B:145:ALA:HA	1:D:131:PRO:HG3	1.77	0.67
2:A:658:GLY:HA3	2:A:684:LEU:H	1.60	0.67
1:D:104:CYS:HB3	1:D:122:LYS:HG3	1.75	0.67
1:D:134:ALA:HB2	1:D:370:ILE:HG21	1.76	0.67
1:D:344:ASP:OD2	1:D:364:HIS:NE2	2.27	0.67
2:C:590:SER:OG	2:C:593:GLU:OE2	2.13	0.66
2:A:252:GLY:O	2:A:493:SER:OG	2.11	0.66
1:B:490:LYS:HD3	1:B:507:ILE:HD13	1.78	0.66
1:D:269:ILE:HG13	1:D:316:LEU:HD23	1.77	0.66
1:B:392:SER:HB3	1:B:409:LEU:HD13	1.76	0.66
2:A:495:ILE:HB	2:A:609:ALA:HB3	1.77	0.66
2:A:136:ILE:HG22	2:A:142:GLU:HA	1.77	0.66
2:A:76:ALA:HB1	2:A:221:LEU:HD13	1.78	0.65
1:D:395:GLY:HA2	1:D:528:GLY:H	1.62	0.65
2:C:621:THR:HG22	2:C:623:LEU:H	1.61	0.65
2:C:351:GLN:O	2:C:354:PRO:HD3	1.96	0.65
1:B:368:ILE:HD13	1:B:370:ILE:HD11	1.78	0.65
1:B:465:VAL:HG22	1:B:511:LEU:HD22	1.79	0.65
1:D:466:VAL:HG23	1:D:509:ASN:HB3	1.78	0.65
2:C:103:ARG:NH2	2:C:108:GLU:OE2	2.30	0.64
1:B:170:LEU:HG	1:B:176:ARG:HD2	1.79	0.64
1:B:132:VAL:HG22	1:B:511:LEU:HD11	1.78	0.64
1:D:278:PHE:CD1	1:D:334:CYS:HB2	2.31	0.64
2:C:476:VAL:HB	2:C:692:LEU:HB2	1.80	0.64
2:A:453:LEU:HD12	2:A:468:ALA:HB2	1.78	0.64
1:B:41:ASP:HB3	1:B:124:HIS:HB2	1.78	0.63
1:B:33:SER:HA	1:B:37:ASN:HB2	1.80	0.63
2:A:310:ARG:O	2:A:444:ARG:NH2	2.31	0.63
2:C:98:ASP:OD1	2:C:126:ARG:NH1	2.30	0.63
2:C:142:GLU:OE2	2:C:179:HIS:NE2	2.28	0.63
1:B:143:ILE:HG22	1:B:331:HIS:HB2	1.81	0.63
2:A:374:THR:N	2:A:377:ASP:OD2	2.32	0.63
1:D:368:ILE:HD12	1:D:468:PHE:CZ	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ALA:O	1:B:331:HIS:N	2.30	0.63
2:C:60:ALA:HA	2:C:63:ILE:HD12	1.81	0.63
2:C:291:VAL:HG12	2:C:452:ALA:HB3	1.80	0.63
2:C:619:LEU:HB2	2:C:657:VAL:HG21	1.79	0.63
2:C:629:ILE:HG22	2:C:650:TYR:HB3	1.81	0.62
1:B:499:VAL:O	1:B:501:GLY:N	2.32	0.62
1:B:104:CYS:SG	1:B:106:TYR:OH	2.55	0.62
1:D:375:PRO:HB3	1:D:428:PRO:HB3	1.82	0.62
1:D:138:PRO:HA	1:D:278:PHE:HE2	1.64	0.62
1:D:73:CYS:O	1:D:77:PHE:HB2	1.99	0.62
1:D:466:VAL:CG2	1:D:509:ASN:HB3	2.29	0.62
1:D:325:ALA:HB3	1:D:330:PRO:HA	1.82	0.62
1:B:221:ASP:HB2	1:B:310:ARG:HD2	1.82	0.61
2:A:140:GLY:O	2:A:176:ASN:ND2	2.27	0.61
1:D:556:ARG:HG2	1:D:562:VAL:HA	1.81	0.61
2:C:300:SER:HA	2:C:337:GLY:H	1.65	0.61
1:D:364:HIS:O	1:D:366:SER:N	2.33	0.61
2:A:521:LEU:HB3	2:A:547:TYR:CE2	2.36	0.60
1:B:244:ASP:HB2	1:B:470:GLU:H	1.66	0.60
2:A:507:LEU:HA	2:A:512:VAL:HG22	1.84	0.60
1:D:86:ASP:HB3	1:D:158:GLN:H	1.66	0.60
1:D:233:ASP:HA	1:D:260:ILE:O	2.00	0.60
2:A:543:ILE:HG22	2:A:609:ALA:HA	1.82	0.60
2:A:301:PHE:CZ	2:A:337:GLY:HA2	2.37	0.60
1:D:38:LEU:HD12	1:D:386:VAL:HG22	1.83	0.60
2:A:629:ILE:HG21	2:A:655:ILE:HG12	1.84	0.59
1:D:215:GLU:O	1:D:219:MET:HG3	2.02	0.59
2:C:586:LYS:HE3	2:C:591:TYR:O	2.03	0.59
1:B:99:HIS:CE1	1:B:101:LEU:HB2	2.37	0.59
2:C:342:ALA:HA	2:C:352:VAL:HG22	1.84	0.59
1:B:23:MET:HE2	1:B:44:ASN:HB3	1.83	0.59
1:B:98:SER:HB2	1:B:102:ASP:HB2	1.83	0.59
1:D:20:GLN:O	1:D:24:THR:OG1	2.20	0.59
2:A:629:ILE:O	2:A:631:ALA:N	2.35	0.59
2:C:512:VAL:O	2:C:514:LEU:N	2.35	0.59
2:C:495:ILE:O	2:C:608:ILE:HA	2.02	0.59
1:B:99:HIS:NE2	1:B:124:HIS:HE1	1.98	0.59
2:A:501:THR:HG22	2:A:524:LEU:HD11	1.85	0.59
2:C:130:ARG:HG2	2:C:154:ALA:CB	2.32	0.59
1:D:474:LEU:HD13	1:D:525:PRO:HB3	1.85	0.58
1:B:506:TYR:O	1:B:508:GLN:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:289:ASP:OD1	2:C:307:LYS:NZ	2.29	0.58
1:B:87:VAL:HG22	1:B:156:TRP:H	1.67	0.58
2:A:19:PHE:HB3	2:A:31:PHE:HB2	1.85	0.58
2:A:290:ASN:HB3	2:A:451:PHE:CE2	2.38	0.58
2:A:380:LEU:HD21	2:A:399:ARG:HA	1.86	0.58
1:B:443:ALA:HB3	1:B:484:ASN:H	1.69	0.58
2:A:20:ILE:HG21	2:A:487:ALA:HB1	1.86	0.57
1:D:134:ALA:CB	1:D:370:ILE:HG21	2.33	0.57
2:C:395:ILE:HG22	2:C:397:LEU:HG	1.87	0.57
1:D:391:ILE:HD11	2:C:102:ILE:HG23	1.85	0.57
2:C:58:THR:HG22	2:C:60:ALA:H	1.69	0.57
1:B:423:LEU:HB2	1:B:431:ILE:HD11	1.85	0.57
1:D:173:MET:SD	1:D:179:GLN:NE2	2.78	0.57
1:B:130:GLY:O	1:B:174:ARG:NH2	2.37	0.57
2:C:482:ALA:HB3	2:C:671:THR:HG21	1.86	0.57
1:D:242:LEU:HA	1:D:470:GLU:OE2	2.03	0.57
1:D:392:SER:HB2	1:D:525:PRO:O	2.04	0.57
1:D:432:HIS:ND1	1:D:457:GLU:OE1	2.38	0.57
2:C:28:VAL:HG21	2:C:481:VAL:HG21	1.85	0.57
2:A:306:SER:O	2:A:312:ASN:ND2	2.37	0.57
1:D:138:PRO:HA	1:D:278:PHE:CE2	2.39	0.57
1:D:216:LEU:HD23	1:D:219:MET:HE1	1.87	0.56
1:B:386:VAL:HG11	1:B:415:LEU:HD11	1.87	0.56
1:D:368:ILE:HD12	1:D:468:PHE:CE1	2.40	0.56
1:D:368:ILE:HG23	1:D:466:VAL:HG12	1.87	0.56
1:D:394:ALA:N	1:D:403:TRP:O	2.36	0.56
2:C:252:GLY:O	2:C:493:SER:OG	2.21	0.56
1:B:127:ASP:OD1	1:B:128:ILE:N	2.38	0.56
2:C:20:ILE:HG12	2:C:487:ALA:HB1	1.87	0.56
2:A:86:VAL:HG13	2:A:164:GLN:HB2	1.87	0.56
1:D:278:PHE:HD1	1:D:334:CYS:HB2	1.70	0.56
1:D:294:LEU:HD11	1:D:312:VAL:HG21	1.86	0.56
1:B:546:ARG:NH2	1:B:567:GLY:O	2.38	0.56
1:D:473:GLN:O	1:D:475:PRO:HD3	2.06	0.56
2:A:86:VAL:HG21	2:A:223:PRO:HG2	1.87	0.56
2:C:374:THR:N	2:C:377:ASP:OD2	2.39	0.56
2:C:484:GLY:O	2:C:487:ALA:HB3	2.06	0.56
2:A:16:PHE:HA	2:A:34:PRO:HG3	1.87	0.56
1:D:161:ARG:HB3	1:D:166:ILE:HD12	1.88	0.56
2:C:494:ASP:HB3	2:C:609:ALA:O	2.05	0.56
2:A:124:VAL:O	2:A:129:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:ALA:HB3	1:D:396:ALA:N	2.20	0.56
1:B:140:ALA:O	1:B:143:ILE:HD13	2.05	0.55
1:B:400:MET:HE2	2:A:116:THR:HG22	1.87	0.55
2:A:91:LEU:HB2	2:A:168:ILE:HG12	1.87	0.55
1:D:362:TRP:CZ3	1:D:406:CYS:HB2	2.40	0.55
1:B:424:GLU:OE2	2:A:135:ARG:NH2	2.37	0.55
2:A:121:HIS:O	2:A:322:TYR:OH	2.16	0.55
1:D:61:PRO:O	1:D:64:LEU:HG	2.07	0.55
1:D:53:MET:SD	1:D:56:GLN:HB2	2.46	0.55
1:D:432:HIS:O	2:C:135:ARG:NH1	2.35	0.55
2:C:6:TYR:HD2	2:C:23:ASP:HB2	1.71	0.55
1:B:420:ILE:HG23	1:B:431:ILE:HD12	1.88	0.55
1:D:386:VAL:O	1:D:390:VAL:HG23	2.06	0.55
1:D:143:ILE:HG21	1:D:331:HIS:HB2	1.89	0.55
2:C:667:ILE:HB	2:C:674:ILE:HB	1.88	0.55
1:B:392:SER:H	1:B:409:LEU:HD21	1.70	0.55
1:D:360:ALA:HB3	1:D:396:ALA:H	1.72	0.55
1:B:101:LEU:HD23	1:B:128:ILE:HB	1.89	0.55
1:B:466:VAL:HG12	1:B:468:PHE:H	1.72	0.55
2:A:340:SER:HA	2:A:356:SER:HA	1.87	0.55
2:A:626:THR:HG22	2:A:656:GLU:HB3	1.88	0.55
1:D:430:LEU:HD21	2:C:137:ILE:HG22	1.87	0.55
2:C:32:LYS:O	2:C:50:GLN:NE2	2.40	0.55
2:A:454:ILE:HG12	2:A:477:LEU:HB2	1.88	0.54
1:D:117:PHE:HE2	1:D:201:LEU:HD21	1.71	0.54
2:A:579:GLU:OE2	2:A:583:GLN:NE2	2.40	0.54
1:D:50:LEU:O	1:D:52:GLU:N	2.41	0.54
2:C:136:ILE:HG22	2:C:142:GLU:HA	1.89	0.54
1:D:301:PRO:HD2	1:D:302:PRO:HD3	1.89	0.54
1:D:391:ILE:HA	1:D:405:ALA:HA	1.88	0.54
1:B:87:VAL:HG13	1:B:156:TRP:HB2	1.89	0.54
2:C:664:PRO:HA	2:C:676:VAL:O	2.08	0.54
1:B:68:ILE:HD12	1:B:291:TYR:HE2	1.71	0.54
1:B:86:ASP:OD2	1:B:154:LYS:NZ	2.31	0.54
1:B:104:CYS:HB3	1:B:122:LYS:HG2	1.89	0.54
2:A:246:ARG:HB3	2:A:254:LEU:HB3	1.89	0.54
2:C:117:TYR:C	2:C:119:PRO:HD3	2.28	0.54
1:B:36:PHE:O	1:B:383:VAL:HG23	2.08	0.54
1:B:104:CYS:CB	1:B:122:LYS:HG2	2.38	0.54
2:A:320:LEU:O	2:A:321:ARG:HG2	2.07	0.54
2:C:352:VAL:HG11	2:C:425:ILE:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:494:ASP:HB2	2:A:609:ALA:O	2.07	0.54
2:A:658:GLY:CA	2:A:684:LEU:H	2.21	0.54
1:B:483:LYS:HB3	1:B:485:VAL:HG23	1.90	0.54
1:D:32:ARG:HG2	2:C:556:GLN:HA	1.88	0.54
2:C:560:CYS:HB2	2:C:581:PHE:HE1	1.73	0.54
1:B:65:GLY:N	1:B:288:SER:OG	2.41	0.53
1:B:407:GLY:HA3	1:B:415:LEU:HB3	1.90	0.53
2:A:106:HIS:CE1	2:A:108:GLU:HB2	2.43	0.53
2:C:423:VAL:HG11	2:C:639:ASN:HB2	1.89	0.53
2:C:315:LYS:NZ	2:C:550:GLU:OE2	2.42	0.53
2:C:365:CYS:SG	2:C:380:LEU:HD23	2.49	0.53
1:B:538:LEU:HD21	1:B:569:LEU:HD11	1.90	0.53
1:D:300:VAL:N	1:D:301:PRO:HD3	2.23	0.53
2:C:660:ILE:HA	2:C:683:SER:HB3	1.90	0.53
1:B:347:ARG:NH1	1:B:351:GLU:OE1	2.42	0.53
2:A:407:ARG:O	2:A:412:GLU:N	2.22	0.53
2:A:551:ILE:HD11	2:A:581:PHE:HB2	1.90	0.53
1:D:206:VAL:HA	1:D:209:VAL:HB	1.91	0.53
1:D:374:ASP:HB2	1:D:380:ASP:OD1	2.08	0.53
2:A:170:PHE:O	2:A:211:ARG:NH2	2.41	0.53
2:A:334:LEU:HD11	2:A:436:GLY:CA	2.39	0.53
2:A:585:HIS:ND1	2:A:593:GLU:HG3	2.24	0.53
2:A:386:ALA:O	2:A:399:ARG:NE	2.42	0.53
2:A:499:GLN:HG2	2:A:527:ARG:HB2	1.91	0.53
1:D:39:ALA:O	1:D:415:LEU:HD12	2.08	0.53
2:A:192:PRO:HB2	2:A:194:VAL:HG23	1.91	0.52
2:A:374:THR:H	2:A:377:ASP:HB2	1.74	0.52
2:A:596:SER:OG	2:A:596:SER:O	2.22	0.52
2:A:634:ARG:NH2	2:A:668:GLU:OE2	2.23	0.52
1:D:4:VAL:CG1	1:D:9:LEU:HG	2.39	0.52
2:C:316:ASP:HB2	2:C:323:ARG:HH21	1.74	0.52
1:D:419:ASP:OD2	2:C:207:ARG:HA	2.10	0.52
1:B:144:TYR:HE2	1:D:174:ARG:HD2	1.73	0.52
2:C:174:VAL:HG11	2:C:205:GLN:O	2.10	0.52
2:A:126:ARG:HA	2:A:129:ARG:HB2	1.91	0.52
1:D:417:SER:N	2:C:104:LEU:O	2.39	0.52
2:C:294:VAL:HA	2:C:303:ILE:HG22	1.91	0.52
2:A:301:PHE:O	2:A:333:THR:HA	2.09	0.52
2:A:70:ILE:HG12	2:A:254:LEU:HD13	1.92	0.52
2:C:55:LEU:HB2	2:C:62:ILE:HD12	1.92	0.52
1:B:35:VAL:HG23	1:B:36:PHE:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:GLY:HA3	1:B:507:ILE:CD1	2.41	0.51
2:A:138:SER:HA	2:A:172:TRP:CE2	2.46	0.51
1:D:421:GLU:OE2	2:C:211:ARG:NH2	2.37	0.51
1:B:38:LEU:HD12	1:B:386:VAL:HG22	1.92	0.51
2:A:248:PHE:CZ	2:A:274:SER:HB3	2.46	0.51
1:D:370:ILE:HG23	1:D:384:THR:HA	1.93	0.51
2:C:345:ASP:HB3	2:C:347:PHE:HD1	1.76	0.51
2:A:135:ARG:CZ	2:A:171:VAL:HG11	2.40	0.51
1:D:402:GLY:HA3	1:D:448:GLY:HA2	1.92	0.51
1:B:368:ILE:HB	1:B:468:PHE:CD2	2.46	0.51
2:A:574:LEU:O	2:A:577:LEU:HB3	2.11	0.51
1:D:24:THR:HG22	1:D:42:TYR:HE2	1.76	0.51
2:C:543:ILE:HG22	2:C:609:ALA:HA	1.92	0.51
2:A:263:ARG:HE	2:A:266:ASN:HB2	1.76	0.51
1:B:104:CYS:SG	1:B:122:LYS:HE3	2.51	0.51
2:A:582:HIS:CE1	2:A:597:PRO:HB3	2.46	0.51
1:D:110:PHE:HA	1:D:114:GLU:O	2.10	0.51
2:C:514:LEU:O	2:C:518:ASN:HB2	2.11	0.51
1:D:366:SER:O	1:D:468:PHE:HB2	2.11	0.51
1:D:386:VAL:HG13	1:D:415:LEU:HD11	1.93	0.51
2:C:17:THR:OG1	2:C:35:SER:HB2	2.10	0.51
2:C:130:ARG:HG2	2:C:154:ALA:HB1	1.92	0.50
2:C:281:CYS:SG	2:C:492:LEU:HD13	2.51	0.50
2:A:583:GLN:O	2:A:586:LYS:HB3	2.11	0.50
1:B:149:ARG:HG2	1:D:172:ASN:ND2	2.26	0.50
1:B:403:TRP:NE1	2:A:119:PRO:HD2	2.26	0.50
1:B:493:ARG:NE	1:B:504:ASP:OD1	2.26	0.50
2:A:244:PRO:HB3	2:A:258:VAL:HG11	1.92	0.50
1:D:143:ILE:HG13	1:D:329:ALA:HA	1.92	0.50
1:D:390:VAL:HG21	1:D:417:SER:HA	1.94	0.50
1:B:69:PRO:HA	1:B:72:LYS:HG2	1.92	0.50
2:A:276:PRO:HD3	2:A:304:THR:HG21	1.94	0.50
1:B:82:ILE:HD12	1:B:108:PRO:HG3	1.93	0.50
1:B:99:HIS:HB2	1:B:333:ASN:HA	1.92	0.50
1:B:340:GLU:CD	1:B:364:HIS:HB3	2.31	0.50
1:D:178:TYR:CE1	2:C:555:GLY:HA3	2.47	0.50
2:C:59:PRO:O	2:C:63:ILE:HG13	2.12	0.50
2:C:218:ASN:OD1	2:C:264:ALA:N	2.45	0.50
1:D:481:GLY:HA2	1:D:531:GLY:O	2.11	0.50
1:B:471:GLY:O	1:B:489:PRO:HB2	2.12	0.50
1:B:497:ARG:N	1:B:518:GLU:OE2	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:6:TYR:N	2:A:23:ASP:HA	2.27	0.50
1:D:496:HIS:HB3	1:D:518:GLU:HG2	1.93	0.50
1:B:351:GLU:HB3	1:B:358:VAL:HG22	1.94	0.50
1:B:552:ILE:HG12	1:B:563:ILE:HB	1.92	0.50
2:A:113:TYR:HA	2:A:117:TYR:CE2	2.47	0.50
1:D:111:TYR:HB3	1:D:116:VAL:HG11	1.94	0.50
2:C:59:PRO:O	2:C:62:ILE:HG22	2.12	0.50
2:A:269:ASN:HD22	2:A:319:PHE:HE1	1.60	0.49
1:B:268:LEU:HD12	1:B:269:ILE:H	1.77	0.49
1:B:375:PRO:HD2	1:B:379:ASN:O	2.12	0.49
1:B:274:GLN:CD	1:B:329:ALA:HB2	2.32	0.49
1:D:368:ILE:HG21	1:D:468:PHE:H	1.77	0.49
2:C:365:CYS:SG	2:C:402:ALA:HB2	2.51	0.49
2:A:36:THR:H	2:A:42:LEU:HD12	1.78	0.49
1:D:443:ALA:HB3	1:D:482:ALA:HB3	1.94	0.49
1:D:466:VAL:HG22	1:D:509:ASN:HD22	1.77	0.49
1:B:548:GLY:O	2:A:126:ARG:NH2	2.45	0.49
1:D:496:HIS:CE1	1:D:501:GLY:HA2	2.47	0.49
2:C:86:VAL:HB	2:C:164:GLN:CB	2.42	0.49
2:C:184:MET:HG2	2:C:196:VAL:HG11	1.95	0.49
1:B:66:SER:N	1:B:288:SER:OG	2.46	0.49
1:B:403:TRP:CE2	2:A:119:PRO:HD2	2.48	0.49
1:B:490:LYS:HB2	1:B:525:PRO:HD3	1.93	0.49
2:A:300:SER:HA	2:A:335:GLY:O	2.12	0.49
1:B:243:GLU:N	1:B:470:GLU:OE2	2.30	0.49
1:B:392:SER:OG	1:B:409:LEU:HD22	2.13	0.49
1:D:365:ALA:HB2	1:D:408:PRO:O	2.12	0.49
1:B:13:ARG:HD3	1:B:216:LEU:HD22	1.95	0.49
1:B:403:TRP:HE1	2:A:118:PRO:HA	1.77	0.49
1:D:362:TRP:HZ3	1:D:406:CYS:HB2	1.76	0.49
2:C:130:ARG:HG2	2:C:154:ALA:HB2	1.94	0.49
2:C:293:THR:OG1	2:C:304:THR:HG22	2.13	0.49
2:C:342:ALA:HB3	2:C:373:PRO:HG2	1.95	0.49
1:B:267:VAL:HG11	1:B:290:VAL:HG11	1.94	0.48
2:A:269:ASN:HB3	2:A:319:PHE:CZ	2.47	0.48
1:B:36:PHE:HE1	1:B:423:LEU:HD23	1.76	0.48
2:C:55:LEU:HD23	2:C:57:ARG:O	2.13	0.48
2:C:250:SER:OG	2:C:266:ASN:ND2	2.47	0.48
1:B:387:LEU:HD12	1:B:387:LEU:H	1.76	0.48
1:D:398:LYS:HG2	1:D:530:TYR:OH	2.13	0.48
2:C:77:LEU:HG	2:C:81:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:509:ASN:ND2	1:D:510:THR:O	2.46	0.48
2:C:600:LEU:HD21	2:C:603:LEU:HD21	1.94	0.48
1:B:286:SER:OG	1:B:323:CYS:O	2.29	0.48
2:A:298:GLY:HA2	2:A:338:GLY:H	1.76	0.48
2:A:551:ILE:HD11	2:A:581:PHE:CB	2.44	0.48
1:D:40:HIS:HA	1:D:42:TYR:CD1	2.47	0.48
1:D:467:GLY:HA2	1:D:508:GLN:HA	1.95	0.48
2:A:292:ILE:HG12	2:A:305:LEU:HG	1.96	0.48
1:D:163:GLU:HA	1:D:166:ILE:HB	1.95	0.48
1:D:433:ARG:HG2	2:C:95:GLY:HA3	1.95	0.48
2:C:131:PRO:O	2:C:132:ILE:HD13	2.14	0.48
1:B:117:PHE:CZ	1:B:197:LEU:HB3	2.49	0.48
1:B:391:ILE:HD13	1:B:404:PRO:O	2.13	0.48
2:A:296:MET:HG2	2:A:460:ALA:HB2	1.95	0.48
2:A:496:ARG:HG2	2:A:608:ILE:HD12	1.96	0.48
1:D:429:VAL:HA	1:D:458:PRO:HA	1.94	0.48
2:A:109:ASP:OD1	2:A:117:TYR:OH	2.29	0.48
1:D:7:ILE:HD11	2:C:420:ARG:O	2.13	0.48
1:D:325:ALA:CB	1:D:330:PRO:HA	2.43	0.48
1:B:368:ILE:HG22	1:B:466:VAL:HG13	1.95	0.47
1:B:458:PRO:HG3	1:B:514:ALA:HB3	1.94	0.47
1:D:413:GLY:O	2:C:106:HIS:HB3	2.13	0.47
1:D:466:VAL:CG2	1:D:509:ASN:HD22	2.26	0.47
2:A:375:VAL:HG22	2:A:429:VAL:HG21	1.96	0.47
2:C:276:PRO:HD3	2:C:304:THR:HG21	1.95	0.47
2:C:393:GLY:O	2:C:395:ILE:HG13	2.14	0.47
2:A:652:GLY:HA3	2:A:669:GLU:HG2	1.96	0.47
1:D:251:GLU:OE2	1:D:253:SER:OG	2.23	0.47
1:D:439:ASP:OD1	1:D:550:VAL:HA	2.14	0.47
1:B:269:ILE:HG13	1:B:316:LEU:HD23	1.97	0.47
1:B:430:LEU:HD13	2:A:137:ILE:HG22	1.95	0.47
2:C:39:ASP:CG	2:C:231:ARG:HH22	2.18	0.47
2:C:553:TYR:OH	2:C:594:PRO:HA	2.15	0.47
1:B:73:CYS:HB2	1:B:96:MET:HE2	1.97	0.47
1:B:139:ASP:OD2	1:B:141:LYS:NZ	2.43	0.47
2:A:189:ALA:C	2:A:191:LEU:H	2.18	0.47
1:D:432:HIS:HB3	1:D:455:GLU:HG2	1.96	0.47
1:B:503:GLU:HG2	1:B:505:HIS:NE2	2.29	0.47
2:A:205:GLN:HG3	2:A:500:LEU:HD13	1.96	0.47
2:A:342:ALA:HA	2:A:352:VAL:HG22	1.95	0.47
1:D:90:HIS:CD2	1:D:106:TYR:HE1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:124:VAL:HG11	2:C:129:ARG:HG3	1.96	0.47
1:B:241:ILE:HG22	1:B:253:SER:HB3	1.96	0.47
1:B:386:VAL:O	1:B:390:VAL:HG23	2.15	0.47
1:B:542:LEU:HD11	1:B:569:LEU:HD22	1.96	0.47
2:A:174:VAL:HG11	2:A:205:GLN:O	2.15	0.47
2:C:102:ILE:HG22	2:C:104:LEU:H	1.80	0.47
2:A:106:HIS:CD2	2:A:108:GLU:H	2.32	0.47
2:C:495:ILE:HB	2:C:609:ALA:HB3	1.97	0.47
1:B:368:ILE:HB	1:B:468:PHE:CE2	2.50	0.47
1:D:407:GLY:CA	1:D:415:LEU:HB3	2.44	0.47
2:C:200:HIS:CD2	2:C:201:GLU:HG3	2.51	0.46
1:B:545:VAL:HA	1:B:550:VAL:O	2.16	0.46
1:D:93:PRO:HA	1:D:96:MET:O	2.15	0.46
2:A:126:ARG:HG3	2:A:129:ARG:HE	1.81	0.46
2:A:554:LEU:HG	2:A:598:VAL:HB	1.97	0.46
2:A:521:LEU:HD22	2:A:547:TYR:CD2	2.51	0.46
2:A:570:ASP:O	2:A:574:LEU:N	2.48	0.46
2:C:246:ARG:HB3	2:C:254:LEU:HB3	1.97	0.46
2:C:649:VAL:HG22	2:C:666:VAL:HB	1.96	0.46
1:B:38:LEU:HB3	1:B:124:HIS:CG	2.51	0.46
1:B:7:ILE:O	1:B:11:VAL:HG23	2.16	0.46
1:B:201:LEU:HD23	1:B:209:VAL:HG21	1.96	0.46
2:C:89:GLY:HA2	2:C:128:LEU:HB3	1.98	0.46
2:C:175:ARG:NH1	2:C:504:PRO:HD2	2.30	0.46
1:D:11:VAL:HG22	2:C:431:LEU:HD11	1.98	0.46
1:B:153:VAL:HG23	1:D:164:ASP:HB3	1.98	0.46
2:C:313:PHE:O	2:C:444:ARG:NH2	2.41	0.46
1:B:225:ARG:NH2	1:B:264:GLU:OE2	2.49	0.46
1:D:260:ILE:HD11	1:D:350:LEU:HD23	1.97	0.46
1:B:403:TRP:NE1	2:A:118:PRO:HA	2.31	0.45
2:A:23:ASP:OD1	2:A:24:HIS:N	2.47	0.45
2:A:352:VAL:HG21	2:A:425:ILE:HG12	1.98	0.45
2:A:664:PRO:HA	2:A:676:VAL:O	2.15	0.45
1:B:50:LEU:O	1:B:52:GLU:N	2.48	0.45
1:B:496:HIS:H	1:B:501:GLY:HA3	1.81	0.45
2:A:310:ARG:HH21	2:A:313:PHE:HD2	1.63	0.45
2:A:629:ILE:N	2:A:630:PRO:HD2	2.32	0.45
1:B:458:PRO:HB3	1:B:462:ALA:HB3	1.97	0.45
1:B:564:ASP:OD1	1:B:565:GLY:N	2.49	0.45
2:A:234:ALA:O	2:A:238:GLU:HB3	2.15	0.45
2:A:247:TYR:HB2	2:A:256:PRO:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:451:PHE:O	2:C:473:SER:OG	2.22	0.45
1:B:407:GLY:O	1:B:409:LEU:N	2.49	0.45
2:A:319:PHE:HB2	2:A:324:ILE:HD12	1.99	0.45
1:D:294:LEU:HD11	1:D:312:VAL:HG11	1.97	0.45
1:D:391:ILE:HG12	1:D:405:ALA:CB	2.46	0.45
1:B:365:ALA:C	1:B:367:GLY:H	2.20	0.45
1:B:478:GLY:HA3	1:B:529:GLY:O	2.17	0.45
1:D:26:THR:O	1:D:30:THR:OG1	2.26	0.45
1:D:493:ARG:HB3	1:D:521:ILE:HB	1.99	0.45
1:B:151:PRO:HD2	1:D:168:LEU:HA	1.99	0.45
2:A:125:PRO:O	2:A:126:ARG:HB2	2.17	0.45
1:D:370:ILE:HG23	1:D:383:VAL:O	2.17	0.45
1:B:408:PRO:HB2	1:B:410:CYS:SG	2.57	0.45
1:B:561:VAL:HG22	1:B:578:ARG:HH21	1.81	0.45
1:D:391:ILE:HD12	1:D:452:THR:HG21	1.98	0.45
2:A:658:GLY:HA3	2:A:683:SER:HB2	1.99	0.45
2:C:184:MET:SD	2:C:198:SER:OG	2.68	0.45
2:C:48:LEU:HA	2:C:51:ILE:HD12	1.99	0.45
1:B:35:VAL:HG23	1:B:36:PHE:CE1	2.52	0.45
2:A:664:PRO:HB3	2:A:678:PRO:HG3	1.98	0.45
1:B:545:VAL:HG11	1:B:563:ILE:HD12	1.99	0.44
2:C:86:VAL:HB	2:C:164:GLN:HB2	1.98	0.44
1:B:130:GLY:O	1:B:174:ARG:NH1	2.49	0.44
1:B:131:PRO:HB3	1:D:145:ALA:HB2	1.99	0.44
2:A:521:LEU:HB3	2:A:547:TYR:HE2	1.82	0.44
2:C:159:ARG:NH2	2:C:190:ALA:O	2.50	0.44
1:B:42:TYR:HB3	1:B:123:GLY:HA2	2.00	0.44
1:B:439:ASP:OD1	1:B:550:VAL:HA	2.18	0.44
2:A:505:MET:O	2:A:600:LEU:HB3	2.18	0.44
1:D:127:ASP:OD1	1:D:128:ILE:N	2.50	0.44
1:D:279:ILE:HA	1:D:334:CYS:HB3	2.00	0.44
1:D:387:LEU:O	1:D:434:TYR:OH	2.22	0.44
2:C:90:LEU:HA	2:C:167:ALA:O	2.17	0.44
2:C:657:VAL:HG11	2:C:686:PRO:HG3	1.99	0.44
2:A:495:ILE:HG12	2:A:611:LEU:HD12	1.99	0.44
1:B:33:SER:CA	1:B:37:ASN:HB2	2.47	0.44
1:B:407:GLY:O	1:B:409:LEU:HG	2.18	0.44
1:B:407:GLY:CA	1:B:415:LEU:HB3	2.48	0.44
2:C:12:ALA:HB3	2:C:73:THR:HA	1.99	0.44
2:C:184:MET:HG2	2:C:196:VAL:CG1	2.48	0.44
1:B:148:LEU:HD23	1:B:173:MET:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:HIS:CD2	1:D:106:TYR:CE1	3.06	0.44
1:D:506:TYR:CG	1:D:507:ILE:HG23	2.53	0.44
1:B:63:HIS:CE1	1:B:122:LYS:HD3	2.53	0.44
1:B:144:TYR:CE2	1:D:174:ARG:HD2	2.51	0.44
1:B:86:ASP:OD1	1:B:158:GLN:N	2.45	0.44
2:A:170:PHE:CD2	2:A:180:GLU:HG2	2.53	0.44
2:C:652:GLY:O	2:C:690:TYR:OH	2.36	0.44
1:B:134:ALA:C	1:B:136:TYR:H	2.21	0.43
2:A:135:ARG:HD2	2:A:135:ARG:HA	1.77	0.43
1:D:472:ARG:HB2	1:D:506:TYR:HE1	1.83	0.43
2:A:550:GLU:HG2	2:A:561:SER:HA	2.00	0.43
1:D:21:ARG:HA	1:D:21:ARG:HD3	1.76	0.43
2:C:525:ARG:O	2:C:529:MET:HG2	2.18	0.43
1:B:218:ASP:HB3	1:B:222:ARG:NH1	2.32	0.43
1:D:283:ALA:O	1:D:287:ILE:HG12	2.18	0.43
1:B:153:VAL:HA	1:D:164:ASP:HB3	2.00	0.43
1:B:490:LYS:HG2	1:B:491:LEU:N	2.34	0.43
1:D:395:GLY:O	1:D:448:GLY:HA2	2.18	0.43
2:C:168:ILE:HD12	2:C:184:MET:HG3	1.99	0.43
1:B:179:GLN:O	1:B:183:LEU:HG	2.18	0.43
1:B:245:SER:O	1:B:249:LEU:N	2.52	0.43
1:B:386:VAL:CG1	1:B:415:LEU:HD11	2.49	0.43
2:A:321:ARG:HA	2:A:321:ARG:HD3	1.84	0.43
2:A:658:GLY:HA3	2:A:684:LEU:N	2.30	0.43
1:D:441:GLY:O	1:D:487:LEU:HD11	2.18	0.43
2:C:447:ASP:OD1	2:C:447:ASP:N	2.51	0.43
2:C:605:CYS:SG	2:C:606:SER:N	2.91	0.43
1:B:556:ARG:HA	1:B:562:VAL:HG22	2.00	0.43
1:D:278:PHE:CE1	1:D:334:CYS:HB2	2.53	0.43
1:D:329:ALA:N	1:D:330:PRO:HD3	2.33	0.43
1:D:392:SER:OG	1:D:409:LEU:HD22	2.18	0.43
1:D:570:ASP:O	1:D:572:ALA:N	2.50	0.43
1:B:278:PHE:HE1	1:B:334:CYS:HG	1.61	0.43
1:B:400:MET:HG3	1:B:402:GLY:N	2.28	0.43
2:A:99:SER:HA	2:A:102:ILE:HD12	2.00	0.43
2:A:345:ASP:OD2	2:A:349:MET:HB2	2.18	0.43
2:A:363:PRO:HD2	2:A:366:TYR:CD2	2.53	0.43
2:C:553:TYR:HE2	2:C:595:ASN:H	1.66	0.43
1:B:87:VAL:HG22	1:B:156:TRP:N	2.34	0.43
1:B:95:TYR:H	1:B:96:MET:CE	2.32	0.43
2:A:42:LEU:O	2:A:46:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:251:ASN:ND2	2:A:496:ARG:O	2.40	0.43
1:D:71:MET:HG2	1:D:106:TYR:HE2	1.84	0.43
1:D:209:VAL:O	1:D:213:ILE:HG12	2.19	0.43
2:C:485:LEU:HD12	2:C:488:PHE:HD2	1.84	0.43
2:C:637:LEU:HB2	2:C:644:TRP:CD2	2.54	0.43
1:D:99:HIS:HD2	1:D:101:LEU:HB2	1.83	0.43
1:D:154:LYS:HD2	1:D:162:ARG:NH2	2.33	0.43
1:D:380:ASP:HB3	1:D:382:TYR:CZ	2.54	0.43
2:C:305:LEU:HD11	2:C:440:VAL:O	2.19	0.43
2:A:681:ARG:HH11	2:A:681:ARG:HG2	1.84	0.43
1:D:53:MET:N	1:D:306:GLU:OE1	2.39	0.43
1:D:78:PHE:HB3	1:D:82:ILE:HG23	2.01	0.43
1:D:327:GLU:HB3	1:D:328:PRO:HD3	2.01	0.43
2:C:378:ALA:HA	2:C:406:ILE:HD11	2.01	0.43
2:A:90:LEU:HB3	2:A:128:LEU:O	2.19	0.42
2:A:494:ASP:OD1	2:A:494:ASP:N	2.37	0.42
2:A:553:TYR:OH	2:A:582:HIS:ND1	2.42	0.42
2:A:581:PHE:O	2:A:584:ARG:HB3	2.19	0.42
2:A:582:HIS:CE1	2:A:594:PRO:HB3	2.54	0.42
1:B:201:LEU:O	1:B:205:GLY:N	2.49	0.42
1:B:416:MET:HG3	2:A:104:LEU:O	2.19	0.42
1:B:564:ASP:O	1:B:566:ASN:N	2.46	0.42
1:D:300:VAL:H	1:D:301:PRO:HD3	1.84	0.42
2:A:408:SER:HA	2:A:412:GLU:HB3	2.02	0.42
2:A:571:ARG:HA	2:A:574:LEU:HB3	2.00	0.42
2:C:76:ALA:HB1	2:C:221:LEU:HD13	2.00	0.42
1:B:46:LEU:HD13	1:B:197:LEU:HD11	2.01	0.42
2:A:514:LEU:HD23	2:A:514:LEU:HA	1.90	0.42
2:A:682:VAL:HG13	2:A:692:LEU:HG	2.01	0.42
1:D:327:GLU:C	1:D:329:ALA:H	2.21	0.42
1:D:545:VAL:HG11	1:D:563:ILE:HD13	2.01	0.42
2:C:71:ASN:O	2:C:247:TYR:HA	2.19	0.42
2:C:551:ILE:HD11	2:C:581:PHE:CG	2.54	0.42
1:D:455:GLU:HA	1:D:521:ILE:HG12	2.02	0.42
2:C:526:GLU:OE1	2:C:526:GLU:HA	2.19	0.42
1:B:82:ILE:HG22	1:B:154:LYS:HE2	2.01	0.42
2:A:192:PRO:HB2	2:A:194:VAL:CG2	2.49	0.42
2:A:373:PRO:HA	2:A:377:ASP:OD2	2.19	0.42
2:C:20:ILE:HG12	2:C:487:ALA:CB	2.50	0.42
1:B:495:ILE:HD13	1:B:502:GLU:H	1.84	0.42
1:D:7:ILE:O	1:D:11:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:419:GLU:O	2:C:423:VAL:HG22	2.20	0.42
1:B:460:LYS:HA	1:B:460:LYS:HD3	1.63	0.42
1:B:496:HIS:HE2	1:B:503:GLU:HB2	1.85	0.42
2:C:300:SER:HA	2:C:337:GLY:N	2.34	0.42
2:C:547:TYR:CB	2:C:564:LEU:HB3	2.42	0.42
1:B:172:ASN:OD1	1:D:149:ARG:HG2	2.20	0.42
1:B:244:ASP:HB2	1:B:470:GLU:N	2.33	0.42
1:B:466:VAL:HB	1:B:509:ASN:HB2	2.02	0.42
2:A:286:PHE:HZ	2:A:689:THR:HB	1.85	0.42
1:D:46:LEU:HD13	1:D:197:LEU:HD21	2.02	0.42
1:D:231:VAL:HG23	1:D:260:ILE:HG21	2.02	0.42
1:D:286:SER:HA	1:D:339:MET:HE1	2.01	0.42
2:C:80:LEU:HD23	2:C:80:LEU:HA	1.90	0.42
2:C:166:VAL:HG23	2:C:194:VAL:HG11	2.01	0.42
2:A:122:MET:HE2	2:A:129:ARG:HH22	1.85	0.42
2:C:551:ILE:HD11	2:C:581:PHE:HB2	2.02	0.42
1:B:39:ALA:HB3	1:B:415:LEU:HD12	2.02	0.41
1:B:215:GLU:O	1:B:219:MET:HG3	2.20	0.41
1:B:494:LEU:HD13	1:B:520:VAL:HG22	2.02	0.41
2:A:138:SER:HA	2:A:172:TRP:CD2	2.54	0.41
2:A:682:VAL:HA	2:A:691:GLU:O	2.19	0.41
1:D:47:PHE:CE1	1:D:53:MET:HG3	2.55	0.41
1:D:447:ARG:HG2	1:D:536:ARG:NH2	2.34	0.41
1:B:375:PRO:HG3	1:B:381:GLU:HG3	2.01	0.41
2:A:132:ILE:HD12	2:A:170:PHE:CZ	2.55	0.41
2:A:341:ILE:HG12	2:A:355:ARG:O	2.20	0.41
1:D:71:MET:HG2	1:D:106:TYR:CE2	2.55	0.41
1:D:128:ILE:O	1:D:148:LEU:HB3	2.19	0.41
2:C:175:ARG:HH11	2:C:504:PRO:HD2	1.85	0.41
2:A:476:VAL:HB	2:A:692:LEU:HB2	2.02	0.41
2:A:582:HIS:ND1	2:A:594:PRO:HB3	2.36	0.41
1:D:153:VAL:HG21	1:D:165:VAL:HG11	2.00	0.41
2:C:345:ASP:HB3	2:C:347:PHE:CD1	2.55	0.41
2:C:384:TYR:HB3	2:C:675:LEU:HD21	2.02	0.41
2:C:485:LEU:HD12	2:C:485:LEU:HA	1.80	0.41
1:B:48:ASP:N	1:B:52:GLU:O	2.53	0.41
2:A:255:ALA:N	2:A:256:PRO:HD3	2.35	0.41
2:A:656:GLU:HG3	2:A:657:VAL:N	2.34	0.41
2:C:285:PRO:HG2	2:C:687:SER:OG	2.21	0.41
2:C:411:ALA:HB1	2:C:416:ILE:O	2.20	0.41
2:C:616:MET:N	2:C:616:MET:SD	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:626:THR:HG22	2:C:630:PRO:HD3	2.01	0.41
1:B:58:GLN:HB3	1:B:304:TYR:CD1	2.56	0.41
1:B:451:GLY:HA3	1:B:524:ASN:O	2.21	0.41
2:C:680:TRP:HA	2:C:694:PRO:HA	2.02	0.41
2:A:425:ILE:O	2:A:429:VAL:HG23	2.21	0.41
1:D:355:PRO:HA	1:D:358:VAL:CG2	2.47	0.41
2:C:353:GLY:N	2:C:354:PRO:CD	2.84	0.41
2:A:600:LEU:HD12	2:A:601:VAL:H	1.86	0.41
1:D:61:PRO:HB2	1:D:292:LEU:HD13	2.02	0.41
1:D:277:TYR:OH	1:D:508:GLN:HG2	2.21	0.41
1:B:132:VAL:HG12	1:B:134:ALA:H	1.86	0.41
1:B:244:ASP:HB2	1:B:470:GLU:HA	2.02	0.41
1:B:570:ASP:HB3	1:B:573:ALA:HB3	2.03	0.41
2:A:48:LEU:CD1	2:A:239:LEU:HD13	2.51	0.41
2:A:138:SER:O	2:A:175:ARG:NH1	2.53	0.41
2:A:506:ARG:HB3	2:A:598:VAL:HG13	2.02	0.41
1:D:155:LEU:O	1:D:166:ILE:HD11	2.21	0.41
1:D:447:ARG:H	1:D:536:ARG:NH1	2.19	0.41
2:C:85:GLY:HA3	2:C:220:TYR:CE2	2.56	0.41
2:C:106:HIS:CE1	2:C:108:GLU:HB2	2.56	0.41
2:C:428:LEU:HD23	2:C:428:LEU:HA	1.84	0.41
2:C:502:THR:HA	2:C:602:ASN:HA	2.03	0.41
2:C:564:LEU:HD11	2:C:569:LEU:HD13	2.03	0.41
2:C:684:LEU:HD13	2:C:690:TYR:CZ	2.55	0.41
1:B:452:THR:H	1:B:524:ASN:HB3	1.86	0.41
2:A:92:CYS:SG	2:A:97:GLU:HA	2.61	0.41
2:A:95:GLY:N	2:A:97:GLU:OE1	2.51	0.41
1:D:490:LYS:HG2	1:D:491:LEU:N	2.35	0.41
1:D:568:GLN:HG2	1:D:569:LEU:HD23	2.02	0.41
2:C:682:VAL:HG13	2:C:692:LEU:HG	2.03	0.41
1:B:129:GLY:HA3	1:B:172:ASN:O	2.20	0.40
1:B:392:SER:OG	1:B:393:GLY:N	2.55	0.40
1:B:464:THR:HG21	1:B:520:VAL:HG11	2.03	0.40
1:B:473:GLN:O	1:B:475:PRO:HD3	2.21	0.40
2:A:334:LEU:HD11	2:A:436:GLY:HA3	2.02	0.40
2:C:210:THR:HG21	2:C:316:ASP:CG	2.41	0.40
2:C:511:PHE:CE2	2:C:513:ASP:HA	2.56	0.40
1:B:433:ARG:HB2	1:B:455:GLU:HB3	2.03	0.40
1:B:543:ALA:O	1:B:547:ASN:N	2.49	0.40
2:A:275:ALA:O	2:A:293:THR:HG21	2.21	0.40
2:A:307:LYS:HB2	2:A:307:LYS:HE3	1.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:374:THR:H	2:A:377:ASP:CG	2.23	0.40
2:A:397:LEU:HD12	2:A:397:LEU:HA	1.82	0.40
1:D:40:HIS:HA	1:D:42:TYR:CE1	2.56	0.40
2:C:101:GLU:HB2	2:C:129:ARG:HH12	1.86	0.40
1:B:274:GLN:NE2	1:B:329:ALA:HB2	2.36	0.40
1:B:381:GLU:OE1	1:B:428:PRO:HD3	2.21	0.40
1:B:392:SER:H	1:B:409:LEU:CD2	2.33	0.40
2:A:170:PHE:N	2:A:180:GLU:OE2	2.41	0.40
1:D:35:VAL:O	1:D:383:VAL:HG21	2.22	0.40
1:D:388:ALA:HA	1:D:454:LEU:HD22	2.04	0.40
1:D:391:ILE:HG12	1:D:405:ALA:HA	2.04	0.40
1:D:468:PHE:HB3	1:D:469:GLY:H	1.58	0.40
2:C:364:VAL:HG22	2:C:377:ASP:CG	2.42	0.40
1:B:362:TRP:CZ2	1:B:394:ALA:HA	2.56	0.40
1:B:383:VAL:HG22	1:B:384:THR:O	2.20	0.40
2:A:374:THR:H	2:A:377:ASP:CB	2.33	0.40
2:A:557:ILE:HD13	2:A:557:ILE:HA	1.91	0.40
1:D:205:GLY:O	1:D:209:VAL:HG23	2.21	0.40
1:D:300:VAL:N	1:D:301:PRO:CD	2.85	0.40
1:D:472:ARG:CB	1:D:506:TYR:HE1	2.34	0.40
1:B:93:PRO:HA	1:B:96:MET:O	2.21	0.40
1:B:243:GLU:HA	1:B:250:GLY:HA2	2.03	0.40
2:A:564:LEU:HD11	2:A:569:LEU:HD13	2.03	0.40
2:A:629:ILE:HG22	2:A:650:TYR:HB3	2.03	0.40
1:D:161:ARG:HB3	1:D:166:ILE:CD1	2.50	0.40
2:C:460:ALA:O	2:C:464:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	577/581 (99%)	510 (88%)	62 (11%)	5 (1%)	17 55
1	D	577/581 (99%)	503 (87%)	65 (11%)	9 (2%)	9 44
2	A	689/696 (99%)	623 (90%)	63 (9%)	3 (0%)	34 71
2	C	689/696 (99%)	625 (91%)	62 (9%)	2 (0%)	41 75
All	All	2532/2554 (99%)	2261 (89%)	252 (10%)	19 (1%)	19 58

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	143	ILE
1	B	366	SER
1	D	367	GLY
1	D	365	ALA
1	D	412	PHE
1	D	571	GLU
1	B	330	PRO
1	B	571	GLU
2	A	321	ARG
2	A	622	PRO
1	D	506	TYR
2	A	118	PRO
1	D	328	PRO
1	B	507	ILE
2	C	118	PRO
2	C	594	PRO
1	D	143	ILE
1	D	327	GLU
1	D	413	GLY

5.3.2 Protein sidechains

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	B	460/462 (100%)	454 (99%)	6 (1%)	69 82
1	D	459/462 (99%)	454 (99%)	5 (1%)	73 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	557/562 (99%)	555 (100%)	2 (0%)	91 94
2	C	557/562 (99%)	551 (99%)	6 (1%)	73 85
All	All	2033/2048 (99%)	2014 (99%)	19 (1%)	78 88

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	20	GLN
1	B	96	MET
1	B	117	PHE
1	B	366	SER
1	B	417	SER
1	B	522	ASN
2	A	605	CYS
2	A	623	LEU
1	D	9	LEU
1	D	96	MET
1	D	382	TYR
1	D	417	SER
1	D	497	ARG
2	C	251	ASN
2	C	312	ASN
2	C	350	LEU
2	C	506	ARG
2	C	545	CYS
2	C	636	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	184	ASN
1	D	331	HIS
2	C	29	GLN
2	C	266	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

Of 2 ligands modelled in this entry, 2 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	B	579/581 (99%)	-0.23	4 (0%)	87	82	16, 38, 88, 140	0
1	D	579/581 (99%)	-0.16	3 (0%)	91	85	22, 46, 88, 146	0
2	A	691/696 (99%)	-0.15	4 (0%)	89	84	23, 50, 103, 154	0
2	C	691/696 (99%)	-0.00	14 (2%)	65	56	39, 65, 111, 151	0
All	All	2540/2554 (99%)	-0.13	25 (0%)	82	74	16, 51, 104, 154	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	33	ALA	3.5
2	C	592	SER	3.2
2	A	113	TYR	3.1
2	C	407	ARG	2.9
1	B	558	GLU	2.8
2	C	110	GLY	2.8
1	D	489	PRO	2.7
2	C	373	PRO	2.6
2	C	134	GLY	2.6
1	B	577	HIS	2.5
1	B	562	VAL	2.5
1	D	527	GLY	2.5
2	C	655	ILE	2.5
2	A	112	ARG	2.4
2	C	333	THR	2.4
2	A	309	GLY	2.3
2	C	366	TYR	2.2
2	A	11	ASP	2.2
2	C	591	TYR	2.2
1	B	563	ILE	2.2
2	C	24	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	32	LYS	2.1
2	C	113	TYR	2.1
1	D	528	GLY	2.0
2	C	637	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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. 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	B-factors(Å^2)	Q<0.9
3	ZN	B	600	1/1	0.86	0.07	48,48,48,48	0
3	ZN	D	600	1/1	0.89	0.13	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.