



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:54 PM UTC

PDB ID : 6YRA / pdb_00006yra
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 types of validation reports are described at

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

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

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

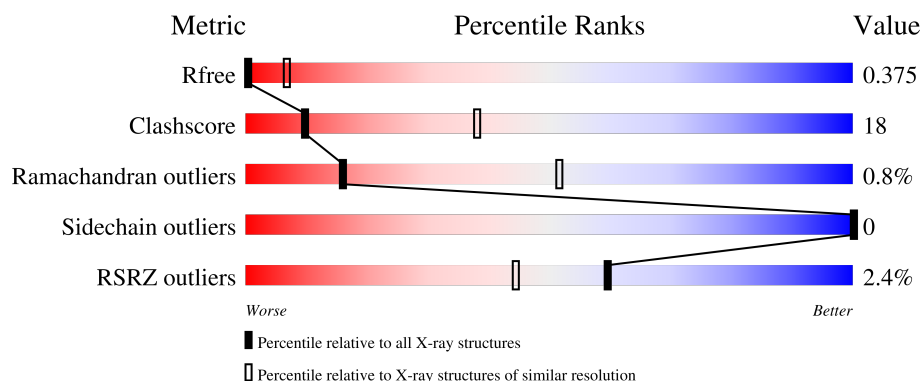
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

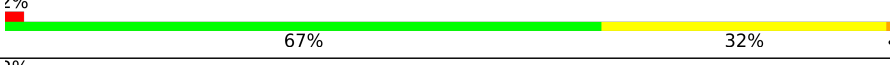
The reported resolution of this entry is 4.00 Å.

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}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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

Mol	Chain	Length	Quality of chain
1	B	581	
1	D	581	
2	A	696	
2	C	696	

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.

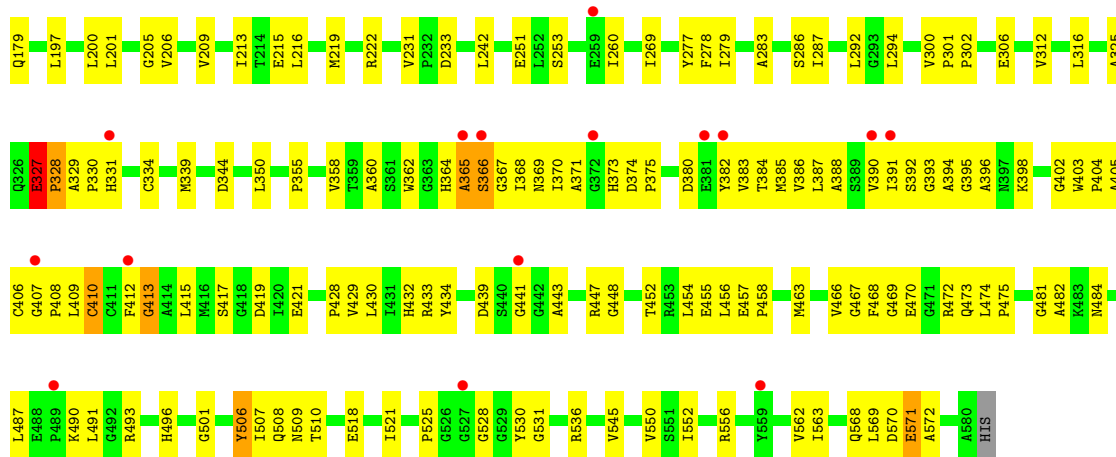
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	579	Total	C	N	O	S	0	0	0
			4385	2750	769	838	28			
1	D	579	Total	C	N	O	S	0	0	0
			4378	2744	769	837	28			

- Molecule 2 is a protein called 5-oxoprolinase.

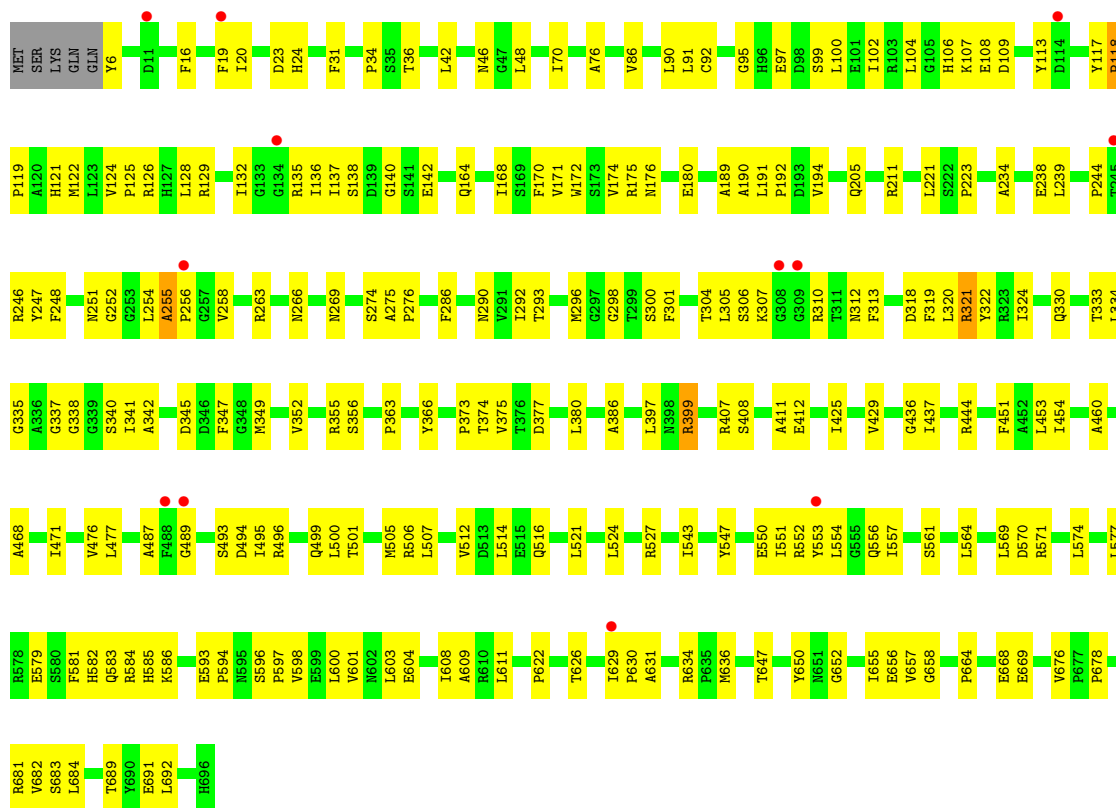
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	691	Total	C	N	O	S	0	0	0
			5250	3285	940	998	27			
2	C	691	Total	C	N	O	S	0	0	0
			5250	3285	940	998	27			

- Molecule 3 is ZINC ION (CCD ID: 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		

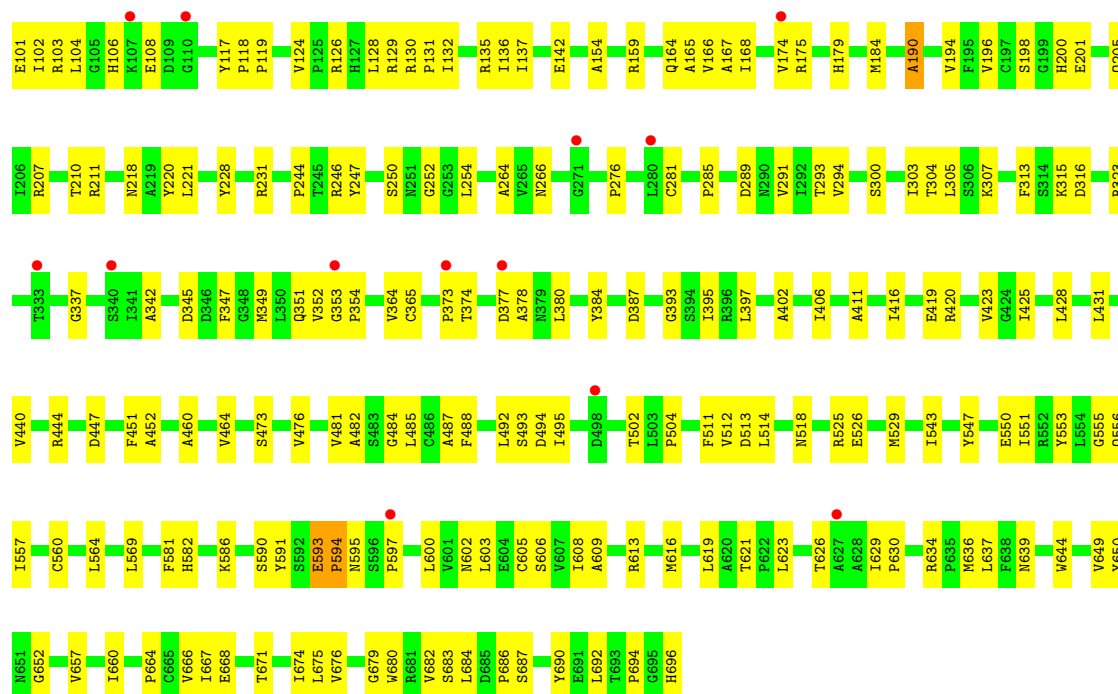


• Molecule 2: 5-oxoprolinase



• Molecule 2: 5-oxoprolinase





4 Data and refinement statistics

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 48.84 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.84-4.00) 98.4 (48.84-4.00)	Depositor EDS
R_{merge}	0.63	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.239 , 0.381 (Not available) , 0.375	Depositor DCC
R_{free} test set	1156 reflections (4.61%)	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)	0.35 , 155.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.27	0/4481	0.68	0/6096
1	D	0.26	0/4473	0.71	3/6085 (0.0%)
2	A	0.23	0/5352	0.64	1/7269 (0.0%)
2	C	0.25	0/5352	0.63	3/7269 (0.0%)
All	All	0.25	0/19658	0.66	7/26719 (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 (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	143	ILE	N-CA-C	7.64	125.24	109.34
1	D	142	GLU	CA-C-N	6.63	133.90	121.97
1	D	142	GLU	C-N-CA	6.63	133.90	121.97
2	C	593	GLU	N-CA-C	6.15	123.40	109.81
2	A	399	ARG	N-CA-C	5.63	119.92	112.72
2	C	190	ALA	CA-C-N	5.44	128.32	123.10
2	C	190	ALA	C-N-CA	5.44	128.32	123.10

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	187	0
1	D	4378	0	4269	191	0
2	A	5250	0	5201	171	0
2	C	5250	0	5201	156	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
All	All	19265	0	18947	671	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 18.

All (671) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:216:LEU:HA	1:D:219:MET:HE2	1.62	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
2:A:122:MET:HE2	2:A:129:ARG:HH22	1.47	0.79
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:286:SER:HA	1:D:339:MET:HE1	1.71	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:A:107:LYS:NZ	2:A:318:ASP:OD2	2.31	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:98:SER:HB2	1:B:102:ASP:HB2	1.83	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
2:C:117:TYR:C	2:C:119:PRO:HD3	2.28	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:373:HIS:HD2	1:D:463:MET:HE2	1.69	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: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
1:B:340:GLU:CD	1:B:364:HIS:HB3	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:124:VAL:O	2:A:129:ARG:NH2	2.39	0.56
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
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:B:339:MET:HE1	1:B:410:CYS:HB2	1.89	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:B:274:GLN:CD	1:B:329:ALA:HB2	2.32	0.54
2:A:122:MET:HE2	2:A:129:ARG:NH2	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:D:219:MET:HE1	2:C:349:MET:HE3	1.90	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
1:B:400:MET:HE1	2:A:118:PRO:HB3	1.91	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:O	2:A:596:SER:OG	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:73:CYS:HB2	1:B:96:MET:HE2	1.91	0.52
1:B:144:TYR:HE2	1:D:174:ARG:HD2	1.73	0.52
2:C:39:ASP:CG	2:C:231:ARG:HH22	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:189:ALA:C	2:A:191:LEU:H	2.18	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:365:ALA:C	1:B:367:GLY:H	2.20	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
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:D:20:GLN:O	1:D:24:THR:OG1	2.20	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:D:373:HIS:CD2	1:D:463:MET:HE2	2.47	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
2:A:347:PHE:HB2	2:A:349:MET:HE2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:134:ALA:C	1:B:136:TYR:H	2.21	0.48
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:C:634:ARG:HB3	2:C:636:MET:HE2	1.95	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
2:A:636:MET:HE3	2:A:647:THR:HB	1.96	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:87:VAL:HG21	1:D:105:MET:HE2	1.95	0.47
1:D:251:GLU:OE2	1:D:253:SER:OG	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:553:TYR:OH	2:C:594:PRO:HA	2.15	0.47
1:B:139:ASP:OD2	1:B:141:LYS:NZ	2.43	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
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
1:D:327:GLU:C	1:D:329:ALA:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:A:374:THR:H	2:A:377:ASP:CG	2.23	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
2:C:210:THR:HG21	2:C:316:ASP:CG	2.41	0.45
1:B:478:GLY:HA3	1:B:529:GLY:O	2.17	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
2:C:364:VAL:HG22	2:C:377:ASP:CG	2.42	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:23:MET:HE2	1:B:44:ASN:HB3	1.98	0.44
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
1:D:569:LEU:C	1:D:571:GLU:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:408:PRO:C	1:D:410:CYS:H	2.26	0.44
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:A:190:ALA:C	2:A:192:PRO:HD3	2.43	0.44
2:C:652:GLY:O	2:C:690:TYR:OH	2.36	0.44
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
1:B:142:GLU:C	1:B:144:TYR:N	2.74	0.43
1:B:365:ALA:C	1:B:367:GLY:N	2.76	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:128:ILE:HD12	1:B:173:MET:HE2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:407:GLY:C	1:D:415:LEU:HB3	2.44	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:A:505:MET:HE1	2:A:516:GLN:HB3	2.01	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
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:B:146:GLU:CD	1:B:331:HIS:HB3	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:274:GLN:HE22	1:B:328:PRO:C	2.27	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: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:B:142:GLU:OE2	1:D:463:MET:HE1	2.19	0.42
1:B:351:GLU:CD	1:B:358:VAL:HA	2.43	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
2:A:189:ALA:C	2:A:191:LEU:N	2.78	0.42
1:D:7:ILE:O	1:D:11:VAL:HG23	2.19	0.42
2:C:419:GLU:O	2:C:423:VAL:HG22	2.20	0.42
1:B:52:GLU:OE1	1:B:217:LYS:NZ	2.35	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:570:ASP:C	1:D:572:ALA:H	2.28	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:274:SER:HB2	2:A:489:GLY:C	2.46	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
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:437:MET:HE3	1:B:437:MET:HB3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:LEU:O	1:D:166:ILE:HD11	2.21	0.41
1:D:385:MET:HE2	1:D:456:LEU:HD22	2.02	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:143:ILE:C	1:B:145:ALA:H	2.29	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:A:603:LEU:C	2:A:604:GLU:HG3	2.45	0.40
1:D:339:MET:HA	1:D:339:MET:HE2	2.04	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:385:MET:HE3	1:D:385:MET:HB3	1.82	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%)	14	48
1	D	577/581 (99%)	503 (87%)	65 (11%)	9 (2%)	7	37
2	A	689/696 (99%)	623 (90%)	63 (9%)	3 (0%)	30	65
2	C	689/696 (99%)	625 (91%)	62 (9%)	2 (0%)	36	70
All	All	2532/2554 (99%)	2261 (89%)	252 (10%)	19 (1%)	16	52

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	143	ILE
1	B	366	SER
1	D	367	GLY

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Mol	Chain	Res	Type
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	D	459/462 (99%)	459 (100%)	0	100	100
2	A	436/562 (78%)	436 (100%)	0	100	100
2	C	557/562 (99%)	557 (100%)	0	100	100
All	All	1452/1586 (92%)	1452 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	181	GLN
2	A	541	ASN
2	A	556	GLN
1	D	179	GLN

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Mol	Chain	Res	Type
1	D	331	HIS
1	D	333	ASN
1	D	352	GLN
1	D	509	ASN
2	C	29	GLN
2	C	111	HIS
2	C	266	ASN
2	C	400	GLN
2	C	499	GLN
2	C	516	GLN
2	C	518	ASN
2	C	633	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	B	579/581 (99%)	0.44	18 (3%)	51 37	16, 38, 88, 140	0
1	D	579/581 (99%)	0.43	16 (2%)	55 40	22, 46, 88, 146	0
2	A	691/696 (99%)	0.31	12 (1%)	69 51	23, 50, 103, 154	0
2	C	691/696 (99%)	0.41	15 (2%)	62 46	39, 65, 111, 151	0
All	All	2540/2554 (99%)	0.39	61 (2%)	59 44	16, 51, 104, 154	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	331	HIS	6.4
1	D	331	HIS	5.4
1	B	366	SER	5.2
2	C	33	ALA	3.6
1	D	390	VAL	3.4
2	A	309	GLY	3.4
1	D	259	GLU	3.4
1	B	329	ALA	3.4
2	C	340	SER	3.2
2	A	489	GLY	3.1
2	C	597	PRO	3.1
1	B	35	VAL	3.1
1	B	301	PRO	3.0
1	B	509	ASN	2.9
2	C	110	GLY	2.9
2	C	353	GLY	2.8
2	A	629	ILE	2.8
1	D	407	GLY	2.7
1	D	381	GLU	2.7
1	B	121	CYS	2.6
2	C	627	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	A	11	ASP	2.6
1	D	145	ALA	2.6
2	C	17	THR	2.6
2	C	174	VAL	2.6
2	C	373	PRO	2.6
1	B	43	SER	2.3
1	D	382	TYR	2.3
1	B	558	GLU	2.3
1	D	527	GLY	2.3
1	B	382	TYR	2.3
2	A	19	PHE	2.3
1	D	489	PRO	2.3
2	A	256	PRO	2.3
2	A	245	THR	2.2
1	B	38	LEU	2.2
2	C	498	ASP	2.2
1	B	256	ALA	2.2
1	D	372	GLY	2.2
2	A	488	PHE	2.2
1	B	462	ALA	2.2
1	D	365	ALA	2.2
2	C	107	LYS	2.1
1	D	441	GLY	2.1
2	A	308	GLY	2.1
2	C	280	LEU	2.1
1	B	122	LYS	2.1
1	B	300	VAL	2.1
2	A	134	GLY	2.1
2	C	271	GLY	2.1
2	A	114	ASP	2.1
1	D	412	PHE	2.1
1	B	332	VAL	2.1
1	D	559	TYR	2.0
2	C	333	THR	2.0
1	B	32	ARG	2.0
1	D	391	ILE	2.0
2	A	553	TYR	2.0
2	C	377	ASP	2.0
1	B	271	SER	2.0
1	D	366	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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, 95th 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($\text{\AA}^2$)	Q<0.9
3	ZN	D	600	1/1	0.90	0.09	52,52,52,52	0
3	ZN	B	600	1/1	0.94	0.07	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.