



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:31 PM UTC

PDB ID : 1BML / pdb_00001bml
Title : COMPLEX OF THE CATALYTIC DOMAIN OF HUMAN PLASMIN AND STREPTOKINASE
Authors : Wang, X.; Zhang, X.C.
Deposited on : 1999-05-25
Resolution : 2.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

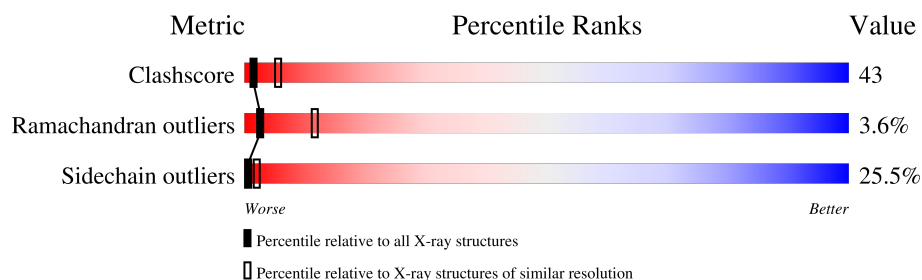
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8940 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 PLASMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1917	1217	339	347	14			
1	B	250	Total	C	N	O	S	0	0	0
			1917	1217	339	347	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	741	ALA	SER	engineered mutation	UNP P00747
B	741	ALA	SER	engineered mutation	UNP P00747

- Molecule 2 is a protein called STREPTOKINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	318	Total	C	N	O	S	0	0	0
			2553	1610	426	514	3			
2	D	318	Total	C	N	O	S	0	0	0
			2553	1610	426	514	3			

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.03Å 125.05Å 86.79Å 90.00° 105.41° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	91.3 (20.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.201 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8940	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

4 Model quality

4.1 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	0.63	0/1967	1.19	19/2673 (0.7%)
1	B	0.61	0/1967	1.17	20/2673 (0.7%)
2	C	0.51	0/2597	0.96	11/3522 (0.3%)
2	D	0.50	0/2597	1.05	22/3522 (0.6%)
All	All	0.56	0/9128	1.08	72/12390 (0.6%)

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
2	C	0	1

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	569	HIS	N-CA-C	-11.21	95.60	109.83
2	D	130	GLN	N-CA-C	9.87	125.59	112.17
1	A	745	LEU	N-CA-C	-9.47	93.09	108.52
2	D	22	VAL	N-CA-C	9.34	120.22	108.82
2	D	335	LEU	N-CA-C	8.59	120.41	111.14
1	B	573	TRP	CA-C-N	8.30	129.10	119.47
1	B	573	TRP	C-N-CA	8.30	129.10	119.47
1	A	558	CYS	CA-C-N	8.27	130.18	119.84
1	A	558	CYS	C-N-CA	8.27	130.18	119.84
2	D	328	ASP	CA-C-N	8.09	127.81	119.56
2	D	328	ASP	C-N-CA	8.09	127.81	119.56
2	D	265	ASN	N-CA-C	7.90	120.40	109.18
1	B	572	SER	N-CA-C	-7.69	103.90	113.28
1	A	708	LYS	N-CA-C	-7.62	102.58	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	327	TYR	N-CA-C	-7.49	104.66	113.88
1	A	707	ASN	N-CA-C	7.33	120.14	111.71
1	B	546	PHE	N-CA-C	-7.01	101.93	113.50
2	C	351	THR	N-CA-C	-6.96	103.46	112.23
2	D	347	ASP	N-CA-C	6.95	121.34	112.86
2	D	346	MET	N-CA-C	6.89	121.27	110.32
2	D	25	THR	N-CA-C	-6.83	97.15	108.34
2	D	96	ASP	N-CA-C	-6.80	104.18	113.30
2	D	288	ASP	N-CA-C	6.78	120.91	110.20
1	A	637	ARG	N-CA-C	6.75	120.53	109.06
2	C	20	VAL	N-CA-C	6.75	113.43	106.21
2	D	136	LEU	N-CA-C	6.42	119.25	108.02
2	D	183	LYS	N-CA-C	6.38	116.42	108.19
1	A	679	GLU	N-CA-C	6.27	118.17	109.15
1	B	708	LYS	N-CA-C	-6.23	103.42	111.02
1	B	597	TRP	N-CA-C	6.20	119.50	109.40
2	C	288	ASP	N-CA-C	6.17	118.87	110.55
2	D	132	VAL	N-CA-C	6.12	122.06	109.34
2	C	327	TYR	N-CA-C	-6.11	106.47	114.04
1	A	641	GLU	CA-C-N	6.10	126.55	119.47
1	A	641	GLU	C-N-CA	6.10	126.55	119.47
2	D	118	PHE	N-CA-C	6.05	119.41	109.85
2	D	26	VAL	N-CA-C	5.97	117.17	108.58
1	A	573	TRP	CA-C-N	5.88	126.03	119.32
1	A	573	TRP	C-N-CA	5.88	126.03	119.32
1	A	744	PRO	N-CA-C	5.85	122.77	112.01
1	B	594	SER	CA-C-N	5.80	127.09	119.84
1	B	594	SER	C-N-CA	5.80	127.09	119.84
1	B	641	GLU	CA-C-N	5.77	125.46	119.05
1	B	641	GLU	C-N-CA	5.77	125.46	119.05
1	B	569	HIS	N-CA-C	-5.77	101.18	109.48
2	C	122	ASP	N-CA-C	-5.72	106.14	113.01
1	B	739	GLY	N-CA-C	-5.66	106.85	115.00
2	D	289	ARG	N-CA-C	-5.65	104.60	113.02
2	D	336	LEU	N-CA-C	5.65	117.89	109.59
1	B	558	CYS	CA-C-N	5.64	126.89	119.84
1	B	558	CYS	C-N-CA	5.64	126.89	119.84
2	D	122	ASP	N-CA-C	-5.62	106.46	113.15
1	B	621	HIS	N-CA-C	-5.61	107.68	114.75
1	A	626	LEU	N-CA-C	5.61	119.06	110.20
1	B	745	LEU	N-CA-C	-5.60	95.99	107.70
1	A	597	TRP	N-CA-C	5.55	117.94	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	546	PHE	N-CA-C	-5.41	104.65	113.19
2	C	336	LEU	N-CA-C	5.39	117.02	108.67
1	B	625	ASN	N-CA-C	-5.30	103.35	110.24
2	C	314	LEU	N-CA-C	-5.28	101.09	109.59
2	D	235	LEU	CA-C-N	5.28	126.44	119.84
2	D	235	LEU	C-N-CA	5.28	126.44	119.84
1	B	720	VAL	N-CA-C	5.18	115.68	108.84
1	A	711	ASN	N-CA-C	5.18	119.47	113.20
2	C	330	ARG	N-CA-C	-5.18	107.09	113.41
1	B	580	ARG	N-CA-C	5.15	117.51	109.52
2	C	265	ASN	N-CA-C	5.14	117.66	109.96
2	C	140	HIS	N-CA-C	5.08	117.40	109.52
1	A	770	LYS	CA-C-N	5.06	125.78	120.11
1	A	770	LYS	C-N-CA	5.06	125.78	120.11
2	C	352	GLY	N-CA-C	-5.04	107.86	115.32
1	B	711	ASN	N-CA-C	5.01	119.26	113.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	327	TYR	Sidechain

4.2 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	A	1917	0	1892	126	0
1	B	1917	0	1892	149	0
2	C	2553	0	2485	252	0
2	D	2553	0	2485	251	0
All	All	8940	0	8754	767	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 43.

All (767) 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)
2:C:170:ASN:HB2	2:C:171:PRO:HD2	1.24	1.13
2:D:170:ASN:HB2	2:D:171:PRO:HD2	1.14	1.10
1:B:749:GLU:HG2	1:B:754:ILE:HD13	1.33	1.05
2:D:186:LYS:HB3	2:D:188:LEU:HD21	1.40	1.03
2:C:302:VAL:HG22	2:C:368:TYR:HB3	1.45	0.96
2:D:170:ASN:HB2	2:D:171:PRO:CD	1.95	0.96
1:B:598:VAL:HB	1:B:650:LEU:HB2	1.48	0.95
2:C:304:THR:HB	2:C:306:GLU:HG2	1.50	0.93
2:D:282:LYS:HB3	2:D:283:PRO:HD2	1.48	0.92
1:B:611:PRO:HB3	1:B:635:VAL:HG12	1.50	0.91
2:C:224:VAL:HG22	2:C:270:ILE:HD12	1.55	0.87
2:C:101:ILE:HD11	2:C:144:ARG:HG2	1.56	0.87
2:C:348:TYR:HB3	2:C:369:MET:HG2	1.56	0.86
2:C:357:ASN:HD21	2:C:359:ASP:HB3	1.39	0.86
2:D:71:PRO:N	2:D:129:THR:HG22	1.91	0.85
2:D:224:VAL:HG22	2:D:270:ILE:HD12	1.58	0.85
1:B:711:ASN:HD21	1:B:720:VAL:H	1.25	0.84
2:C:282:LYS:HB3	2:C:283:PRO:HD2	1.57	0.84
1:A:682:ILE:HD11	1:A:702:LEU:HG	1.61	0.82
2:D:323:PHE:CD1	2:D:350:LEU:HD11	2.15	0.81
2:C:170:ASN:HB2	2:C:171:PRO:CD	2.06	0.81
2:C:36:LYS:HZ1	2:C:89:ALA:HB3	1.46	0.80
2:D:247:ASN:O	2:D:248:ARG:HB3	1.80	0.80
2:C:283:PRO:HG2	2:C:286:PRO:HG3	1.63	0.80
2:D:186:LYS:HB3	2:D:188:LEU:CD2	2.12	0.79
2:D:357:ASN:HD22	2:D:359:ASP:H	1.27	0.79
2:C:302:VAL:CG2	2:C:368:TYR:HB3	2.11	0.79
2:D:170:ASN:CB	2:D:171:PRO:HD2	2.06	0.79
2:C:226:HIS:HB3	2:C:248:ARG:NH1	1.99	0.78
2:D:196:SER:HB2	2:D:240:GLU:OE2	1.83	0.77
2:C:36:LYS:NZ	2:C:89:ALA:HB3	1.99	0.76
1:A:637:ARG:HB2	1:A:651:LYS:HB3	1.68	0.75
1:A:577:VAL:HG22	1:A:618:LEU:HD23	1.67	0.75
1:B:746:VAL:CG1	1:B:753:TYR:HB3	2.17	0.75
1:B:681:PHE:C	1:B:682:ILE:HD13	2.12	0.75
1:B:586:HIS:CD2	1:B:587:PHE:N	2.54	0.75
2:D:91:VAL:HG13	2:D:96:ASP:HB2	1.68	0.75
2:C:91:VAL:HG13	2:C:96:ASP:HB2	1.67	0.74
1:A:622:GLN:HG3	2:C:313:LEU:HD21	1.69	0.74
2:C:238:ASP:O	2:C:239:GLN:HB3	1.87	0.74
2:D:351:THR:HG22	2:D:353:LYS:HD3	1.69	0.73
1:B:549:GLY:HA2	1:B:575:TRP:CZ3	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:104:ALA:C	2:C:106:ASP:H	1.97	0.73
1:B:746:VAL:HG11	1:B:753:TYR:HB3	1.71	0.73
1:A:666:CYS:SG	1:A:752:LYS:HD3	2.29	0.72
2:D:75:GLU:HB2	2:D:78:ASP:OD2	1.89	0.72
1:A:711:ASN:HD21	1:A:720:VAL:H	1.35	0.72
2:C:340:LEU:HG	2:C:345:ILE:HD12	1.72	0.71
2:D:106:ASP:HB3	2:D:140:HIS:H	1.55	0.71
2:D:130:GLN:O	2:D:132:VAL:HG23	1.90	0.71
2:C:247:ASN:O	2:C:248:ARG:HB3	1.88	0.71
1:B:634:GLU:HG2	1:B:635:VAL:H	1.54	0.71
2:C:245:VAL:HG12	2:C:246:LYS:H	1.56	0.71
2:D:348:TYR:HB3	2:D:369:MET:HG2	1.72	0.71
2:C:170:ASN:CB	2:C:171:PRO:HD2	2.13	0.71
1:A:595:PRO:HG3	1:A:658:ILE:HD11	1.74	0.70
1:A:637:ARG:NH2	1:A:638:LEU:H	1.89	0.70
2:C:132:VAL:HG12	2:C:132:VAL:O	1.89	0.70
1:A:741:ALA:HA	1:A:759:THR:HG22	1.72	0.70
2:D:264:ILE:HG22	2:D:265:ASN:H	1.54	0.70
1:B:679:GLU:OE1	1:B:679:GLU:HA	1.91	0.70
2:D:281:GLU:O	2:D:282:LYS:HG3	1.92	0.70
1:B:769:ASN:O	1:B:770:LYS:HG2	1.90	0.70
1:A:733:GLY:H	1:A:766:ALA:HB1	1.57	0.70
2:C:350:LEU:HA	2:C:369:MET:HE2	1.74	0.70
2:D:196:SER:O	2:D:200:LEU:HB2	1.91	0.70
2:C:94:ASN:HD21	2:C:234:ILE:H	1.40	0.69
2:C:291:HIS:ND1	2:C:292:LEU:HD23	2.07	0.69
2:C:16:SER:OG	2:C:132:VAL:HA	1.92	0.69
2:C:184:LEU:HD12	2:C:185:LEU:N	2.07	0.69
1:B:634:GLU:HG2	1:B:635:VAL:N	2.06	0.69
1:B:682:ILE:HD13	1:B:682:ILE:N	2.07	0.68
2:D:104:ALA:C	2:D:106:ASP:H	2.02	0.68
2:D:263:GLU:HG3	2:D:264:ILE:N	2.07	0.68
2:D:302:VAL:HG22	2:D:368:TYR:HB3	1.76	0.68
2:D:338:ASN:HB3	2:D:350:LEU:HG	1.76	0.68
2:C:297:ILE:O	2:C:310:SER:HA	1.93	0.68
2:D:101:ILE:HD11	2:D:144:ARG:HG2	1.76	0.68
1:A:543:ALA:HB3	1:A:544:PRO:HD3	1.75	0.67
2:C:23:ALA:HB3	2:C:140:HIS:CD2	2.30	0.67
2:D:190:ILE:O	2:D:245:VAL:HB	1.93	0.67
2:D:331:ASP:HA	2:D:334:LYS:HD3	1.76	0.67
2:C:172:ASP:CG	2:C:173:ASP:H	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:172:ASP:CG	2:C:173:ASP:N	2.53	0.67
1:B:745:LEU:HD23	1:B:774:TYR:CE2	2.30	0.67
2:C:338:ASN:HD22	2:C:338:ASN:C	2.02	0.67
2:D:153:ASN:O	2:D:249:GLU:HG3	1.95	0.67
2:C:339:ASN:ND2	2:C:341:ASP:HB2	2.10	0.66
2:D:152:GLN:HA	2:D:152:GLN:NE2	2.10	0.66
2:D:223:ILE:HG23	2:D:234:ILE:HA	1.75	0.66
2:D:35:LEU:HD22	2:D:87:LEU:HD13	1.76	0.66
2:D:198:GLU:O	2:D:201:ALA:HB3	1.95	0.66
2:C:269:LEU:C	2:C:270:ILE:HD13	2.21	0.66
1:A:725:LEU:CD2	1:A:774:TYR:HB2	2.24	0.66
1:B:580:ARG:HD2	1:B:617:ILE:HD13	1.76	0.66
2:C:282:LYS:HB3	2:C:283:PRO:CD	2.25	0.66
2:D:151:ILE:HG23	2:D:249:GLU:OE1	1.95	0.66
1:A:676:ASP:HB2	1:A:706:GLU:HB2	1.78	0.65
1:B:707:ASN:H	1:B:707:ASN:HD22	1.44	0.65
2:D:162:TYR:CE1	2:D:164:VAL:HB	2.31	0.65
1:A:572:SER:C	1:A:574:PRO:HD3	2.21	0.65
2:C:148:GLU:CD	2:C:148:GLU:H	2.04	0.65
2:C:226:HIS:CD2	2:C:246:LYS:HD3	2.32	0.65
2:C:357:ASN:ND2	2:C:359:ASP:HB3	2.10	0.65
1:B:774:TYR:CD1	1:B:774:TYR:N	2.65	0.65
2:C:196:SER:HB2	2:C:240:GLU:OE2	1.96	0.65
2:D:162:TYR:HE1	2:D:164:VAL:HB	1.62	0.64
1:A:605:LEU:HD13	1:A:638:LEU:HD22	1.78	0.64
1:A:637:ARG:HH21	1:A:638:LEU:H	1.45	0.64
1:A:682:ILE:HD11	1:A:702:LEU:CG	2.27	0.64
2:C:111:ASP:OD2	2:C:115:LYS:HB3	1.98	0.64
1:B:626:LEU:HD11	1:B:630:VAL:HG11	1.80	0.64
2:C:284:TYR:C	2:C:286:PRO:HD2	2.22	0.64
2:D:137:LEU:HD12	2:D:137:LEU:C	2.22	0.64
2:C:153:ASN:O	2:C:249:GLU:HA	1.97	0.64
2:D:92:HIS:O	2:D:234:ILE:HD13	1.97	0.64
2:C:77:ALA:O	2:C:81:LYS:HB2	1.98	0.64
1:A:562:VAL:O	1:A:688:THR:HA	1.98	0.64
1:A:586:HIS:CE1	1:A:685:TRP:HB2	2.31	0.64
2:D:163:THR:HB	2:D:182:THR:HB	1.80	0.64
1:B:616:VAL:C	1:B:617:ILE:HD12	2.23	0.64
2:D:144:ARG:HG3	2:D:144:ARG:HH11	1.62	0.64
1:B:626:LEU:CD1	1:B:630:VAL:HG11	2.28	0.63
1:B:603:HIS:HA	1:B:606:GLU:HG3	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:347:ASP:O	2:C:371:LYS:HA	1.98	0.63
2:D:172:ASP:CG	2:D:173:ASP:H	2.06	0.63
2:D:163:THR:CB	2:D:182:THR:HB	2.29	0.63
1:A:761:TRP:CZ2	1:A:773:VAL:HG21	2.34	0.63
2:D:245:VAL:HG12	2:D:246:LYS:H	1.64	0.63
1:B:682:ILE:HG23	1:B:745:LEU:HD22	1.80	0.63
1:B:711:ASN:HD21	1:B:720:VAL:N	1.96	0.63
2:C:112:ARG:O	2:C:112:ARG:HG2	1.98	0.63
2:C:284:TYR:O	2:C:286:PRO:HD2	1.98	0.63
1:B:668:PRO:HB3	1:B:754:ILE:HG21	1.80	0.62
2:D:192:ASP:O	2:D:245:VAL:HG23	1.99	0.62
1:A:725:LEU:HD21	1:A:774:TYR:HB2	1.80	0.62
2:D:145:PRO:O	2:D:147:LYS:HG2	1.99	0.62
2:C:207:LEU:HD11	2:C:214:TYR:O	1.99	0.62
1:B:628:PRO:O	1:B:630:VAL:N	2.32	0.62
2:D:15:ASN:HD22	2:D:16:SER:H	1.45	0.62
1:A:756:GLN:HE21	1:A:756:GLN:HA	1.65	0.62
1:A:759:THR:HA	1:A:774:TYR:CD2	2.35	0.62
2:C:190:ILE:O	2:C:245:VAL:HB	1.99	0.62
1:B:633:ILE:HG22	1:B:634:GLU:H	1.62	0.62
2:C:158:VAL:HG11	2:C:268:ASP:OD1	2.00	0.62
2:C:188:LEU:HB3	2:C:192:ASP:OD2	2.00	0.62
2:C:302:VAL:HG23	2:C:369:MET:O	1.99	0.62
2:D:163:THR:HG22	2:D:269:LEU:HD11	1.80	0.62
1:A:586:HIS:C	1:A:586:HIS:CD2	2.77	0.61
1:B:748:PHE:HB2	1:B:753:TYR:CE1	2.35	0.61
2:D:282:LYS:HB3	2:D:283:PRO:CD	2.28	0.61
1:B:709:VAL:O	1:B:712:ARG:HG3	2.00	0.61
2:D:357:ASN:OD1	2:D:364:ILE:HB	2.01	0.61
1:A:756:GLN:HA	1:A:756:GLN:NE2	2.16	0.61
1:B:637:ARG:HA	1:B:637:ARG:NE	2.16	0.61
2:D:187:THR:O	2:D:187:THR:HG22	2.01	0.61
2:C:344:GLY:HA2	2:C:346:MET:HE2	1.81	0.61
2:D:20:VAL:HA	2:D:137:LEU:HB3	1.83	0.61
2:D:184:LEU:O	2:D:185:LEU:HD23	2.01	0.61
2:D:238:ASP:O	2:D:239:GLN:HB3	1.99	0.61
2:D:269:LEU:HD12	2:D:270:ILE:N	2.16	0.61
2:C:309:LYS:HG2	2:C:310:SER:H	1.65	0.60
1:B:639:PHE:HB2	1:B:649:LEU:HB2	1.84	0.60
1:A:554:GLU:OE2	1:A:555:PRO:HD2	2.00	0.60
1:B:581:THR:HG23	1:B:585:MET:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:286:PRO:HB2	2:C:287:PHE:CE1	2.37	0.60
2:D:264:ILE:HG22	2:D:265:ASN:N	2.16	0.60
1:B:626:LEU:HD11	1:B:630:VAL:CG1	2.32	0.60
2:C:162:TYR:CE1	2:C:164:VAL:HB	2.36	0.60
1:A:637:ARG:HH21	1:A:638:LEU:HB2	1.65	0.60
1:A:593:ILE:HG22	1:A:594:SER:N	2.17	0.60
1:A:549:GLY:HA2	1:A:575:TRP:CZ3	2.37	0.60
1:B:556:LYS:O	1:B:699:GLU:OE2	2.20	0.60
1:B:749:GLU:CG	1:B:754:ILE:HD13	2.23	0.59
2:D:75:GLU:HA	2:D:75:GLU:OE1	2.02	0.59
2:C:101:ILE:HD11	2:C:144:ARG:CG	2.31	0.59
2:D:188:LEU:HB3	2:D:192:ASP:CG	2.26	0.59
1:A:603:HIS:HA	1:A:606:GLU:HG3	1.84	0.59
2:D:155:ALA:O	2:D:190:ILE:HD11	2.02	0.59
2:D:323:PHE:CE1	2:D:350:LEU:HD21	2.37	0.59
2:D:159:ASP:OD1	2:D:187:THR:HG23	2.02	0.59
2:D:283:PRO:CG	2:D:286:PRO:HG3	2.33	0.59
1:B:633:ILE:HG22	1:B:634:GLU:N	2.15	0.59
1:B:754:ILE:HD12	1:B:754:ILE:N	2.18	0.59
2:C:192:ASP:N	2:C:192:ASP:OD1	2.34	0.59
2:D:357:ASN:ND2	2:D:359:ASP:H	1.99	0.59
2:C:284:TYR:CD2	2:C:285:ASP:HB2	2.37	0.59
2:D:31:GLN:HA	2:D:31:GLN:OE1	2.01	0.59
1:A:577:VAL:CG2	1:A:618:LEU:HD23	2.33	0.59
1:B:615:LYS:HG2	1:B:617:ILE:HD11	1.85	0.59
2:C:153:ASN:O	2:C:249:GLU:HG3	2.03	0.59
2:C:248:ARG:NH1	2:C:268:ASP:OD1	2.36	0.59
2:C:331:ASP:HA	2:C:334:LYS:HD3	1.83	0.59
2:D:173:ASP:O	2:D:174:ASP:HB2	2.03	0.59
2:D:204:GLN:NE2	2:D:207:LEU:HD12	2.18	0.59
2:D:357:ASN:ND2	2:D:359:ASP:HB3	2.18	0.59
2:C:37:PHE:CD1	2:C:37:PHE:C	2.81	0.58
2:C:302:VAL:O	2:C:302:VAL:HG12	2.03	0.58
2:D:263:GLU:O	2:D:264:ILE:HD13	2.04	0.58
2:C:159:ASP:HA	2:C:187:THR:HG23	1.83	0.58
1:A:709:VAL:O	1:A:712:ARG:HG3	2.02	0.58
2:D:236:PRO:HB3	2:D:239:GLN:NE2	2.17	0.58
2:C:151:ILE:HG21	2:C:248:ARG:O	2.03	0.58
2:C:198:GLU:O	2:C:201:ALA:HB3	2.04	0.58
2:C:294:LEU:HD12	2:C:295:PHE:N	2.19	0.58
2:D:172:ASP:CG	2:D:173:ASP:N	2.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:THR:HG22	2:D:244:HIS:HB3	1.86	0.58
1:A:641:GLU:HB2	1:A:647:ILE:CG2	2.34	0.58
1:B:710:CYS:SG	1:B:716:LEU:HD12	2.44	0.58
2:D:91:VAL:HG13	2:D:96:ASP:CB	2.34	0.58
2:D:214:TYR:CD1	2:D:278:LYS:HA	2.38	0.58
2:D:340:LEU:HB3	2:D:345:ILE:HB	1.84	0.58
2:C:76:LYS:HE3	2:C:103:PHE:HD2	1.69	0.57
2:C:162:TYR:HE2	2:C:199:LEU:HD22	1.69	0.57
2:C:323:PHE:HA	2:C:336:LEU:O	2.04	0.57
2:D:265:ASN:H	2:D:265:ASN:HD22	1.52	0.57
2:C:324:ARG:N	2:C:336:LEU:O	2.35	0.57
2:C:152:GLN:HA	2:C:152:GLN:NE2	2.19	0.57
1:B:543:ALA:HB3	1:B:544:PRO:HD3	1.86	0.57
2:D:189:ALA:H	2:D:192:ASP:CG	2.12	0.57
2:C:121:LYS:HE2	2:C:121:LYS:HA	1.86	0.57
1:B:725:LEU:HD21	1:B:774:TYR:HB2	1.86	0.57
2:D:285:ASP:O	2:D:286:PRO:C	2.48	0.57
2:C:154:GLN:OE1	2:C:154:GLN:HA	2.05	0.57
2:C:164:VAL:HG23	2:C:272:GLU:HB3	1.87	0.57
1:B:759:THR:HA	1:B:774:TYR:CD2	2.40	0.56
2:C:284:TYR:CE2	2:C:285:ASP:HB2	2.40	0.56
2:C:328:ASP:OD1	2:C:330:ARG:HD3	2.05	0.56
1:A:563:VAL:O	1:A:734:THR:HA	2.06	0.56
2:D:15:ASN:ND2	2:D:16:SER:H	2.03	0.56
2:D:284:TYR:C	2:D:286:PRO:HD2	2.31	0.56
1:A:586:HIS:CD2	1:A:587:PHE:N	2.73	0.56
1:A:640:LEU:O	1:A:641:GLU:C	2.48	0.56
1:A:668:PRO:HD2	1:A:781:VAL:HG22	1.86	0.56
1:B:577:VAL:CG1	1:B:616:VAL:HG13	2.35	0.56
2:D:304:THR:HB	2:D:306:GLU:HG2	1.86	0.56
2:D:100:VAL:HG13	2:D:141:VAL:HG11	1.87	0.56
2:D:165:GLN:CB	2:D:273:LYS:HG3	2.36	0.56
1:A:685:TRP:CE2	1:A:697:LEU:HB2	2.40	0.56
1:B:784:ILE:HG22	1:B:785:GLU:N	2.19	0.56
2:C:246:LYS:HB3	2:C:248:ARG:NH2	2.21	0.56
1:B:649:LEU:O	1:B:650:LEU:HD23	2.05	0.56
1:A:687:GLU:HB3	1:A:737:CYS:HB3	1.87	0.56
2:C:363:ARG:HH11	2:C:363:ARG:CG	2.18	0.56
2:D:15:ASN:ND2	2:D:16:SER:N	2.53	0.56
1:A:733:GLY:N	1:A:766:ALA:HB1	2.21	0.56
1:B:562:VAL:HG23	1:B:740:ASP:OD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:ARG:CZ	1:A:638:LEU:H	2.19	0.55
2:C:35:LEU:HD12	2:C:36:LYS:H	1.72	0.55
2:D:88:ILE:O	2:D:91:VAL:HG23	2.05	0.55
1:B:682:ILE:HD11	1:B:702:LEU:HG	1.88	0.55
2:C:71:PRO:N	2:C:129:THR:HG22	2.21	0.55
2:C:72:HIS:HD2	2:C:73:LYS:N	2.04	0.55
2:C:88:ILE:HG23	2:C:88:ILE:O	2.06	0.55
1:A:756:GLN:HE21	1:A:756:GLN:CA	2.19	0.55
2:C:183:LYS:H	2:C:183:LYS:HD3	1.70	0.55
2:C:226:HIS:HB3	2:C:248:ARG:HH12	1.70	0.55
2:D:130:GLN:O	2:D:132:VAL:N	2.40	0.55
2:C:183:LYS:HG2	2:C:184:LEU:N	2.22	0.55
1:B:581:THR:HG21	1:B:585:MET:HE2	1.89	0.55
1:B:591:THR:HG21	1:B:755:LEU:HD13	1.89	0.55
2:D:23:ALA:HB3	2:D:140:HIS:CD2	2.41	0.55
2:D:130:GLN:OE1	2:D:130:GLN:HA	2.07	0.54
2:C:302:VAL:HG21	2:C:351:THR:OG1	2.07	0.54
2:D:171:PRO:O	2:D:172:ASP:HB2	2.07	0.54
2:D:219:ARG:NH2	2:D:274:TYR:OH	2.40	0.54
2:D:265:ASN:H	2:D:265:ASN:ND2	2.05	0.54
2:C:226:HIS:NE2	2:C:246:LYS:HD3	2.23	0.54
2:C:192:ASP:O	2:C:244:HIS:HA	2.06	0.54
2:C:108:THR:HG23	2:C:116:VAL:HG13	1.89	0.54
1:B:599:LEU:HD11	1:B:647:ILE:HG12	1.89	0.54
2:C:28:GLY:O	2:C:30:ASN:N	2.41	0.54
2:C:294:LEU:HD12	2:C:295:PHE:H	1.73	0.54
1:A:761:TRP:NE1	1:A:773:VAL:HG11	2.23	0.54
2:C:204:GLN:HE22	2:C:207:LEU:HD12	1.73	0.54
2:C:325:ASP:HB3	2:C:331:ASP:OD2	2.08	0.54
2:D:165:GLN:HB2	2:D:273:LYS:HG3	1.89	0.54
2:D:269:LEU:C	2:D:270:ILE:HD13	2.33	0.54
1:B:668:PRO:HD2	1:B:781:VAL:CG2	2.38	0.53
2:D:244:HIS:O	2:D:245:VAL:C	2.51	0.53
1:A:711:ASN:ND2	1:A:718:GLY:HA2	2.23	0.53
1:B:691:THR:HG22	1:B:692:PHE:N	2.23	0.53
1:B:711:ASN:ND2	1:B:718:GLY:CA	2.71	0.53
2:C:188:LEU:HD13	2:C:192:ASP:HB2	1.90	0.53
2:C:236:PRO:HB3	2:C:239:GLN:NE2	2.22	0.53
2:C:323:PHE:HA	2:C:336:LEU:HB2	1.90	0.53
2:D:284:TYR:O	2:D:286:PRO:HD2	2.07	0.53
2:C:106:ASP:HB3	2:C:140:HIS:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:183:LYS:HE2	2:C:206:ILE:HD11	1.90	0.53
2:D:161:GLU:HB3	2:D:269:LEU:HD13	1.90	0.53
2:D:245:VAL:HG12	2:D:246:LYS:N	2.23	0.53
1:B:686:GLY:HA3	1:B:740:ASP:OD1	2.09	0.53
1:B:782:THR:HG22	1:B:783:TRP:N	2.23	0.53
2:D:73:LYS:HA	2:D:125:VAL:O	2.09	0.53
1:B:681:PHE:CD1	1:B:681:PHE:N	2.76	0.53
2:C:94:ASN:ND2	2:C:234:ILE:H	2.06	0.53
2:C:244:HIS:O	2:C:245:VAL:C	2.51	0.53
1:A:627:GLU:O	1:A:630:VAL:HB	2.08	0.53
2:C:151:ILE:HG13	2:C:248:ARG:N	2.24	0.53
2:C:357:ASN:ND2	2:C:359:ASP:CB	2.71	0.53
2:D:101:ILE:HB	2:D:142:ARG:HB3	1.90	0.53
2:D:151:ILE:HD12	2:D:249:GLU:N	2.22	0.53
2:D:351:THR:CG2	2:D:353:LYS:HD3	2.35	0.53
2:D:338:ASN:CB	2:D:350:LEU:HG	2.39	0.53
2:C:127:LEU:HD22	2:C:135:PHE:CD2	2.44	0.53
1:B:711:ASN:ND2	1:B:718:GLY:HA2	2.24	0.52
1:A:605:LEU:HD12	1:A:640:LEU:HD21	1.91	0.52
1:B:609:PRO:HB2	2:D:237:MET:HE1	1.91	0.52
1:B:707:ASN:HD21	1:B:776:ARG:HH22	1.56	0.52
2:D:155:ALA:HB1	2:D:266:ASN:OD1	2.08	0.52
2:D:188:LEU:HB3	2:D:192:ASP:OD2	2.09	0.52
1:B:581:THR:CG2	1:B:585:MET:HB2	2.40	0.52
2:D:100:VAL:HG13	2:D:141:VAL:CG1	2.40	0.52
2:C:186:LYS:HB3	2:C:188:LEU:HD21	1.91	0.52
2:C:204:GLN:HA	2:C:204:GLN:HE21	1.74	0.52
2:C:237:MET:HG3	2:C:238:ASP:H	1.75	0.52
2:D:122:ASP:C	2:D:124:SER:H	2.16	0.52
1:A:586:HIS:HD2	1:A:587:PHE:N	2.08	0.52
1:B:711:ASN:HD22	1:B:718:GLY:CA	2.23	0.52
2:D:186:LYS:HD2	2:D:188:LEU:HD21	1.91	0.52
2:C:159:ASP:CA	2:C:187:THR:HG23	2.39	0.52
2:D:309:LYS:HG2	2:D:310:SER:H	1.75	0.52
1:A:641:GLU:HB2	1:A:647:ILE:HG23	1.90	0.52
1:B:594:SER:HB2	1:B:595:PRO:HD2	1.91	0.52
2:C:72:HIS:HD2	2:C:73:LYS:H	1.58	0.52
2:C:104:ALA:C	2:C:106:ASP:N	2.66	0.52
2:C:288:ASP:HB3	2:C:291:HIS:NE2	2.25	0.52
2:D:246:LYS:O	2:D:247:ASN:HB2	2.09	0.52
2:C:137:LEU:HD12	2:C:138:SER:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:161:GLU:HG3	2:C:183:LYS:O	2.09	0.52
2:C:346:MET:O	2:C:347:ASP:HB2	2.10	0.52
2:D:207:LEU:HD11	2:D:214:TYR:C	2.35	0.52
2:D:163:THR:OG1	2:D:182:THR:HB	2.10	0.51
1:B:641:GLU:HA	1:B:783:TRP:CZ2	2.45	0.51
2:C:184:LEU:HD12	2:C:185:LEU:H	1.71	0.51
2:D:79:LEU:O	2:D:83:ILE:HG13	2.11	0.51
1:A:637:ARG:NE	1:A:638:LEU:H	2.08	0.51
2:C:161:GLU:HB3	2:C:269:LEU:CD1	2.40	0.51
1:B:602:ALA:HB3	1:B:646:ASP:HA	1.93	0.51
2:C:251:ALA:C	2:C:263:GLU:HB3	2.34	0.51
2:D:99:GLU:HG3	2:D:146:TYR:HA	1.93	0.51
2:D:269:LEU:HD12	2:D:270:ILE:H	1.74	0.51
2:D:302:VAL:CG2	2:D:368:TYR:HB3	2.40	0.51
1:A:706:GLU:OE1	1:A:708:LYS:HB2	2.10	0.51
1:B:668:PRO:O	1:B:781:VAL:HG21	2.10	0.51
2:C:151:ILE:HG21	2:C:248:ARG:C	2.35	0.51
2:C:162:TYR:HE1	2:C:164:VAL:HB	1.74	0.51
1:A:682:ILE:HD11	1:A:702:LEU:CD1	2.40	0.51
1:A:774:TYR:CD1	1:A:774:TYR:N	2.78	0.51
2:D:15:ASN:HD22	2:D:16:SER:N	2.08	0.51
1:A:686:GLY:O	1:A:687:GLU:C	2.54	0.51
1:B:560:GLY:O	1:B:561:ARG:C	2.54	0.51
2:C:13:VAL:O	2:C:15:ASN:N	2.43	0.51
2:C:207:LEU:HD11	2:C:214:TYR:C	2.36	0.51
2:C:214:TYR:CD1	2:C:278:LYS:HA	2.45	0.51
2:C:284:TYR:C	2:C:286:PRO:CD	2.84	0.51
1:A:556:LYS:O	1:A:556:LYS:HG3	2.10	0.51
1:A:640:LEU:HD23	1:A:648:ALA:HB2	1.93	0.51
2:C:163:THR:HG23	2:C:163:THR:O	2.10	0.51
2:D:76:LYS:HB2	2:D:123:GLY:O	2.10	0.51
2:D:283:PRO:HG2	2:D:286:PRO:HG3	1.93	0.51
1:B:637:ARG:HB2	1:B:651:LYS:CB	2.41	0.50
2:C:145:PRO:O	2:C:147:LYS:HG2	2.11	0.50
2:C:184:LEU:C	2:C:185:LEU:HG	2.30	0.50
2:D:159:ASP:HA	2:D:187:THR:HG23	1.93	0.50
2:D:211:HIS:HB2	2:D:214:TYR:CD2	2.46	0.50
2:D:324:ARG:HG3	2:D:331:ASP:O	2.11	0.50
1:A:641:GLU:OE1	1:A:643:THR:N	2.43	0.50
2:D:293:LYS:HD2	2:D:293:LYS:N	2.26	0.50
1:A:579:LEU:HD23	1:A:587:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:TRP:CZ2	1:A:697:LEU:HB2	2.47	0.50
1:B:641:GLU:HB2	1:B:647:ILE:HG22	1.93	0.50
1:B:598:VAL:CB	1:B:650:LEU:HB2	2.32	0.50
2:C:153:ASN:HB3	2:C:249:GLU:CG	2.42	0.50
2:D:26:VAL:HG11	2:D:98:PHE:HE2	1.76	0.50
2:D:99:GLU:CD	2:D:144:ARG:NH2	2.70	0.50
2:D:104:ALA:C	2:D:106:ASP:N	2.69	0.50
2:D:163:THR:HG23	2:D:163:THR:O	2.11	0.50
2:D:194:ILE:HG22	2:D:195:THR:N	2.27	0.50
2:D:216:ILE:HG23	2:D:274:TYR:HB3	1.93	0.50
2:D:323:PHE:CG	2:D:350:LEU:HD11	2.46	0.50
2:C:245:VAL:HG12	2:C:246:LYS:N	2.25	0.50
2:D:144:ARG:HG3	2:D:144:ARG:NH1	2.26	0.50
2:D:153:ASN:O	2:D:249:GLU:HA	2.12	0.50
1:A:686:GLY:HA3	1:A:740:ASP:OD1	2.12	0.50
2:C:338:ASN:HD22	2:C:339:ASN:N	2.09	0.50
2:D:99:GLU:O	2:D:143:VAL:HA	2.12	0.50
2:C:155:ALA:HA	2:C:250:GLN:HA	1.93	0.50
2:D:357:ASN:ND2	2:D:359:ASP:CB	2.75	0.50
2:C:219:ARG:NH2	2:C:274:TYR:OH	2.45	0.49
2:C:311:GLU:OE2	2:C:313:LEU:HD11	2.12	0.49
2:D:71:PRO:HA	2:D:127:LEU:O	2.12	0.49
2:D:111:ASP:HB3	2:D:135:PHE:HE1	1.77	0.49
2:D:158:VAL:HA	2:D:266:ASN:O	2.11	0.49
2:D:130:GLN:C	2:D:132:VAL:N	2.68	0.49
2:D:309:LYS:HG2	2:D:310:SER:N	2.27	0.49
2:D:357:ASN:HD21	2:D:359:ASP:HB3	1.75	0.49
2:D:75:GLU:HB2	2:D:78:ASP:CG	2.36	0.49
2:D:226:HIS:CD2	2:D:246:LYS:HD3	2.47	0.49
1:A:676:ASP:O	1:A:677:ARG:HB2	2.12	0.49
2:C:162:TYR:CE2	2:C:199:LEU:HD22	2.46	0.49
2:C:195:THR:H	2:C:198:GLU:HG3	1.78	0.49
2:C:338:ASN:C	2:C:338:ASN:ND2	2.71	0.49
1:A:660:ASP:OD1	1:A:660:ASP:N	2.46	0.49
2:C:300:VAL:HG12	2:C:301:ASP:O	2.12	0.49
2:D:26:VAL:O	2:D:29:THR:O	2.30	0.49
2:D:277:LEU:C	2:D:279:LYS:H	2.21	0.49
2:D:284:TYR:CD2	2:D:285:ASP:N	2.80	0.49
1:B:628:PRO:C	1:B:630:VAL:H	2.20	0.49
2:C:244:HIS:CD2	2:C:244:HIS:N	2.79	0.49
2:C:247:ASN:O	2:C:248:ARG:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:TRP:CZ3	1:A:651:LYS:HB2	2.47	0.49
1:B:564:GLY:H	1:B:691:THR:HG21	1.77	0.49
2:C:338:ASN:HB3	2:C:350:LEU:HD11	1.94	0.49
2:D:117:TYR:N	2:D:117:TYR:CD1	2.80	0.49
1:B:586:HIS:CD2	1:B:586:HIS:C	2.90	0.49
2:D:36:LYS:NZ	2:D:89:ALA:HB3	2.27	0.49
2:D:163:THR:HA	2:D:182:THR:HA	1.95	0.49
2:C:204:GLN:NE2	2:C:207:LEU:HD12	2.28	0.49
2:D:91:VAL:CG1	2:D:96:ASP:HB2	2.39	0.49
1:B:757:GLY:HA2	1:B:775:VAL:O	2.13	0.49
2:C:88:ILE:O	2:C:88:ILE:CG2	2.59	0.49
2:C:157:SER:OG	2:C:187:THR:HG22	2.12	0.49
2:D:265:ASN:N	2:D:265:ASN:ND2	2.58	0.49
1:B:641:GLU:OE1	1:B:643:THR:N	2.46	0.48
1:B:682:ILE:N	1:B:682:ILE:CD1	2.72	0.48
1:A:600:THR:OG1	1:A:601:ALA:N	2.46	0.48
1:B:629:HIS:CD2	1:B:661:LYS:HD2	2.48	0.48
2:C:286:PRO:HB2	2:C:287:PHE:CD1	2.47	0.48
2:C:338:ASN:HB3	2:C:350:LEU:CD1	2.43	0.48
2:D:73:LYS:HG3	2:D:125:VAL:O	2.14	0.48
2:D:93:SER:OG	2:D:94:ASN:N	2.46	0.48
1:A:557:LYS:O	1:A:559:PRO:HD3	2.14	0.48
1:B:663:ILE:CG2	1:B:664:PRO:HD2	2.44	0.48
2:C:359:ASP:HB3	2:C:362:ASN:O	2.13	0.48
2:C:363:ARG:CG	2:C:363:ARG:NH1	2.77	0.48
2:D:130:GLN:O	2:D:131:PRO:C	2.55	0.48
1:A:781:VAL:O	1:A:785:GLU:HG3	2.14	0.48
2:C:154:GLN:O	2:C:250:GLN:HB2	2.12	0.48
2:D:210:THR:O	2:D:212:PRO:HD3	2.13	0.48
2:D:327:TYR:O	2:D:329:PRO:HD3	2.13	0.48
1:B:543:ALA:N	1:B:544:PRO:HD2	2.29	0.48
1:B:577:VAL:HG13	1:B:616:VAL:HG13	1.95	0.48
2:C:17:GLN:HB2	2:C:40:ILE:O	2.13	0.48
2:C:76:LYS:HE2	2:C:102:ASP:OD1	2.13	0.48
2:D:161:GLU:HB2	2:D:268:ASP:O	2.13	0.48
2:C:101:ILE:O	2:C:102:ASP:HB2	2.14	0.48
2:C:151:ILE:HG13	2:C:248:ARG:CA	2.44	0.48
2:C:94:ASN:OD1	2:C:234:ILE:O	2.32	0.48
2:C:153:ASN:HB3	2:C:249:GLU:HG3	1.94	0.48
2:D:202:GLN:HE21	2:D:202:GLN:HB2	1.51	0.48
2:D:202:GLN:O	2:D:206:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:298:LYS:HE3	2:D:364:ILE:CG2	2.43	0.48
1:A:609:PRO:O	1:A:638:LEU:HD12	2.14	0.48
2:C:132:VAL:HG12	2:D:330:ARG:HB3	1.96	0.48
1:A:677:ARG:HD3	1:A:677:ARG:N	2.29	0.48
1:B:707:ASN:HD22	1:B:707:ASN:N	2.11	0.48
1:B:758:VAL:O	1:B:759:THR:C	2.56	0.48
2:D:99:GLU:OE1	2:D:144:ARG:NH2	2.46	0.48
1:B:575:TRP:O	1:B:577:VAL:HG23	2.14	0.47
1:B:711:ASN:ND2	1:B:720:VAL:H	2.03	0.47
2:C:109:ILE:O	2:C:110:THR:HG23	2.14	0.47
2:D:226:HIS:HB3	2:D:248:ARG:NH1	2.29	0.47
2:D:320:ASN:HB3	2:D:333:ALA:O	2.13	0.47
1:A:629:HIS:CD2	1:A:661:LYS:HD2	2.49	0.47
1:B:785:GLU:O	1:B:786:GLY:C	2.57	0.47
2:C:330:ARG:C	2:C:332:LYS:H	2.22	0.47
1:A:636:SER:OG	1:A:653:SER:HA	2.14	0.47
2:D:336:LEU:HD22	2:D:367:VAL:CG2	2.44	0.47
1:B:563:VAL:HG22	1:B:689:GLN:HB2	1.96	0.47
2:C:357:ASN:HD21	2:C:359:ASP:CB	2.19	0.47
1:A:577:VAL:CG1	1:A:578:SER:N	2.78	0.47
1:A:623:GLU:OE1	2:C:332:LYS:HE2	2.13	0.47
1:A:668:PRO:HD2	1:A:781:VAL:CG2	2.44	0.47
1:B:563:VAL:O	1:B:734:THR:HA	2.14	0.47
2:C:110:THR:HG22	2:C:116:VAL:HA	1.96	0.47
2:C:122:ASP:HB2	2:C:124:SER:OG	2.14	0.47
1:B:543:ALA:HB3	1:B:544:PRO:CD	2.44	0.47
2:C:244:HIS:CD2	2:C:244:HIS:H	2.33	0.47
1:B:628:PRO:C	1:B:630:VAL:N	2.73	0.47
1:B:788:MET:C	1:B:790:ASN:H	2.23	0.47
2:C:169:LEU:HD12	2:C:277:LEU:HD13	1.96	0.47
2:C:118:PHE:CD1	2:C:118:PHE:N	2.82	0.47
2:C:158:VAL:HA	2:C:266:ASN:O	2.14	0.47
2:C:165:GLN:CB	2:C:273:LYS:HG3	2.44	0.47
2:D:16:SER:O	2:D:42:LEU:HB2	2.15	0.47
1:A:551:PRO:HA	1:A:574:PRO:HG2	1.96	0.47
1:A:711:ASN:ND2	1:A:719:ARG:H	2.12	0.47
2:C:224:VAL:HG23	2:C:235:LEU:HD11	1.97	0.47
2:D:195:THR:HG22	2:D:242:THR:HB	1.97	0.47
2:C:193:THR:HG22	2:C:244:HIS:HB3	1.97	0.47
2:C:329:PRO:O	2:C:332:LYS:HD2	2.15	0.47
1:A:679:GLU:HA	1:A:679:GLU:OE1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:ASN:O	1:B:717:ASN:HA	2.14	0.46
2:C:84:GLN:O	2:C:85:GLU:C	2.58	0.46
2:C:363:ARG:NH1	2:C:363:ARG:HG3	2.30	0.46
1:B:637:ARG:NE	1:B:637:ARG:CA	2.78	0.46
2:C:324:ARG:HB2	2:C:334:LYS:HB2	1.96	0.46
2:D:94:ASN:HD21	2:D:234:ILE:H	1.62	0.46
2:D:222:SER:HB3	2:D:272:GLU:HG2	1.97	0.46
2:D:227:ASP:C	2:D:228:ASN:CG	2.82	0.46
1:B:708:LYS:HD2	1:B:708:LYS:HA	1.61	0.46
1:B:789:ARG:O	1:B:789:ARG:HG3	2.15	0.46
2:D:111:ASP:HB3	2:D:135:PHE:CE1	2.50	0.46
1:A:706:GLU:CD	1:A:708:LYS:H	2.23	0.46
2:C:72:HIS:CD2	2:C:73:LYS:N	2.82	0.46
2:C:80:LEU:HD23	2:C:80:LEU:HA	1.75	0.46
2:D:26:VAL:HG23	2:D:31:GLN:O	2.16	0.46
2:D:111:ASP:CB	2:D:135:PHE:HE1	2.28	0.46
2:D:226:HIS:NE2	2:D:246:LYS:HD3	2.31	0.46
2:D:284:TYR:C	2:D:286:PRO:CD	2.88	0.46
2:D:344:GLY:HA2	2:D:346:MET:HE2	1.97	0.46
1:A:761:TRP:CE2	1:A:773:VAL:HG11	2.51	0.46
2:D:122:ASP:C	2:D:124:SER:N	2.72	0.46
2:D:197:GLN:O	2:D:200:LEU:HB3	2.15	0.46
2:D:354:VAL:HG12	2:D:367:VAL:HA	1.97	0.46
1:A:556:LYS:HB3	1:A:569:HIS:CE1	2.51	0.46
1:B:564:GLY:O	1:B:565:GLY:C	2.58	0.46
1:B:745:LEU:CD1	1:B:745:LEU:C	2.89	0.46
2:D:151:ILE:CD1	2:D:248:ARG:HA	2.46	0.46
1:A:580:ARG:HD2	1:A:617:ILE:HD13	1.98	0.46
2:D:281:GLU:C	2:D:282:LYS:HG3	2.41	0.46
1:A:568:ALA:HB3	1:A:697:LEU:HD23	1.98	0.46
1:B:592:LEU:HD23	1:B:664:PRO:HB3	1.96	0.46
1:B:627:GLU:HB3	1:B:628:PRO:HD2	1.98	0.46
1:B:741:ALA:HA	1:B:759:THR:HG22	1.97	0.46
2:C:158:VAL:HG23	2:C:189:ALA:O	2.15	0.46
2:C:196:SER:HG	2:C:241:PHE:H	1.64	0.46
1:A:597:TRP:CZ2	1:A:788:MET:HA	2.50	0.46
2:D:244:HIS:H	2:D:244:HIS:CD2	2.34	0.46
2:C:250:GLN:NE2	2:C:251:ALA:C	2.74	0.46
2:C:264:ILE:HD12	2:C:264:ILE:O	2.16	0.46
2:D:132:VAL:O	2:D:132:VAL:HG12	2.15	0.46
2:D:207:LEU:HD11	2:D:214:TYR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:284:TYR:CD2	2:D:285:ASP:HB2	2.51	0.46
1:A:702:LEU:HD13	1:A:728:GLY:HA2	1.97	0.45
1:B:746:VAL:HG13	1:B:753:TYR:HB3	1.93	0.45
1:A:587:PHE:HE1	1:A:604:CYS:HB3	1.81	0.45
1:B:624:VAL:HG21	2:D:332:LYS:HB3	1.97	0.45
2:C:161:GLU:HB3	2:C:269:LEU:HD12	1.98	0.45
1:B:587:PHE:CD1	1:B:587:PHE:C	2.93	0.45
2:C:165:GLN:HB3	2:C:273:LYS:HG3	1.99	0.45
1:A:726:CYS:HA	1:A:772:GLY:O	2.17	0.45
2:D:193:THR:HG22	2:D:244:HIS:CB	2.46	0.45
1:A:713:TYR:HA	1:A:717:ASN:OD1	2.16	0.45
1:B:745:LEU:HD23	1:B:774:TYR:CD2	2.52	0.45
2:C:331:ASP:OD1	2:C:334:LYS:HE2	2.17	0.45
2:C:339:ASN:C	2:C:341:ASP:H	2.25	0.45
2:D:247:ASN:HD22	2:D:247:ASN:HA	1.59	0.45
1:A:687:GLU:OE2	1:A:689:GLN:N	2.42	0.45
1:B:746:VAL:HG22	1:B:755:LEU:HA	1.98	0.45
2:C:73:LYS:HA	2:C:125:VAL:O	2.16	0.45
1:B:644:ARG:HD3	2:D:33:ILE:HG23	1.98	0.45
2:D:118:PHE:CD1	2:D:118:PHE:N	2.84	0.45
1:A:583:PHE:CD1	1:A:583:PHE:N	2.85	0.44
1:B:711:ASN:HD22	1:B:718:GLY:N	2.15	0.44
2:D:75:GLU:O	2:D:76:LYS:C	2.60	0.44
2:D:226:HIS:CE1	2:D:233:THR:OG1	2.70	0.44
1:B:580:ARG:CD	1:B:617:ILE:HD13	2.46	0.44
2:C:100:VAL:HA	2:C:143:VAL:HG12	1.99	0.44
2:C:246:LYS:HB3	2:C:247:ASN:H	1.66	0.44
2:C:284:TYR:CD2	2:C:285:ASP:N	2.85	0.44
1:A:682:ILE:HG23	1:A:745:LEU:CD2	2.47	0.44
2:C:71:PRO:HA	2:C:127:LEU:O	2.17	0.44
2:C:101:ILE:O	2:C:102:ASP:CB	2.66	0.44
1:A:688:THR:O	1:A:691:THR:OG1	2.26	0.44
1:B:592:LEU:CD2	1:B:664:PRO:HB3	2.47	0.44
2:C:104:ALA:O	2:C:106:ASP:N	2.46	0.44
2:D:109:ILE:HG21	2:D:127:LEU:HD21	1.99	0.44
2:D:292:LEU:C	2:D:293:LYS:HD2	2.42	0.44
1:A:638:LEU:HD23	1:A:650:LEU:CD2	2.47	0.44
1:B:692:PHE:CD1	1:B:692:PHE:C	2.96	0.44
2:C:270:ILE:HD13	2:C:270:ILE:N	2.32	0.44
2:D:117:TYR:CD2	2:D:127:LEU:HD23	2.52	0.44
1:A:745:LEU:HA	1:A:745:LEU:HD22	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:207:LEU:O	2:D:207:LEU:HD22	2.17	0.44
2:D:263:GLU:HG3	2:D:264:ILE:H	1.80	0.44
1:A:581:THR:OG1	1:A:585:MET:SD	2.58	0.44
1:A:783:TRP:O	1:A:787:VAL:HG23	2.18	0.44
1:B:566:CYS:O	1:B:698:LYS:HG3	2.18	0.44
1:B:687:GLU:OE2	1:B:689:GLN:N	2.49	0.44
2:C:202:GLN:HE21	2:C:202:GLN:HB2	1.57	0.44
2:D:194:ILE:O	2:D:242:THR:HA	2.18	0.44
2:D:320:ASN:N	2:D:320:ASN:HD22	2.16	0.44
1:A:641:GLU:CD	1:A:643:THR:H	2.25	0.44
1:B:586:HIS:HD2	1:B:587:PHE:N	2.09	0.44
1:B:769:ASN:C	1:B:770:LYS:HG2	2.41	0.44
2:C:39:GLU:H	2:C:39:GLU:HG2	1.52	0.44
2:C:204:GLN:O	2:C:205:SER:C	2.59	0.44
2:C:250:GLN:HE21	2:C:263:GLU:N	2.16	0.44
2:D:188:LEU:HD13	2:D:192:ASP:HB3	1.98	0.44
2:D:265:ASN:N	2:D:265:ASN:HD22	2.12	0.44
1:B:660:ASP:HA	1:B:663:ILE:HD11	2.00	0.43
2:D:111:ASP:OD1	2:D:111:ASP:C	2.61	0.43
1:B:592:LEU:HD23	1:B:664:PRO:CA	2.48	0.43
1:B:691:THR:HG22	1:B:692:PHE:H	1.82	0.43
2:C:151:ILE:HG22	2:C:151:ILE:O	2.17	0.43
2:D:76:LYS:HE3	2:D:103:PHE:HD2	1.83	0.43
1:A:676:ASP:OD1	1:A:677:ARG:NH1	2.51	0.43
2:D:121:LYS:C	2:D:123:GLY:H	2.25	0.43
2:D:244:HIS:CD2	2:D:244:HIS:N	2.85	0.43
1:A:595:PRO:HG3	1:A:658:ILE:CD1	2.44	0.43
1:B:623:GLU:O	1:B:623:GLU:HG2	2.18	0.43
2:C:159:ASP:HA	2:C:187:THR:HA	1.99	0.43
2:C:196:SER:OG	2:C:240:GLU:HG3	2.18	0.43
2:C:204:GLN:O	2:C:207:LEU:HB3	2.17	0.43
2:D:130:GLN:C	2:D:132:VAL:H	2.26	0.43
1:A:707:ASN:N	1:A:707:ASN:HD22	2.16	0.43
2:C:101:ILE:HG12	2:C:143:VAL:HA	2.00	0.43
2:C:155:ALA:HB1	2:C:266:ASN:OD1	2.17	0.43
2:C:75:GLU:CD	2:C:124:SER:HB3	2.43	0.43
2:C:323:PHE:CE2	2:C:350:LEU:HD22	2.53	0.43
2:D:75:GLU:OE1	2:D:124:SER:HB3	2.18	0.43
1:A:570:PRO:HG3	1:A:621:HIS:NE2	2.34	0.43
1:A:658:ILE:CD1	1:A:658:ILE:N	2.80	0.43
1:A:681:PHE:N	1:A:681:PHE:CD1	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:725:LEU:H	1:B:725:LEU:HD23	1.84	0.43
1:B:784:ILE:O	1:B:785:GLU:C	2.62	0.43
2:C:121:LYS:HE2	2:C:121:LYS:CA	2.49	0.43
2:C:169:LEU:HD23	2:C:275:TYR:CD1	2.54	0.43
2:C:320:ASN:N	2:C:320:ASN:HD22	2.17	0.43
2:C:339:ASN:HD21	2:C:341:ASP:HB2	1.81	0.43
2:D:36:LYS:HZ1	2:D:89:ALA:HB3	1.84	0.43
2:C:12:SER:O	2:C:13:VAL:C	2.62	0.43
2:C:156:LYS:HB2	2:C:265:ASN:ND2	2.33	0.43
2:D:99:GLU:CD	2:D:144:ARG:NH1	2.77	0.43
1:A:741:ALA:HA	1:A:759:THR:CG2	2.45	0.43
1:B:555:PRO:HA	1:B:572:SER:HB2	2.00	0.43
2:C:167:THR:HA	2:C:168:PRO:HD3	1.81	0.43
2:C:283:PRO:CG	2:C:286:PRO:HG3	2.39	0.43
2:C:287:PHE:CD1	2:C:287:PHE:N	2.86	0.43
2:D:76:LYS:O	2:D:77:ALA:C	2.62	0.43
2:D:115:LYS:HG2	2:D:117:TYR:CE1	2.53	0.43
2:D:224:VAL:HG11	2:D:243:TYR:CZ	2.54	0.43
1:A:672:TYR:H	1:A:778:SER:HB2	1.83	0.43
1:A:673:VAL:O	1:A:673:VAL:HG12	2.19	0.43
1:B:682:ILE:HD12	1:B:745:LEU:HD22	2.00	0.43
2:C:289:ARG:HA	2:C:292:LEU:HG	2.01	0.43
1:B:558:CYS:HA	1:B:559:PRO:HD2	1.74	0.42
2:C:107:ALA:HA	2:C:138:SER:O	2.19	0.42
2:D:155:ALA:HB1	2:D:266:ASN:CG	2.44	0.42
2:C:16:SER:HG	2:C:132:VAL:HA	1.83	0.42
2:C:351:THR:HG22	2:C:353:LYS:HD3	2.01	0.42
2:D:12:SER:O	2:D:13:VAL:C	2.62	0.42
2:D:165:GLN:HB3	2:D:273:LYS:HG3	2.01	0.42
2:D:193:THR:HA	2:D:243:TYR:O	2.19	0.42
1:A:599:LEU:HD12	1:A:648:ALA:O	2.19	0.42
2:C:155:ALA:HB1	2:C:266:ASN:CG	2.44	0.42
2:C:161:GLU:HB2	2:C:268:ASP:O	2.18	0.42
2:D:196:SER:HG	2:D:241:PHE:H	1.66	0.42
2:D:206:ILE:HA	2:D:209:LYS:HB2	2.01	0.42
1:A:788:MET:C	1:A:790:ASN:H	2.28	0.42
1:A:761:TRP:NE1	1:A:773:VAL:CG1	2.82	0.42
1:B:685:TRP:CZ2	1:B:697:LEU:HD13	2.55	0.42
1:B:689:GLN:C	1:B:691:THR:H	2.27	0.42
1:B:711:ASN:ND2	1:B:719:ARG:N	2.67	0.42
1:B:725:LEU:CD2	1:B:774:TYR:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:127:LEU:HD22	2:C:135:PHE:CE2	2.54	0.42
2:C:130:GLN:C	2:C:132:VAL:N	2.78	0.42
2:C:184:LEU:C	2:C:185:LEU:CG	2.93	0.42
2:C:292:LEU:HD12	2:C:314:LEU:CD1	2.49	0.42
2:D:29:THR:O	2:D:29:THR:HG23	2.20	0.42
2:D:99:GLU:CD	2:D:144:ARG:HH22	2.28	0.42
1:A:713:TYR:CE1	2:C:134:GLU:HG2	2.54	0.42
1:B:583:PHE:HE1	2:D:170:ASN:HA	1.85	0.42
1:B:709:VAL:HG12	1:B:715:PHE:CE2	2.54	0.42
2:C:81:LYS:O	2:C:85:GLU:HG3	2.20	0.42
2:C:92:HIS:O	2:C:234:ILE:HD13	2.20	0.42
2:C:163:THR:HG22	2:C:269:LEU:HD11	2.00	0.42
2:D:162:TYR:CD1	2:D:162:TYR:C	2.98	0.42
2:D:326:LEU:HD23	2:D:326:LEU:HA	1.85	0.42
1:A:573:TRP:N	1:A:574:PRO:HD3	2.33	0.42
2:D:88:ILE:HA	2:D:88:ILE:HD12	1.76	0.42
1:A:624:VAL:HG21	2:C:332:LYS:HB3	2.02	0.42
2:C:349:THR:O	2:C:350:LEU:C	2.63	0.42
1:B:570:PRO:HG3	1:B:621:HIS:CD2	2.55	0.42
1:B:573:TRP:CG	1:B:683:THR:HG21	2.54	0.42
2:C:243:TYR:CE2	2:C:245:VAL:HA	2.55	0.42
2:D:217:TYR:N	2:D:275:TYR:O	2.51	0.42
1:B:580:ARG:HG2	1:B:586:HIS:HA	2.02	0.41
1:B:668:PRO:HD2	1:B:781:VAL:HG22	2.02	0.41
1:B:754:ILE:N	1:B:754:ILE:CD1	2.83	0.41
2:C:169:LEU:HD23	2:C:169:LEU:HA	1.91	0.41
2:D:87:LEU:HD12	2:D:87:LEU:HA	1.91	0.41
1:A:560:GLY:O	1:A:561:ARG:C	2.62	0.41
1:A:782:THR:HG22	1:A:783:TRP:N	2.35	0.41
2:C:24:GLY:O	2:C:32:ASP:HA	2.20	0.41
2:D:196:SER:O	2:D:200:LEU:CB	2.63	0.41
2:D:286:PRO:HB2	2:D:287:PHE:CE1	2.56	0.41
1:B:682:ILE:HG12	1:B:700:ALA:O	2.19	0.41
2:C:30:ASN:HD22	2:C:30:ASN:HA	1.65	0.41
2:D:76:LYS:O	2:D:79:LEU:HB2	2.20	0.41
2:D:200:LEU:HD12	2:D:200:LEU:O	2.21	0.41
2:D:226:HIS:HE1	2:D:233:THR:OG1	2.04	0.41
2:D:328:ASP:OD1	2:D:330:ARG:HD3	2.21	0.41
2:D:353:LYS:O	2:D:368:TYR:HD2	2.04	0.41
1:A:704:VAL:CG1	1:A:705:ILE:N	2.84	0.41
1:A:711:ASN:ND2	1:A:718:GLY:CA	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:788:MET:O	1:B:790:ASN:N	2.54	0.41
2:D:119:ALA:HA	2:D:124:SER:O	2.21	0.41
2:D:153:ASN:HB3	2:D:249:GLU:HG3	2.02	0.41
2:D:247:ASN:O	2:D:248:ARG:CB	2.57	0.41
2:D:293:LYS:N	2:D:293:LYS:CD	2.83	0.41
2:D:299:TYR:HA	2:D:367:VAL:O	2.19	0.41
1:A:637:ARG:HE	1:A:638:LEU:H	1.66	0.41
2:C:216:ILE:HG23	2:C:274:TYR:HB3	2.02	0.41
2:C:243:TYR:CE1	2:C:245:VAL:O	2.73	0.41
2:C:357:ASN:C	2:C:359:ASP:H	2.28	0.41
2:D:183:LYS:HB2	2:D:184:LEU:H	1.64	0.41
1:B:579:LEU:HD12	1:B:579:LEU:HA	1.82	0.41
1:B:632:GLU:OE2	1:B:632:GLU:O	2.38	0.41
2:C:102:ASP:CG	2:C:103:PHE:N	2.78	0.41
2:C:148:GLU:OE1	2:C:148:GLU:N	2.50	0.41
2:C:206:ILE:HA	2:C:209:LYS:HB2	2.03	0.41
2:C:229:ASP:O	2:C:230:ILE:C	2.64	0.41
2:C:320:ASN:HB3	2:C:333:ALA:O	2.20	0.41
2:D:352:GLY:C	2:D:353:LYS:HD2	2.45	0.41
2:D:367:VAL:HG12	2:D:369:MET:HE3	2.03	0.41
2:C:156:LYS:HB2	2:C:157:SER:H	1.68	0.41
2:C:281:GLU:O	2:C:282:LYS:HG3	2.20	0.41
2:D:159:ASP:OD1	2:D:187:THR:CG2	2.69	0.41
1:A:606:GLU:O	2:C:92:HIS:HE1	2.04	0.41
1:A:626:LEU:HD11	1:A:630:VAL:HG11	2.03	0.41
1:A:711:ASN:HD21	1:A:720:VAL:N	2.12	0.41
1:B:548:CYS:C	1:B:666:CYS:SG	3.04	0.41
1:B:624:VAL:O	1:B:625:ASN:C	2.61	0.41
1:B:660:ASP:N	1:B:660:ASP:OD1	2.53	0.41
2:C:26:VAL:CG1	2:C:29:THR:HG23	2.51	0.41
2:C:71:PRO:CA	2:C:129:THR:HG22	2.50	0.41
2:C:323:PHE:CD2	2:C:350:LEU:CD1	3.04	0.41
2:D:37:PHE:CD1	2:D:37:PHE:C	2.99	0.41
2:D:227:ASP:C	2:D:229:ASP:H	2.29	0.41
2:D:245:VAL:CG1	2:D:246:LYS:H	2.28	0.41
2:D:357:ASN:HD22	2:D:359:ASP:N	2.06	0.41
1:B:581:THR:HG21	1:B:585:MET:HB2	2.03	0.41
1:B:711:ASN:OD1	1:B:720:VAL:HB	2.21	0.41
2:C:161:GLU:HB3	2:C:269:LEU:HD13	2.03	0.41
2:D:33:ILE:N	2:D:33:ILE:CD1	2.84	0.41
1:A:641:GLU:HG3	1:A:780:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:GLY:CA	1:A:766:ALA:HB1	2.50	0.40
1:B:593:ILE:HG12	1:B:599:LEU:HB2	2.03	0.40
1:B:600:THR:OG1	1:B:601:ALA:N	2.54	0.40
2:C:183:LYS:HD3	2:C:183:LYS:N	2.34	0.40
2:C:220:ASP:HB3	2:C:273:LYS:O	2.21	0.40
2:C:323:PHE:CD1	2:C:323:PHE:N	2.88	0.40
2:D:157:SER:OG	2:D:187:THR:HG22	2.21	0.40
2:D:336:LEU:HD22	2:D:367:VAL:HG21	2.02	0.40
2:D:357:ASN:ND2	2:D:359:ASP:N	2.68	0.40
1:A:637:ARG:HH21	1:A:638:LEU:CB	2.32	0.40
1:A:640:LEU:HD23	1:A:648:ALA:CB	2.51	0.40
1:B:705:ILE:HG22	1:B:710:CYS:HB2	2.04	0.40
2:C:188:LEU:HD13	2:C:192:ASP:CB	2.50	0.40
2:D:196:SER:OG	2:D:240:GLU:HG3	2.20	0.40
1:A:543:ALA:N	1:A:544:PRO:CD	2.84	0.40
1:B:569:HIS:O	1:B:572:SER:HB3	2.21	0.40
1:B:609:PRO:HB3	2:D:92:HIS:CD2	2.56	0.40
2:C:36:LYS:HZ3	2:C:89:ALA:HB3	1.83	0.40
2:C:285:ASP:N	2:C:286:PRO:CD	2.85	0.40
2:D:160:VAL:HG23	2:D:186:LYS:O	2.21	0.40
1:A:577:VAL:HG22	1:A:618:LEU:CD2	2.47	0.40
1:B:593:ILE:HD12	1:B:667:LEU:HD21	2.03	0.40
2:D:151:ILE:HG13	2:D:248:ARG:N	2.36	0.40
1:A:558:CYS:HA	1:A:559:PRO:HD2	1.90	0.40
1:A:637:ARG:HH21	1:A:638:LEU:N	2.15	0.40
1:A:651:LYS:HE3	1:A:791:ASN:OXT	2.21	0.40
1:B:569:HIS:O	1:B:570:PRO:C	2.64	0.40
1:B:637:ARG:HB2	1:B:651:LYS:HB3	2.02	0.40

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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	246/250 (98%)	212 (86%)	28 (11%)	6 (2%)	4	18
1	B	128/250 (51%)	105 (82%)	18 (14%)	5 (4%)	2	10
2	C	58/186 (31%)	45 (78%)	11 (19%)	2 (3%)	3	12
2	D	62/186 (33%)	44 (71%)	13 (21%)	5 (8%)	1	1
All	All	494/872 (57%)	406 (82%)	70 (14%)	18 (4%)	2	11

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	629	HIS
2	D	188	LEU
1	B	628	PRO
1	B	644	ARG
2	D	185	LEU
1	A	547	ASP
1	A	789	ARG
1	B	587	PHE
2	C	279	LYS
2	D	283	PRO
1	A	559	PRO
1	A	749	GLU
2	D	192	ASP
1	A	687	GLU
2	D	279	LYS
1	A	787	VAL
2	C	132	VAL
1	B	690	GLY

4.3.2 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	A	209/209 (100%)	157 (75%)	52 (25%)	0	2
1	B	209/209 (100%)	168 (80%)	41 (20%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	288/162 (178%)	204 (71%)	84 (29%)	0	1
2	D	288/162 (178%)	212 (74%)	76 (26%)	0	2
All	All	994/742 (134%)	741 (74%)	253 (26%)	0	2

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	546	PHE
1	A	552	GLN
1	A	554	GLU
1	A	556	LYS
1	A	558	CYS
1	A	561	ARG
1	A	567	VAL
1	A	579	LEU
1	A	585	MET
1	A	593	ILE
1	A	605	LEU
1	A	608	SER
1	A	613	SER
1	A	618	LEU
1	A	624	VAL
1	A	626	LEU
1	A	627	GLU
1	A	630	VAL
1	A	632	GLU
1	A	633	ILE
1	A	634	GLU
1	A	636	SER
1	A	637	ARG
1	A	653	SER
1	A	654	SER
1	A	658	ILE
1	A	659	THR
1	A	669	SER
1	A	673	VAL
1	A	674	VAL
1	A	677	ARG
1	A	682	ILE
1	A	688	THR
1	A	691	THR

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Mol	Chain	Res	Type
1	A	697	LEU
1	A	698	LYS
1	A	707	ASN
1	A	712	ARG
1	A	714	GLU
1	A	720	VAL
1	A	721	GLN
1	A	725	LEU
1	A	738	GLN
1	A	746	VAL
1	A	749	GLU
1	A	752	LYS
1	A	756	GLN
1	A	774	TYR
1	A	779	ARG
1	A	782	THR
1	A	788	MET
1	A	789	ARG
1	B	546	PHE
1	B	547	ASP
1	B	552	GLN
1	B	554	GLU
1	B	556	LYS
1	B	558	CYS
1	B	585	MET
1	B	591	THR
1	B	593	ILE
1	B	613	SER
1	B	627	GLU
1	B	630	VAL
1	B	632	GLU
1	B	636	SER
1	B	637	ARG
1	B	650	LEU
1	B	653	SER
1	B	654	SER
1	B	669	SER
1	B	681	PHE
1	B	682	ILE
1	B	688	THR
1	B	698	LYS
1	B	704	VAL

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Mol	Chain	Res	Type
1	B	706	GLU
1	B	707	ASN
1	B	708	LYS
1	B	712	ARG
1	B	719	ARG
1	B	722	SER
1	B	738	GLN
1	B	745	LEU
1	B	746	VAL
1	B	752	LYS
1	B	756	GLN
1	B	763	LEU
1	B	770	LYS
1	B	774	TYR
1	B	779	ARG
1	B	782	THR
1	B	789	ARG
2	C	12	SER
2	C	21	SER
2	C	27	GLU
2	C	29	THR
2	C	31	GLN
2	C	36	LYS
2	C	39	GLU
2	C	81	LYS
2	C	88	ILE
2	C	94	ASN
2	C	95	ASP
2	C	110	THR
2	C	112	ARG
2	C	121	LYS
2	C	122	ASP
2	C	124	SER
2	C	130	GLN
2	C	133	GLN
2	C	141	VAL
2	C	147	LYS
2	C	152	GLN
2	C	156	LYS
2	C	157	SER
2	C	159	ASP
2	C	161	GLU

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Mol	Chain	Res	Type
2	C	165	GLN
2	C	167	THR
2	C	169	LEU
2	C	173	ASP
2	C	182	THR
2	C	183	LYS
2	C	184	LEU
2	C	185	LEU
2	C	192	ASP
2	C	195	THR
2	C	196	SER
2	C	198	GLU
2	C	202	GLN
2	C	204	GLN
2	C	205	SER
2	C	207	LEU
2	C	209	LYS
2	C	210	THR
2	C	211	HIS
2	C	219	ARG
2	C	222	SER
2	C	226	HIS
2	C	227	ASP
2	C	228	ASN
2	C	230	ILE
2	C	232	ARG
2	C	235	LEU
2	C	239	GLN
2	C	240	GLU
2	C	242	THR
2	C	244	HIS
2	C	246	LYS
2	C	247	ASN
2	C	249	GLU
2	C	250	GLN
2	C	264	ILE
2	C	265	ASN
2	C	268	ASP
2	C	272	GLU
2	C	273	LYS
2	C	281	GLU
2	C	282	LYS

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Mol	Chain	Res	Type
2	C	287	PHE
2	C	288	ASP
2	C	290	SER
2	C	293	LYS
2	C	298	LYS
2	C	304	THR
2	C	324	ARG
2	C	330	ARG
2	C	334	LYS
2	C	338	ASN
2	C	345	ILE
2	C	349	THR
2	C	354	VAL
2	C	357	ASN
2	C	363	ARG
2	C	369	MET
2	C	371	LYS
2	D	25	THR
2	D	26	VAL
2	D	31	GLN
2	D	33	ILE
2	D	35	LEU
2	D	39	GLU
2	D	74	LEU
2	D	78	ASP
2	D	81	LYS
2	D	83	ILE
2	D	88	ILE
2	D	93	SER
2	D	95	ASP
2	D	108	THR
2	D	110	THR
2	D	112	ARG
2	D	120	ASP
2	D	122	ASP
2	D	130	GLN
2	D	133	GLN
2	D	137	LEU
2	D	147	LYS
2	D	152	GLN
2	D	156	LYS
2	D	159	ASP

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Mol	Chain	Res	Type
2	D	161	GLU
2	D	164	VAL
2	D	165	GLN
2	D	167	THR
2	D	169	LEU
2	D	182	THR
2	D	183	LYS
2	D	185	LEU
2	D	188	LEU
2	D	192	ASP
2	D	195	THR
2	D	196	SER
2	D	198	GLU
2	D	200	LEU
2	D	202	GLN
2	D	205	SER
2	D	207	LEU
2	D	209	LYS
2	D	210	THR
2	D	211	HIS
2	D	215	THR
2	D	219	ARG
2	D	223	ILE
2	D	227	ASP
2	D	228	ASN
2	D	232	ARG
2	D	239	GLN
2	D	240	GLU
2	D	242	THR
2	D	244	HIS
2	D	246	LYS
2	D	247	ASN
2	D	249	GLU
2	D	265	ASN
2	D	267	THR
2	D	273	LYS
2	D	277	LEU
2	D	281	GLU
2	D	282	LYS
2	D	287	PHE
2	D	288	ASP
2	D	330	ARG

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Mol	Chain	Res	Type
2	D	334	LYS
2	D	338	ASN
2	D	340	LEU
2	D	345	ILE
2	D	347	ASP
2	D	351	THR
2	D	357	ASN
2	D	363	ARG
2	D	369	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	569	HIS
1	A	586	HIS
1	A	625	ASN
1	A	701	GLN
1	A	707	ASN
1	A	711	ASN
1	A	729	HIS
1	A	756	GLN
1	A	769	ASN
1	B	569	HIS
1	B	571	HIS
1	B	586	HIS
1	B	621	HIS
1	B	625	ASN
1	B	671	ASN
1	B	707	ASN
1	B	711	ASN
1	B	738	GLN
1	B	756	GLN
1	B	769	ASN
2	C	17	GLN
2	C	30	ASN
2	C	72	HIS
2	C	86	GLN
2	C	94	ASN
2	C	133	GLN
2	C	152	GLN
2	C	204	GLN
2	C	208	ASN

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Mol	Chain	Res	Type
2	C	228	ASN
2	C	239	GLN
2	C	247	ASN
2	C	250	GLN
2	C	265	ASN
2	C	303	ASN
2	C	320	ASN
2	C	338	ASN
2	C	357	ASN
2	C	358	HIS
2	D	15	ASN
2	D	30	ASN
2	D	86	GLN
2	D	92	HIS
2	D	94	ASN
2	D	152	GLN
2	D	204	GLN
2	D	226	HIS
2	D	239	GLN
2	D	247	ASN
2	D	250	GLN
2	D	265	ASN
2	D	305	ASN
2	D	320	ASN
2	D	338	ASN
2	D	357	ASN
2	D	358	HIS

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

4.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	561:ARG	C	562:VAL	N	19.28
1	B	561:ARG	C	562:VAL	N	18.27

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates

EDS was not executed - this section is therefore empty.

5.4 Ligands

EDS was not executed - this section is therefore empty.

5.5 Other polymers

EDS was not executed - this section is therefore empty.