



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:59 PM GMT

PDB ID : 1I7S
Title : ANTHRANILATE SYNTHASE FROM SERRATIA MARCESCENS IN
COMPLEX WITH ITS END PRODUCT INHIBITOR L-TRYPTOPHAN
Authors : Spraggon, G.; Kim, C.; Nguyen-Huu, X.; Yee, M.-C.; Yanofsky, C.; Mills, S.E.
Deposited on : 2001-03-10
Resolution : 2.40 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

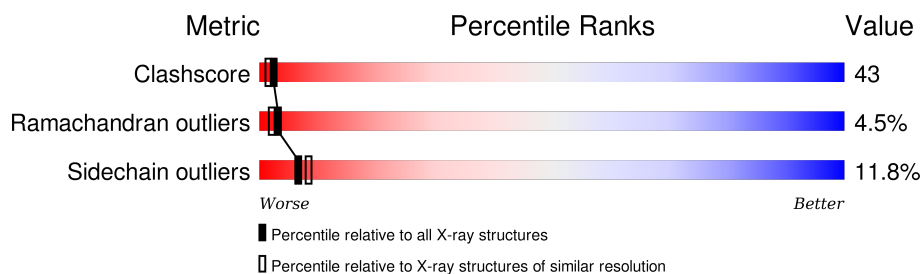
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	519	
1	C	519	
2	B	193	
2	D	193	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10880 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 ANTHRANILATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	0	0
			3966	2474	721	753	18			
1	C	511	Total	C	N	O	S	0	0	0
			3966	2474	721	753	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ARG	PRO	SEE REMARK 999	UNP P00897
A	83	LEU	VAL	see remark 999	UNP P00897
A	130	ILE	LEU	see remark 999	UNP P00897
A	164	LEU	VAL	see remark 999	UNP P00897
A	459	VAL	HIS	see remark 999	UNP P00897
A	461	ASN	HIS	see remark 999	UNP P00897
A	492	PRO	ARG	see remark 999	UNP P00897
A	493	GLU	ARG	see remark 999	UNP P00897
C	60	ARG	PRO	see remark 999	UNP P00897
C	83	LEU	VAL	see remark 999	UNP P00897
C	130	ILE	LEU	see remark 999	UNP P00897
C	164	LEU	VAL	see remark 999	UNP P00897
C	459	VAL	HIS	see remark 999	UNP P00897
C	461	ASN	HIS	see remark 999	UNP P00897
C	492	PRO	ARG	see remark 999	UNP P00897
C	493	GLU	ARG	see remark 999	UNP P00897

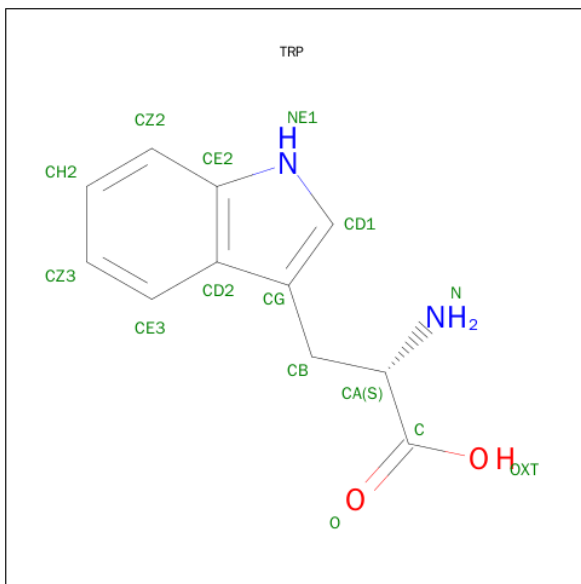
- Molecule 2 is a protein called TRPG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	192	Total	C	N	O	S	0	0	0
			1459	917	265	267	10			
2	D	192	Total	C	N	O	S	0	0	0
			1459	917	265	267	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	152	PHE	SER	see remark 999	UNP P00900
D	152	PHE	SER	see remark 999	UNP P00900

- Molecule 3 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



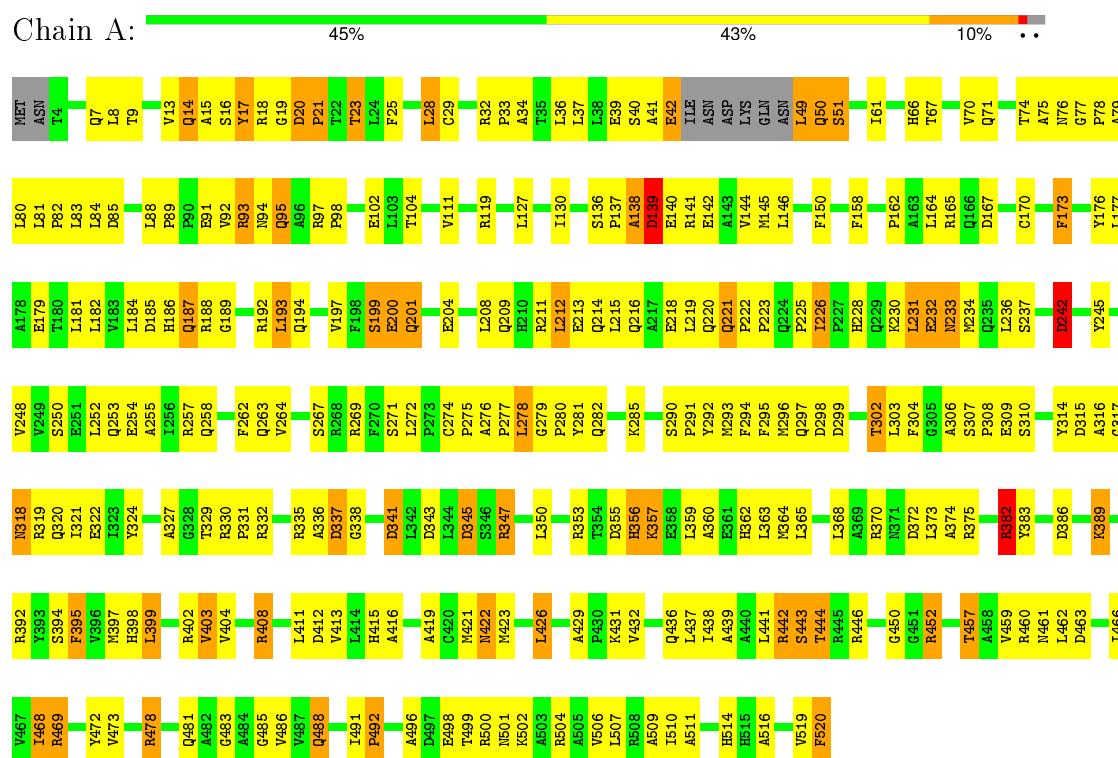
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	2	2		
3	C	1	Total	C	N	O	0	0
			15	11	2	2		

3 Residue-property plots

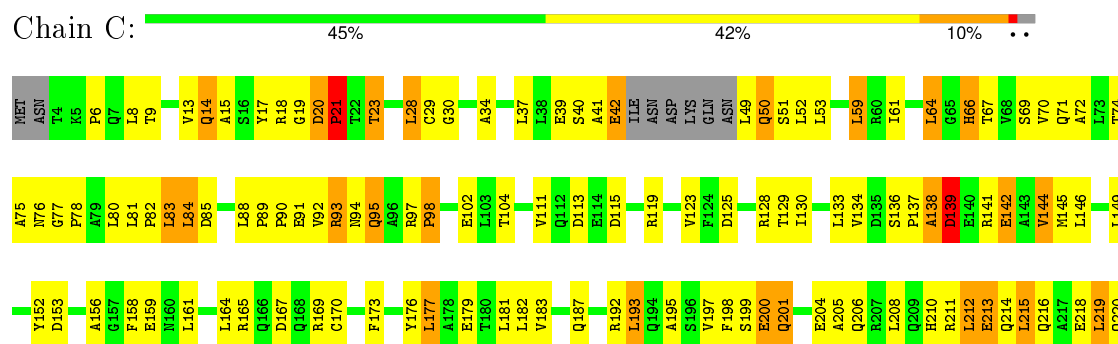
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

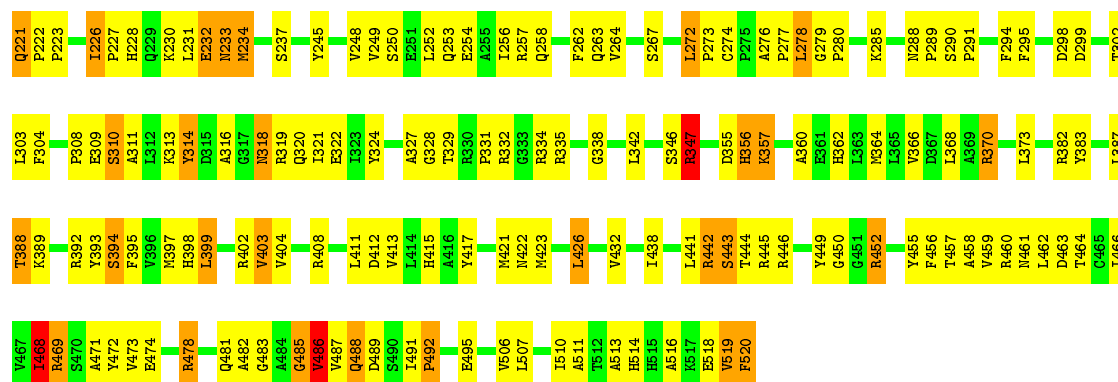
Note EDS was not executed.

• Molecule 1: ANTHRANILATE SYNTHASE



• Molecule 1: ANTHRANILATE SYNTHASE





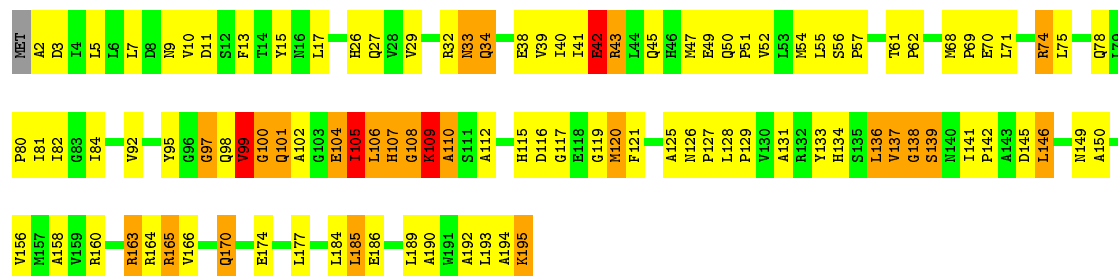
• Molecule 2: TRPG

Chain B: 45% 41% 11% ••



• Molecule 2: TRPG

Chain D: 46% 40% 12% ••



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.27 Å 123.56 Å 179.65 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.90 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (44.90-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0, REFMAC	Depositor
R, R_{free}	0.247 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10880	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.84	0/4035	1.00	9/5474 (0.2%)
1	C	0.86	1/4035 (0.0%)	1.02	13/5474 (0.2%)
2	B	1.05	4/1487 (0.3%)	1.11	8/2015 (0.4%)
2	D	0.92	3/1487 (0.2%)	1.05	5/2015 (0.2%)
All	All	0.89	8/11044 (0.1%)	1.03	35/14978 (0.2%)

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

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	42	GLU	CD-OE1	10.95	1.37	1.25
2	B	42	GLU	CD-OE2	8.64	1.35	1.25
2	B	42	GLU	CD-OE1	8.27	1.34	1.25
2	B	42	GLU	CB-CG	6.91	1.65	1.52
2	D	42	GLU	CB-CG	6.02	1.63	1.52
2	D	42	GLU	CD-OE2	5.69	1.31	1.25
2	B	45	GLN	CD-OE1	5.54	1.36	1.24
1	C	403	VAL	CB-CG2	-5.33	1.41	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	146	LEU	N-CA-C	-10.50	82.66	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	146	LEU	N-CA-C	-9.77	84.62	111.00
1	A	408	ARG	NE-CZ-NH2	-8.41	116.09	120.30
2	B	47	MET	CG-SD-CE	-8.08	87.27	100.20
1	C	370	ARG	NE-CZ-NH1	8.06	124.33	120.30
2	D	43	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	408	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	C	347	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	C	347	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	A	382	ARG	NE-CZ-NH1	-7.45	116.58	120.30
1	C	370	ARG	NE-CZ-NH2	-7.06	116.77	120.30
2	B	100	GLY	N-CA-C	6.50	129.35	113.10
1	C	335	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	A	242	ASP	CB-CG-OD1	-6.16	112.76	118.30
1	C	272	LEU	CA-CB-CG	6.13	129.40	115.30
1	C	64	LEU	CA-CB-CG	-5.98	101.55	115.30
1	C	59	LEU	CA-CB-CG	5.94	128.96	115.30
2	D	100	GLY	N-CA-C	5.89	127.83	113.10
1	C	489	ASP	CB-CG-OD2	5.89	123.60	118.30
2	D	138	GLY	N-CA-C	-5.67	98.92	113.10
2	D	47	MET	CG-SD-CE	-5.57	91.29	100.20
2	B	43	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	370	ARG	NE-CZ-NH2	5.49	123.04	120.30
2	B	151	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	A	345	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	242	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	372	ASP	CB-CG-OD2	5.44	123.20	118.30
1	C	486	VAL	CB-CA-C	-5.39	101.17	111.40
1	C	332	ARG	NE-CZ-NH2	5.29	122.95	120.30
2	B	107	HIS	N-CA-C	5.22	125.09	111.00
2	B	43	ARG	CD-NE-CZ	5.20	130.87	123.60
1	C	468	ILE	N-CA-C	-5.10	97.22	111.00
1	C	332	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	A	341	ASP	CB-CG-OD2	5.04	122.84	118.30
2	B	138	GLY	N-CA-C	-5.03	100.52	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	PHE	Sidechain
1	C	314	TYR	Sidechain
2	D	15	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3966	0	3940	337	0
1	C	3966	0	3940	324	0
2	B	1459	0	1459	137	0
2	D	1459	0	1459	145	0
3	A	15	0	9	1	0
3	C	15	0	9	2	0
All	All	10880	0	10816	923	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 (923) 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:A:263:GLN:NE2	1:A:364:MET:HG2	1.42	1.32
1:C:263:GLN:NE2	1:C:364:MET:HG2	1.44	1.28
2:D:41:ILE:HG22	2:D:45:GLN:HE21	1.15	1.09
1:C:263:GLN:HE22	1:C:364:MET:HG2	0.92	1.06
2:B:163:ARG:NH1	2:B:163:ARG:H	1.54	1.05
1:A:422:ASN:HA	1:A:452:ARG:HH22	1.19	1.04
2:D:41:ILE:HG22	2:D:45:GLN:NE2	1.74	1.03
1:A:263:GLN:HE22	1:A:364:MET:CG	1.73	1.02
1:C:442:ARG:H	1:C:442:ARG:HD2	1.21	1.01
2:B:105:ILE:HG12	2:B:134:HIS:HA	1.40	1.01
1:A:459:VAL:HG23	1:A:461:ASN:HD22	1.22	1.01
1:A:442:ARG:HD2	1:A:442:ARG:H	1.22	1.00
2:D:70:GLU:HG2	2:D:74:ARG:HH21	1.25	1.00
1:A:263:GLN:HE22	1:A:364:MET:HG2	0.83	0.99
2:B:163:ARG:HH11	2:B:163:ARG:H	1.00	0.98
2:D:163:ARG:H	2:D:163:ARG:NH1	1.62	0.97
2:D:105:ILE:HG12	2:D:134:HIS:HA	1.42	0.97
2:B:163:ARG:HH11	2:B:163:ARG:N	1.61	0.96
1:A:254:GLU:O	1:A:258:GLN:HG2	1.64	0.96
1:C:442:ARG:HH22	1:C:446:ARG:HH21	1.00	0.96
2:D:2:ALA:HB2	2:D:193:LEU:HD11	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:GLN:HG3	2:B:170:GLN:O	1.68	0.94
2:D:40:ILE:HG21	2:D:71:LEU:HD21	1.50	0.94
1:A:357:LYS:HD2	1:A:357:LYS:H	1.30	0.93
1:A:20:ASP:H	1:A:21:PRO:HD2	1.30	0.93
1:C:459:VAL:HG23	1:C:461:ASN:HD22	1.33	0.93
2:D:163:ARG:HH11	2:D:163:ARG:N	1.67	0.93
1:C:263:GLN:HE22	1:C:364:MET:CG	1.83	0.93
2:B:34:GLN:H	2:B:34:GLN:HE21	1.07	0.92
1:A:364:MET:SD	2:B:133:TYR:HE2	1.94	0.91
2:B:119:GLY:HA3	2:B:160:ARG:HH12	1.36	0.90
1:C:254:GLU:O	1:C:258:GLN:HG2	1.72	0.90
1:A:74:THR:O	1:A:78:PRO:HD3	1.71	0.90
2:B:119:GLY:HA3	2:B:160:ARG:NH1	1.87	0.90
1:A:412:ASP:H	1:A:415:HIS:HD2	1.20	0.90
1:C:442:ARG:NH2	1:C:446:ARG:HH21	1.69	0.89
1:C:478:ARG:NE	1:C:510:ILE:HG12	1.86	0.89
1:C:422:ASN:HA	1:C:452:ARG:HH22	1.36	0.89
2:B:3:ASP:HB3	2:B:47:MET:CE	2.02	0.88
1:A:457:THR:OG1	1:A:459:VAL:HG22	1.71	0.88
1:A:221:GLN:O	1:A:223:PRO:HD3	1.74	0.88
1:A:422:ASN:HA	1:A:452:ARG:NH2	1.89	0.88
1:A:74:THR:HG21	1:A:179:GLU:OE1	1.73	0.87
2:B:3:ASP:HB3	2:B:47:MET:HE2	1.57	0.87
1:A:442:ARG:O	1:A:444:THR:HG22	1.73	0.86
1:C:442:ARG:N	1:C:442:ARG:HD2	1.86	0.86
1:A:442:ARG:N	1:A:442:ARG:HD2	1.88	0.86
2:D:163:ARG:H	2:D:163:ARG:HH11	0.87	0.86
1:C:364:MET:SD	2:D:133:TYR:HE2	1.98	0.86
1:C:20:ASP:OD1	1:C:23:THR:HG22	1.76	0.86
1:C:459:VAL:HG23	1:C:461:ASN:ND2	1.90	0.85
1:A:267:SER:H	1:A:442:ARG:HH21	1.21	0.85
1:C:193:LEU:HD11	1:C:215:LEU:HD13	1.58	0.85
1:C:20:ASP:H	1:C:21:PRO:CD	1.89	0.85
1:A:20:ASP:H	1:A:21:PRO:CD	1.89	0.84
1:A:20:ASP:N	1:A:21:PRO:HD2	1.88	0.84
2:B:2:ALA:N	2:B:26:HIS:HD1	1.73	0.84
2:D:99:VAL:HA	2:D:137:VAL:HG11	1.58	0.84
1:C:327:ALA:HB3	1:C:399:LEU:HB3	1.58	0.84
2:B:40:ILE:HG21	2:B:71:LEU:HD21	1.59	0.84
1:A:459:VAL:HG23	1:A:461:ASN:ND2	1.92	0.84
1:C:74:THR:HG21	1:C:179:GLU:OE1	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ALA:HB2	1:A:362:HIS:ND1	1.92	0.83
2:B:70:GLU:HG2	2:B:74:ARG:HH21	1.43	0.83
1:C:304:PHE:HZ	1:C:478:ARG:HH12	1.25	0.83
1:C:413:VAL:HG21	1:C:462:LEU:HB3	1.59	0.83
2:B:41:ILE:HG22	2:B:45:GLN:NE2	1.95	0.82
2:B:136:LEU:O	2:B:137:VAL:HG23	1.80	0.81
1:A:74:THR:O	1:A:78:PRO:CD	2.28	0.81
1:A:221:GLN:CB	1:A:222:PRO:HD2	2.10	0.81
1:C:221:GLN:O	1:C:223:PRO:HD3	1.80	0.81
1:C:234:MET:CE	1:C:514:HIS:HB2	2.09	0.81
1:A:442:ARG:HH12	1:A:446:ARG:HE	1.28	0.81
1:C:322:GLU:HG2	1:C:404:VAL:HG12	1.63	0.81
2:D:5:LEU:HD22	2:D:29:VAL:HG23	1.63	0.81
1:C:164:LEU:CD2	1:C:443:SER:HA	2.10	0.80
1:A:442:ARG:HH22	1:A:446:ARG:HH21	1.25	0.80
1:C:442:ARG:HH12	1:C:446:ARG:HE	1.27	0.80
1:A:78:PRO:O	1:A:82:PRO:HD3	1.82	0.80
2:D:115:HIS:CD2	2:D:121:PHE:HB3	2.17	0.79
2:B:5:LEU:HD22	2:B:29:VAL:HG23	1.64	0.79
1:A:193:LEU:HD11	1:A:215:LEU:HD13	1.65	0.79
1:C:357:LYS:HD2	1:C:357:LYS:H	1.47	0.79
2:B:38:GLU:O	2:B:42:GLU:HG3	1.82	0.79
1:A:478:ARG:NE	1:A:510:ILE:HG12	1.98	0.78
1:A:248:VAL:HG22	1:A:441:LEU:HD21	1.66	0.78
2:D:170:GLN:O	2:D:170:GLN:HG3	1.81	0.78
1:C:8:LEU:HD23	1:C:9:THR:N	1.98	0.78
1:C:478:ARG:CZ	1:C:510:ILE:HG23	2.13	0.78
1:A:248:VAL:HG21	1:A:441:LEU:HD11	1.66	0.78
1:A:355:ASP:O	1:A:356:HIS:HB2	1.82	0.78
2:B:100:GLY:H	2:B:137:VAL:HG21	1.48	0.77
1:C:478:ARG:NE	1:C:510:ILE:CG1	2.46	0.77
1:C:478:ARG:CD	1:C:510:ILE:HG12	2.15	0.77
1:C:441:LEU:O	1:C:441:LEU:HD13	1.82	0.77
2:B:95:TYR:OH	2:B:164:ARG:HD3	1.85	0.77
2:D:70:GLU:HG2	2:D:74:ARG:NH2	1.98	0.77
2:B:42:GLU:HA	2:B:45:GLN:OE1	1.85	0.77
1:C:413:VAL:HG21	1:C:462:LEU:CB	2.15	0.76
1:A:322:GLU:HG2	1:A:404:VAL:HG12	1.68	0.76
1:A:478:ARG:CZ	1:A:510:ILE:HG23	2.16	0.76
2:D:115:HIS:HE1	2:D:125:ALA:O	1.69	0.75
1:C:355:ASP:OD2	1:C:357:LYS:HD3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:GLN:HE21	2:D:170:GLN:HA	1.52	0.75
2:D:95:TYR:OH	2:D:164:ARG:HD3	1.87	0.75
1:A:234:MET:CE	1:A:514:HIS:HB2	2.17	0.74
1:C:272:LEU:HD11	1:C:510:ILE:HD13	1.69	0.74
1:C:214:GLN:O	1:C:218:GLU:HG3	1.88	0.74
1:C:329:THR:OG1	1:C:398:HIS:HD2	1.71	0.74
1:A:441:LEU:HD13	1:A:441:LEU:C	2.09	0.73
1:A:329:THR:O	1:A:330:ARG:HG2	1.88	0.73
1:A:442:ARG:NH2	1:A:446:ARG:HH21	1.85	0.73
1:A:263:GLN:NE2	1:A:364:MET:CG	2.37	0.73
1:C:20:ASP:N	1:C:21:PRO:HD2	2.01	0.73
2:B:173:PRO:O	1:C:347:ARG:NH2	2.20	0.73
1:C:422:ASN:HA	1:C:452:ARG:NH2	2.03	0.73
2:B:115:HIS:HE1	2:B:125:ALA:O	1.72	0.73
2:B:115:HIS:HD2	2:B:117:GLY:H	1.35	0.73
2:D:70:GLU:CG	2:D:74:ARG:HH21	2.00	0.72
1:A:187:GLN:NE2	1:A:188:ARG:HG3	2.04	0.72
1:A:276:ALA:H	1:A:514:HIS:HE1	1.36	0.72
1:C:272:LEU:CD1	1:C:510:ILE:HD13	2.20	0.72
2:D:104:GLU:O	2:D:105:ILE:HD12	1.89	0.72
1:C:220:GLN:O	1:C:221:GLN:O	2.07	0.72
1:A:364:MET:SD	2:B:133:TYR:CE2	2.81	0.72
1:A:141:ARG:HA	1:A:459:VAL:HG11	1.70	0.72
2:D:119:GLY:HA3	2:D:160:ARG:HH12	1.55	0.72
1:C:40:SER:HG	3:C:701:TRP:N	1.88	0.71
1:C:276:ALA:O	1:C:280:PRO:HD3	1.90	0.71
1:C:248:VAL:HG21	1:C:441:LEU:HD11	1.71	0.71
1:A:329:THR:OG1	1:A:398:HIS:HD2	1.74	0.71
1:A:277:PRO:C	1:A:280:PRO:HD2	2.11	0.71
2:D:105:ILE:HG22	2:D:106:LEU:H	1.53	0.71
2:B:70:GLU:HG2	2:B:74:ARG:HE	1.55	0.71
1:C:41:ALA:O	1:C:42:GLU:HB2	1.91	0.71
1:C:264:VAL:O	1:C:485:GLY:O	2.08	0.71
1:A:214:GLN:O	1:A:218:GLU:HG3	1.91	0.70
1:A:267:SER:H	1:A:442:ARG:NH2	1.89	0.70
1:C:74:THR:O	1:C:78:PRO:HD3	1.92	0.70
2:B:41:ILE:HG22	2:B:45:GLN:HE21	1.56	0.70
2:B:141:ILE:HG13	2:B:156:VAL:HG21	1.73	0.70
2:B:128:LEU:HD12	2:B:129:PRO:HD2	1.72	0.70
2:D:105:ILE:CG1	2:D:134:HIS:HA	2.21	0.70
1:A:327:ALA:HB2	1:A:362:HIS:CG	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:LEU:C	1:C:441:LEU:HD13	2.12	0.70
1:C:40:SER:OG	3:C:701:TRP:N	2.25	0.70
1:A:40:SER:HG	3:A:601:TRP:N	1.89	0.70
1:C:20:ASP:H	1:C:21:PRO:HD2	1.55	0.70
1:A:264:VAL:O	1:A:485:GLY:O	2.10	0.70
2:B:100:GLY:N	2:B:137:VAL:HG11	2.07	0.69
2:D:42:GLU:HA	2:D:45:GLN:OE1	1.91	0.69
1:A:510:ILE:HD12	1:A:511:ALA:H	1.58	0.69
1:C:318:ASN:ND2	1:C:320:GLN:H	1.89	0.69
1:C:355:ASP:O	1:C:356:HIS:HB2	1.90	0.69
1:A:164:LEU:CD2	1:A:443:SER:HA	2.23	0.69
2:D:100:GLY:H	2:D:137:VAL:HG21	1.57	0.69
2:B:34:GLN:HE21	2:B:34:GLN:N	1.87	0.69
1:A:71:GLN:HE21	1:A:97:ARG:HH22	1.40	0.69
2:B:61:THR:HB	2:B:62:PRO:HD2	1.74	0.69
2:D:99:VAL:CA	2:D:137:VAL:HG11	2.21	0.69
2:B:39:VAL:HA	2:B:42:GLU:CD	2.12	0.69
1:C:8:LEU:HD13	1:C:136:SER:OG	1.92	0.69
1:C:308:PRO:HD2	1:C:468:ILE:HD11	1.74	0.69
1:C:226:ILE:HD13	1:C:228:HIS:HE1	1.56	0.68
2:D:2:ALA:HB2	2:D:193:LEU:CD1	2.21	0.68
1:A:478:ARG:NE	1:A:510:ILE:CG1	2.56	0.68
1:A:272:LEU:O	1:A:478:ARG:HB3	1.93	0.68
1:C:277:PRO:C	1:C:280:PRO:HD2	2.14	0.68
1:A:422:ASN:CA	1:A:452:ARG:HH22	2.01	0.68
1:C:314:TYR:HB2	1:C:321:ILE:HD12	1.73	0.68
2:B:70:GLU:CG	2:B:74:ARG:HH21	2.07	0.68
1:A:413:VAL:HG21	1:A:462:LEU:HB3	1.76	0.68
1:A:77:GLY:N	1:A:78:PRO:HD2	2.09	0.67
1:C:234:MET:HE3	1:C:514:HIS:HB2	1.74	0.67
1:A:15:ALA:HB1	1:A:219:LEU:HD12	1.75	0.67
1:C:221:GLN:CB	1:C:222:PRO:HD2	2.25	0.67
1:C:272:LEU:O	1:C:478:ARG:HB3	1.95	0.67
1:A:488:GLN:HA	1:A:488:GLN:HE21	1.60	0.67
1:A:277:PRO:O	1:A:280:PRO:HD2	1.95	0.67
1:C:74:THR:O	1:C:78:PRO:CD	2.43	0.67
2:B:105:ILE:CG1	2:B:134:HIS:HA	2.20	0.66
1:C:28:LEU:HD13	1:C:215:LEU:HD21	1.77	0.66
1:A:280:PRO:HG2	1:A:281:TYR:H	1.58	0.66
1:A:29:CYS:HA	1:A:32:ARG:HH21	1.59	0.66
1:A:279:GLY:N	1:A:280:PRO:HD2	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:VAL:CG2	1:C:441:LEU:HD11	2.26	0.66
1:A:314:TYR:HB2	1:A:321:ILE:HD12	1.77	0.66
2:B:3:ASP:HB3	2:B:47:MET:HE1	1.78	0.66
1:A:373:LEU:HD12	1:A:403:VAL:HG23	1.76	0.66
2:D:99:VAL:HG12	2:D:100:GLY:H	1.59	0.66
1:A:507:LEU:O	1:A:510:ILE:HD12	1.95	0.66
1:C:182:LEU:HD13	1:C:193:LEU:HG	1.77	0.66
1:C:20:ASP:N	1:C:21:PRO:CD	2.55	0.66
2:B:70:GLU:HG2	2:B:74:ARG:NH2	2.10	0.66
1:A:413:VAL:HG22	1:A:462:LEU:HD13	1.76	0.66
1:C:412:ASP:H	1:C:415:HIS:CD2	2.14	0.66
2:D:39:VAL:HA	2:D:42:GLU:HG3	1.78	0.66
1:C:442:ARG:O	1:C:444:THR:HG22	1.96	0.65
1:A:272:LEU:HD11	1:A:510:ILE:HD13	1.79	0.65
1:C:412:ASP:H	1:C:415:HIS:HD2	1.43	0.65
1:A:426:LEU:CD2	1:A:468:ILE:HG23	2.26	0.65
1:A:412:ASP:H	1:A:415:HIS:CD2	2.09	0.65
1:C:276:ALA:O	1:C:280:PRO:CD	2.44	0.65
1:A:272:LEU:CD1	1:A:510:ILE:HD13	2.26	0.65
1:A:137:PRO:HG2	1:A:140:GLU:HB2	1.78	0.65
2:B:115:HIS:CD2	2:B:117:GLY:H	2.14	0.65
2:B:119:GLY:CA	2:B:160:ARG:HH12	2.08	0.65
1:A:220:GLN:O	1:A:221:GLN:O	2.14	0.65
1:A:478:ARG:CD	1:A:510:ILE:HG12	2.26	0.65
1:C:89:PRO:HG2	1:C:92:VAL:HG23	1.78	0.65
1:A:212:LEU:O	1:A:216:GLN:HG3	1.97	0.64
1:C:413:VAL:HG22	1:C:462:LEU:HD13	1.78	0.64
1:C:360:ALA:HB2	2:D:108:GLY:HA2	1.79	0.64
1:C:373:LEU:HD12	1:C:403:VAL:HG23	1.80	0.64
1:A:41:ALA:O	1:A:42:GLU:HB2	1.96	0.64
1:A:89:PRO:HG2	1:A:92:VAL:HG23	1.80	0.64
1:A:327:ALA:HB3	1:A:399:LEU:HB3	1.79	0.64
2:D:92:VAL:HG12	2:D:97:GLY:HA3	1.78	0.64
2:B:104:GLU:O	2:B:105:ILE:HD12	1.97	0.64
2:B:99:VAL:C	2:B:137:VAL:HG11	2.18	0.64
1:A:28:LEU:O	1:A:32:ARG:NH2	2.30	0.64
1:C:218:GLU:C	1:C:220:GLN:H	2.00	0.64
2:D:115:HIS:HD2	2:D:121:PHE:HB3	1.62	0.64
1:A:355:ASP:OD2	1:A:357:LYS:HD3	1.97	0.64
2:D:119:GLY:HA3	2:D:160:ARG:NH1	2.13	0.64
2:D:2:ALA:CB	2:D:193:LEU:HD11	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ARG:HD2	1:C:387:LEU:HD23	1.79	0.63
1:A:262:PHE:HD1	1:A:364:MET:HE2	1.62	0.63
1:C:510:ILE:HD12	1:C:511:ALA:N	2.13	0.63
2:D:99:VAL:C	2:D:137:VAL:HG11	2.18	0.63
1:A:248:VAL:CG2	1:A:441:LEU:HD11	2.29	0.63
1:C:442:ARG:NH1	1:C:446:ARG:HE	1.96	0.63
1:C:18:ARG:HH22	1:C:223:PRO:HB3	1.64	0.63
1:A:36:LEU:HD13	1:A:296:MET:HG3	1.80	0.63
1:C:276:ALA:H	1:C:514:HIS:HE1	1.45	0.63
1:A:510:ILE:HD12	1:A:511:ALA:N	2.12	0.63
1:C:145:MET:CE	1:C:181:LEU:HD22	2.29	0.63
1:A:360:ALA:HB2	2:B:108:GLY:HA2	1.80	0.63
1:C:478:ARG:CZ	1:C:510:ILE:CG2	2.77	0.62
1:A:290:SER:HB2	1:A:291:PRO:HD2	1.80	0.62
2:B:98:GLN:HE22	2:B:101:GLN:NE2	1.96	0.62
1:C:77:GLY:N	1:C:78:PRO:HD2	2.15	0.62
1:C:164:LEU:HD22	1:C:443:SER:HA	1.79	0.62
1:C:364:MET:SD	2:D:133:TYR:CE2	2.86	0.62
2:D:100:GLY:N	2:D:137:VAL:HG11	2.14	0.62
1:A:18:ARG:HH22	1:A:223:PRO:HB3	1.64	0.62
1:C:459:VAL:CG2	1:C:461:ASN:ND2	2.62	0.62
1:C:84:LEU:HD22	1:C:88:LEU:HG	1.82	0.62
1:A:506:VAL:O	1:A:509:ALA:HB3	2.00	0.62
1:A:267:SER:N	1:A:442:ARG:HH21	1.97	0.62
1:A:357:LYS:CD	1:A:357:LYS:H	2.07	0.62
1:A:412:ASP:N	1:A:415:HIS:HD2	1.96	0.62
1:A:230:LYS:C	1:A:232:GLU:H	2.01	0.62
1:C:248:VAL:HG13	1:C:441:LEU:HG	1.82	0.61
1:C:262:PHE:CD1	1:C:364:MET:HE2	2.35	0.61
1:A:226:ILE:HD13	1:A:228:HIS:HE1	1.64	0.61
1:C:426:LEU:HD23	1:C:450:GLY:HA2	1.82	0.61
2:B:99:VAL:HA	2:B:137:VAL:HG11	1.82	0.61
2:B:115:HIS:CD2	2:B:121:PHE:HB3	2.36	0.61
1:A:441:LEU:HD13	1:A:441:LEU:O	2.01	0.61
1:A:193:LEU:HD21	1:A:215:LEU:HD13	1.83	0.61
1:C:61:ILE:HD13	1:C:130:ILE:HD12	1.81	0.61
1:C:37:LEU:HD13	1:C:53:LEU:HD11	1.82	0.61
1:A:276:ALA:O	1:A:280:PRO:HD3	2.01	0.61
1:A:383:TYR:CE2	1:C:342:LEU:HD13	2.35	0.61
1:C:95:GLN:HB2	1:C:102:GLU:HB3	1.80	0.61
2:B:105:ILE:HG12	2:B:134:HIS:CA	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:LEU:C	2:B:137:VAL:HG23	2.21	0.60
2:B:50:GLN:N	2:B:51:PRO:CD	2.64	0.60
1:A:394:SER:O	1:A:395:PHE:HB2	2.01	0.60
2:D:107:HIS:O	2:D:109:LYS:N	2.33	0.60
1:C:78:PRO:O	1:C:82:PRO:HD3	2.02	0.60
1:A:164:LEU:HD23	1:A:443:SER:HA	1.83	0.60
1:C:488:GLN:HE21	1:C:488:GLN:HA	1.66	0.60
1:A:250:SER:HA	1:A:253:GLN:HE21	1.65	0.60
1:C:6:PRO:HB2	1:C:134:VAL:HG22	1.84	0.60
1:A:262:PHE:CD1	1:A:364:MET:HE2	2.36	0.60
1:A:82:PRO:HA	1:A:85:ASP:OD2	2.01	0.60
1:A:119:ARG:CZ	1:A:411:LEU:HD21	2.31	0.60
1:A:231:LEU:HG	1:A:231:LEU:O	2.02	0.60
1:C:426:LEU:CD2	1:C:468:ILE:HG23	2.31	0.60
1:C:81:LEU:HB2	1:C:82:PRO:HD3	1.84	0.59
1:C:357:LYS:CD	1:C:357:LYS:H	2.16	0.59
2:D:141:ILE:HG13	2:D:156:VAL:HG21	1.84	0.59
2:B:105:ILE:HG22	2:B:106:LEU:H	1.67	0.59
1:C:457:THR:OG1	1:C:459:VAL:HG22	2.01	0.59
1:A:221:GLN:CB	1:A:222:PRO:CD	2.80	0.59
2:D:29:VAL:HG11	2:D:43:ARG:HH21	1.68	0.59
1:A:248:VAL:HG13	1:A:441:LEU:HG	1.85	0.59
1:A:75:ALA:HA	1:A:78:PRO:HG3	1.85	0.59
2:B:39:VAL:HA	2:B:42:GLU:HG3	1.85	0.59
1:C:322:GLU:OE1	1:C:402:ARG:HD2	2.03	0.59
2:B:107:HIS:C	2:B:109:LYS:H	2.06	0.59
1:A:74:THR:HG21	1:A:179:GLU:CD	2.23	0.58
1:C:164:LEU:HD23	1:C:443:SER:HA	1.85	0.58
1:A:478:ARG:CZ	1:A:510:ILE:CG2	2.81	0.58
2:B:34:GLN:H	2:B:34:GLN:NE2	1.91	0.58
2:B:3:ASP:CB	2:B:47:MET:CE	2.80	0.58
1:A:185:ASP:OD2	1:A:188:ARG:NH1	2.37	0.58
2:B:101:GLN:O	2:B:137:VAL:HA	2.03	0.58
2:B:100:GLY:C	2:B:137:VAL:HG22	2.24	0.58
2:D:131:ALA:HB2	2:D:177:LEU:HB2	1.86	0.58
2:B:50:GLN:N	2:B:51:PRO:HD3	2.18	0.58
1:A:304:PHE:HZ	1:A:478:ARG:HH12	1.52	0.58
1:A:84:LEU:HD22	1:A:88:LEU:HG	1.86	0.58
1:A:20:ASP:OD1	1:A:23:THR:HG22	2.04	0.57
2:B:98:GLN:HE22	2:B:101:GLN:HE22	1.51	0.57
2:D:107:HIS:C	2:D:109:LYS:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:186:GLU:HA	2:D:186:GLU:OE1	2.04	0.57
1:C:324:TYR:CE2	1:C:402:ARG:HD3	2.39	0.57
1:C:165:ARG:NH1	1:C:167:ASP:OD1	2.38	0.57
2:B:100:GLY:N	2:B:137:VAL:CG1	2.67	0.57
2:B:2:ALA:HB2	2:B:193:LEU:HD11	1.86	0.57
2:D:34:GLN:NE2	2:D:34:GLN:H	2.03	0.57
1:C:71:GLN:HE21	1:C:97:ARG:HH22	1.50	0.57
2:D:55:LEU:HD13	2:D:68:MET:SD	2.43	0.57
1:C:388:THR:HB	1:C:399:LEU:HD22	1.87	0.57
1:A:34:ALA:HA	1:A:176:TYR:CZ	2.38	0.57
1:C:254:GLU:OE1	1:C:257:ARG:HD3	2.04	0.57
1:C:74:THR:HG21	1:C:179:GLU:CD	2.24	0.57
2:D:137:VAL:CG1	2:D:139:SER:HB2	2.35	0.57
2:D:149:ASN:HB2	2:D:160:ARG:HH21	1.69	0.57
1:A:520:PHE:N	1:A:520:PHE:CD1	2.73	0.57
1:C:438:ILE:HG23	1:C:442:ARG:CZ	2.35	0.57
2:D:170:GLN:HE21	2:D:170:GLN:CA	2.17	0.57
1:A:322:GLU:OE1	1:A:402:ARG:HD2	2.05	0.57
1:C:327:ALA:HB2	1:C:362:HIS:ND1	2.19	0.56
1:A:39:GLU:HA	1:A:51:SER:OG	2.05	0.56
1:A:79:ALA:O	1:A:82:PRO:HD2	2.05	0.56
1:A:276:ALA:O	1:A:280:PRO:CD	2.53	0.56
2:D:50:GLN:OE1	2:D:50:GLN:HA	2.03	0.56
1:C:507:LEU:O	1:C:510:ILE:HD12	2.05	0.56
1:A:29:CYS:HA	1:A:32:ARG:NH2	2.19	0.56
2:B:150:ALA:HB3	2:B:158:ALA:HB3	1.87	0.56
1:A:277:PRO:O	1:A:280:PRO:HG2	2.06	0.56
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.69	0.56
2:B:101:GLN:N	2:B:137:VAL:HG13	2.20	0.56
2:B:99:VAL:CA	2:B:137:VAL:HG11	2.35	0.56
2:D:57:PRO:HD3	2:D:84:ILE:HB	1.86	0.56
1:C:478:ARG:HE	1:C:510:ILE:CG1	2.19	0.56
2:D:142:PRO:HD2	2:D:146:LEU:HD23	1.88	0.56
2:D:74:ARG:HG3	2:D:74:ARG:HH11	1.71	0.56
1:A:33:PRO:HB2	1:A:299:ASP:OD2	2.06	0.56
1:A:145:MET:HE1	1:A:181:LEU:HD13	1.86	0.56
1:C:17:TYR:CG	1:C:18:ARG:N	2.73	0.56
2:B:3:ASP:CB	2:B:47:MET:HE2	2.33	0.56
1:C:15:ALA:HB1	1:C:219:LEU:HD12	1.88	0.56
1:A:248:VAL:HG13	1:A:441:LEU:CD2	2.36	0.56
1:C:441:LEU:CD1	1:C:441:LEU:C	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:ARG:HB2	2:B:163:ARG:NH1	2.21	0.56
1:C:193:LEU:HD21	1:C:215:LEU:HD13	1.88	0.56
1:A:394:SER:O	1:A:395:PHE:CB	2.53	0.56
1:A:20:ASP:N	1:A:21:PRO:CD	2.58	0.55
1:A:145:MET:HE2	1:A:181:LEU:HD22	1.89	0.55
1:C:510:ILE:HD12	1:C:511:ALA:H	1.70	0.55
1:A:280:PRO:HG2	1:A:281:TYR:N	2.21	0.55
1:A:426:LEU:HD22	1:A:468:ILE:HG23	1.87	0.55
1:C:69:SER:HB3	1:C:97:ARG:NH2	2.21	0.55
1:C:52:LEU:HD12	1:C:52:LEU:N	2.21	0.55
1:A:332:ARG:NH2	1:A:392:ARG:HB3	2.21	0.55
1:A:442:ARG:NH1	1:A:446:ARG:HE	2.01	0.55
1:C:145:MET:HE2	1:C:181:LEU:HD22	1.87	0.55
1:C:366:VAL:O	1:C:370:ARG:HG3	2.06	0.55
1:A:67:THR:CG2	1:A:102:GLU:OE2	2.55	0.55
2:D:163:ARG:HB2	2:D:163:ARG:NH1	2.21	0.55
1:A:478:ARG:HG3	1:A:478:ARG:HH11	1.71	0.55
2:D:149:ASN:HB3	2:D:160:ARG:HE	1.72	0.55
2:D:100:GLY:N	2:D:137:VAL:CG1	2.70	0.55
1:C:248:VAL:HG13	1:C:441:LEU:CG	2.37	0.55
1:C:426:LEU:HD21	1:C:468:ILE:HG23	1.88	0.55
1:C:13:VAL:HG12	1:C:14:GLN:O	2.06	0.55
2:B:70:GLU:HG2	2:B:74:ARG:NE	2.20	0.55
2:D:149:ASN:CB	2:D:160:ARG:HE	2.19	0.55
1:A:426:LEU:HD21	1:A:468:ILE:HG23	1.89	0.55
2:B:100:GLY:H	2:B:137:VAL:CG2	2.19	0.54
1:C:97:ARG:HB2	1:C:98:PRO:CD	2.37	0.54
1:C:302:THR:OG1	1:C:473:VAL:HB	2.07	0.54
2:D:98:GLN:HE22	2:D:101:GLN:HE22	1.56	0.54
1:C:327:ALA:HB2	1:C:362:HIS:CG	2.42	0.54
1:C:134:VAL:HG11	1:C:198:PHE:O	2.07	0.54
2:D:104:GLU:HG2	2:D:136:LEU:HD12	1.90	0.54
2:D:11:ASP:HB2	2:D:57:PRO:O	2.08	0.54
1:C:179:GLU:O	1:C:195:ALA:HA	2.07	0.54
1:A:507:LEU:O	1:A:510:ILE:CD1	2.54	0.54
1:A:324:TYR:CE2	1:A:402:ARG:HD3	2.43	0.54
1:A:248:VAL:HG13	1:A:441:LEU:HD21	1.89	0.54
1:C:192:ARG:HG2	1:C:192:ARG:HH21	1.71	0.54
1:A:478:ARG:HG3	1:A:478:ARG:NH1	2.22	0.54
1:C:49:LEU:O	1:C:50:GLN:HB3	2.08	0.54
1:C:276:ALA:H	1:C:514:HIS:CE1	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:VAL:HA	2:B:42:GLU:CG	2.36	0.54
2:D:92:VAL:CG1	2:D:97:GLY:HA3	2.38	0.54
1:A:297:GLN:HA	1:A:302:THR:HG22	1.90	0.54
1:A:182:LEU:HD13	1:A:193:LEU:HG	1.90	0.54
1:A:37:LEU:O	1:A:294:PHE:HA	2.08	0.54
1:C:42:GLU:O	1:C:49:LEU:N	2.40	0.54
1:A:111:VAL:O	1:A:111:VAL:HG12	2.07	0.54
2:D:136:LEU:O	2:D:137:VAL:HG23	2.08	0.54
1:A:357:LYS:HD2	1:A:357:LYS:N	2.12	0.54
1:A:422:ASN:OD1	1:A:452:ARG:NH2	2.41	0.53
1:A:459:VAL:CG2	1:A:461:ASN:ND2	2.68	0.53
1:C:426:LEU:HD21	1:C:468:ILE:CG2	2.38	0.53
2:B:105:ILE:HD13	2:B:133:TYR:O	2.08	0.53
1:C:193:LEU:HD21	1:C:215:LEU:CD1	2.38	0.53
1:C:462:LEU:HD23	1:C:462:LEU:C	2.28	0.53
1:A:478:ARG:HH11	1:A:478:ARG:CG	2.21	0.53
1:A:373:LEU:HD12	1:A:403:VAL:CG2	2.37	0.53
2:D:119:GLY:CA	2:D:160:ARG:HH12	2.21	0.53
1:C:394:SER:O	1:C:395:PHE:HB2	2.09	0.53
1:A:488:GLN:HA	1:A:488:GLN:NE2	2.24	0.53
1:A:341:ASP:C	1:A:341:ASP:OD1	2.46	0.53
1:A:13:VAL:HG12	1:A:14:GLN:N	2.24	0.53
1:A:170:CYS:HB2	1:A:472:TYR:CZ	2.43	0.53
1:A:267:SER:OG	1:A:442:ARG:NH2	2.42	0.53
1:C:277:PRO:O	1:C:280:PRO:HD2	2.09	0.53
1:C:75:ALA:O	1:C:78:PRO:HG2	2.08	0.53
1:A:441:LEU:C	1:A:441:LEU:CD1	2.77	0.53
1:A:93:ARG:HB2	1:A:104:THR:HB	1.89	0.53
1:C:20:ASP:H	1:C:21:PRO:HD3	1.70	0.53
1:C:193:LEU:CD1	1:C:215:LEU:HD13	2.35	0.53
1:A:232:GLU:O	1:A:233:ASN:HB2	2.09	0.53
2:B:10:VAL:HG22	2:B:32:ARG:HD2	1.90	0.53
2:D:17:LEU:HD23	2:D:174:GLU:HB3	1.91	0.53
2:D:100:GLY:C	2:D:137:VAL:HG22	2.30	0.53
1:C:37:LEU:HD13	1:C:53:LEU:CD1	2.39	0.53
1:A:17:TYR:CG	1:A:18:ARG:N	2.76	0.53
1:A:469:ARG:CG	1:A:469:ARG:HH11	2.21	0.53
2:D:105:ILE:HG12	2:D:134:HIS:CA	2.29	0.52
1:C:183:VAL:HG11	1:C:192:ARG:NH1	2.25	0.52
2:D:105:ILE:HD13	2:D:133:TYR:O	2.08	0.52
1:A:277:PRO:O	1:A:280:PRO:CG	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:ILE:HB	2:D:166:VAL:HG22	1.89	0.52
2:B:99:VAL:HG12	2:B:100:GLY:N	2.24	0.52
1:A:192:ARG:HH21	1:A:192:ARG:HG2	1.74	0.52
2:D:61:THR:HB	2:D:62:PRO:HD2	1.90	0.52
1:A:432:VAL:O	1:A:436:GLN:HG3	2.09	0.52
2:B:150:ALA:HB3	2:B:158:ALA:CB	2.40	0.52
1:C:298:ASP:CG	1:C:299:ASP:H	2.12	0.52
1:A:61:ILE:HD13	1:A:130:ILE:HD12	1.91	0.52
1:C:76:ASN:HB2	1:C:204:GLU:OE1	2.08	0.52
2:B:101:GLN:H	2:B:137:VAL:HG13	1.72	0.52
2:B:11:ASP:OD2	2:B:13:PHE:HB2	2.09	0.52
2:D:150:ALA:HB3	2:D:158:ALA:HB3	1.91	0.52
1:A:318:ASN:ND2	1:A:320:GLN:H	2.08	0.52
2:B:120:MET:O	2:B:187:GLN:NE2	2.41	0.52
1:A:276:ALA:H	1:A:514:HIS:CE1	2.23	0.52
2:B:61:THR:CB	2:B:62:PRO:HD2	2.40	0.52
1:C:170:CYS:HB2	1:C:472:TYR:CZ	2.45	0.52
1:A:248:VAL:HG13	1:A:441:LEU:CG	2.39	0.52
1:C:8:LEU:HD23	1:C:9:THR:C	2.30	0.52
1:A:187:GLN:HE21	1:A:188:ARG:HG3	1.75	0.52
1:A:426:LEU:HD21	1:A:468:ILE:CG2	2.40	0.52
1:C:113:ASP:OD1	1:C:113:ASP:C	2.47	0.52
2:B:81:ILE:HB	2:B:166:VAL:HG22	1.91	0.52
1:C:211:ARG:O	1:C:215:LEU:HB2	2.10	0.52
1:A:469:ARG:NH1	1:A:469:ARG:HG3	2.24	0.52
2:B:12:SER:O	2:B:13:PHE:CD2	2.62	0.52
1:A:242:ASP:OD1	1:A:242:ASP:N	2.41	0.52
2:D:137:VAL:HG12	2:D:139:SER:N	2.25	0.52
1:C:75:ALA:C	1:C:78:PRO:HD2	2.30	0.52
1:A:234:MET:HG2	1:A:516:ALA:HB2	1.92	0.52
1:A:335:ARG:HB2	1:A:337:ASP:OD1	2.10	0.52
2:D:109:LYS:HB2	2:D:177:LEU:HD13	1.91	0.52
2:B:29:VAL:HG11	2:B:43:ARG:NH2	2.25	0.52
1:A:39:GLU:OE1	1:A:285:LYS:HE3	2.10	0.51
1:A:278:LEU:HD23	1:A:295:PHE:CD2	2.44	0.51
2:B:55:LEU:HD13	2:B:68:MET:SD	2.50	0.51
1:C:364:MET:HE3	2:D:13:PHE:HZ	1.75	0.51
2:D:34:GLN:HE21	2:D:34:GLN:H	1.58	0.51
1:C:93:ARG:HB3	1:C:104:THR:HB	1.92	0.51
2:D:99:VAL:HA	2:D:139:SER:HB2	1.92	0.51
1:C:298:ASP:CG	1:C:299:ASP:N	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:ASP:OD2	2:D:13:PHE:HB2	2.10	0.51
1:A:423:MET:HG3	1:A:466:ILE:CD1	2.40	0.51
2:B:149:ASN:HB2	2:B:160:ARG:HH21	1.75	0.51
2:B:39:VAL:HG13	2:B:42:GLU:OE1	2.10	0.51
1:A:277:PRO:O	1:A:280:PRO:CD	2.58	0.51
1:A:13:VAL:HG12	1:A:14:GLN:O	2.11	0.51
1:C:518:GLU:O	1:C:519:VAL:O	2.28	0.51
1:C:232:GLU:HA	1:C:516:ALA:HA	1.92	0.51
1:A:221:GLN:O	1:A:223:PRO:CD	2.55	0.51
1:A:165:ARG:NH1	1:A:167:ASP:OD2	2.38	0.51
2:B:98:GLN:NE2	2:B:101:GLN:HE22	2.08	0.51
1:C:267:SER:H	1:C:442:ARG:HH21	1.59	0.51
1:A:51:SER:HB2	1:A:186:HIS:CE1	2.45	0.51
2:D:9:ASN:ND2	2:D:56:SER:O	2.42	0.51
1:C:59:LEU:HD12	1:C:177:LEU:HD12	1.92	0.51
1:A:438:ILE:O	1:A:442:ARG:HD2	2.10	0.51
2:D:49:GLU:O	2:D:50:GLN:HB2	2.10	0.51
1:C:316:ALA:CB	1:C:460:ARG:HB2	2.41	0.51
1:C:75:ALA:HA	1:C:78:PRO:HG3	1.92	0.51
1:A:97:ARG:NH1	1:A:97:ARG:HG3	2.26	0.51
1:A:308:PRO:O	1:A:309:GLU:HB2	2.11	0.51
1:A:426:LEU:HD23	1:A:450:GLY:HA2	1.93	0.51
1:C:66:HIS:N	1:C:66:HIS:CD2	2.79	0.50
1:C:388:THR:HB	1:C:399:LEU:CD2	2.41	0.50
1:A:374:ALA:HB1	2:B:19:ASP:HB2	1.91	0.50
1:A:413:VAL:CG2	1:A:462:LEU:HD13	2.41	0.50
1:C:80:LEU:HD23	1:C:83:LEU:HD12	1.93	0.50
2:D:2:ALA:N	2:D:26:HIS:HD1	2.10	0.50
2:D:71:LEU:HG	2:D:75:LEU:HD12	1.94	0.50
2:D:120:MET:CE	2:D:149:ASN:HD21	2.25	0.50
1:A:307:SER:OG	1:A:308:PRO:HD2	2.11	0.50
2:D:102:ALA:O	2:D:136:LEU:HD12	2.11	0.50
1:C:267:SER:HA	1:C:483:GLY:HA2	1.93	0.50
1:A:164:LEU:HD22	1:A:443:SER:HA	1.94	0.50
1:C:232:GLU:O	1:C:233:ASN:HB2	2.11	0.50
1:C:152:TYR:CE1	1:C:422:ASN:ND2	2.80	0.50
2:D:142:PRO:O	2:D:146:LEU:HB3	2.12	0.50
1:C:153:ASP:OD2	1:C:445:ARG:HB3	2.12	0.50
1:A:263:GLN:HE21	1:A:364:MET:HG2	1.63	0.50
2:B:120:MET:CE	2:B:149:ASN:HD21	2.25	0.50
1:C:97:ARG:HG3	1:C:97:ARG:HH11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ARG:HG2	1:A:257:ARG:HH11	1.77	0.50
1:C:314:TYR:HB2	1:C:321:ILE:CD1	2.40	0.50
2:B:11:ASP:HB2	2:B:57:PRO:O	2.11	0.50
1:A:262:PHE:CD1	1:A:364:MET:CE	2.94	0.49
2:B:131:ALA:HB2	2:B:177:LEU:HB2	1.93	0.49
2:B:88:HIS:CE1	2:B:170:GLN:HB2	2.47	0.49
1:C:329:THR:OG1	1:C:398:HIS:CD2	2.59	0.49
1:C:97:ARG:HB2	1:C:98:PRO:HD2	1.93	0.49
1:C:159:GLU:HG3	1:C:432:VAL:HG22	1.94	0.49
1:A:364:MET:HE2	1:A:429:ALA:HB1	1.93	0.49
1:C:318:ASN:ND2	1:C:318:ASN:C	2.65	0.49
1:A:332:ARG:HD2	1:A:345:ASP:OD2	2.13	0.49
2:B:104:GLU:HG2	2:B:136:LEU:HD12	1.93	0.49
1:A:274:CYS:SG	1:A:510:ILE:CG2	3.00	0.49
1:A:290:SER:CB	1:A:291:PRO:HD2	2.42	0.49
2:D:128:LEU:HD12	2:D:129:PRO:HD2	1.94	0.49
1:C:520:PHE:N	1:C:520:PHE:CD1	2.80	0.49
1:A:421:MET:O	1:A:422:ASN:HB2	2.12	0.49
1:C:141:ARG:HA	1:C:459:VAL:HG11	1.94	0.49
1:C:234:MET:HG2	1:C:516:ALA:HB2	1.94	0.49
2:D:150:ALA:HB3	2:D:158:ALA:CB	2.42	0.49
1:C:169:ARG:NH1	1:C:474:GLU:HG2	2.27	0.49
1:A:442:ARG:O	1:A:444:THR:N	2.45	0.49
1:C:80:LEU:HD22	1:C:133:LEU:HD12	1.94	0.49
1:C:221:GLN:CB	1:C:222:PRO:CD	2.91	0.49
1:C:248:VAL:HG22	1:C:441:LEU:HD21	1.94	0.49
1:A:139:ASP:O	1:A:139:ASP:CG	2.50	0.49
1:A:28:LEU:HD13	1:A:215:LEU:HD21	1.94	0.49
1:C:462:LEU:HD23	1:C:463:ASP:N	2.28	0.49
2:D:68:MET:HB3	2:D:69:PRO:HD3	1.93	0.49
1:C:66:HIS:H	1:C:66:HIS:CD2	2.31	0.49
1:C:212:LEU:O	1:C:216:GLN:HG3	2.12	0.49
1:C:262:PHE:CD1	1:C:364:MET:CE	2.95	0.49
1:C:215:LEU:O	1:C:218:GLU:HB2	2.12	0.49
1:C:309:GLU:HG3	1:C:310:SER:N	2.28	0.49
1:C:137:PRO:O	1:C:139:ASP:N	2.44	0.49
1:C:469:ARG:HG3	1:C:469:ARG:HH11	1.78	0.49
2:B:146:LEU:HG	2:B:159:VAL:HG13	1.93	0.49
1:C:469:ARG:NH1	1:C:469:ARG:HG3	2.26	0.49
1:C:253:GLN:HA	1:C:256:ILE:HD12	1.95	0.49
2:D:98:GLN:HE22	2:D:101:GLN:NE2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:ASP:O	2:B:51:PRO:HA	2.13	0.49
1:A:49:LEU:O	1:A:50:GLN:HB3	2.13	0.49
1:C:67:THR:CG2	1:C:102:GLU:OE2	2.61	0.49
2:B:163:ARG:CZ	2:B:163:ARG:HB2	2.42	0.48
1:C:488:GLN:NE2	1:C:488:GLN:HA	2.28	0.48
2:B:80:PRO:HB2	2:B:192:ALA:HB1	1.95	0.48
1:A:298:ASP:CG	1:A:299:ASP:N	2.66	0.48
1:A:13:VAL:CG1	1:A:14:GLN:N	2.76	0.48
1:A:426:LEU:HD23	1:A:450:GLY:CA	2.43	0.48
1:A:267:SER:N	1:A:442:ARG:NH2	2.59	0.48
1:C:218:GLU:C	1:C:220:GLN:N	2.67	0.48
1:C:290:SER:HB2	1:C:291:PRO:HD2	1.95	0.48
2:D:100:GLY:CA	2:D:137:VAL:HG22	2.43	0.48
2:D:100:GLY:H	2:D:137:VAL:CG2	2.25	0.48
1:A:422:ASN:CA	1:A:452:ARG:NH2	2.67	0.48
1:A:272:LEU:HD13	1:A:272:LEU:C	2.34	0.48
1:C:93:ARG:CB	1:C:104:THR:HB	2.42	0.48
2:B:102:ALA:O	2:B:104:GLU:HG2	2.13	0.48
2:D:70:GLU:HG2	2:D:74:ARG:HE	1.77	0.48
1:A:95:GLN:HB2	1:A:102:GLU:HB3	1.95	0.48
2:D:74:ARG:HG3	2:D:74:ARG:NH1	2.28	0.48
1:A:216:GLN:C	1:A:218:GLU:N	2.65	0.48
1:C:75:ALA:HA	1:C:78:PRO:CG	2.44	0.48
1:A:248:VAL:CG1	1:A:441:LEU:HG	2.43	0.48
1:C:226:ILE:HD12	1:C:226:ILE:H	1.78	0.48
2:D:194:ALA:O	2:D:195:LYS:OXT	2.31	0.48
1:C:364:MET:HE3	2:D:13:PHE:CZ	2.49	0.48
1:C:278:LEU:HD23	1:C:295:PHE:CE2	2.47	0.48
1:C:423:MET:HG3	1:C:466:ILE:CD1	2.43	0.48
1:A:75:ALA:C	1:A:78:PRO:HD2	2.34	0.48
1:A:193:LEU:HD21	1:A:215:LEU:CD1	2.44	0.48
2:D:33:ASN:CB	2:D:34:GLN:HE21	2.26	0.48
1:A:234:MET:HE3	1:A:514:HIS:HB2	1.92	0.47
2:B:149:ASN:OD1	2:B:149:ASN:N	2.46	0.47
1:C:422:ASN:CA	1:C:452:ARG:HH22	2.16	0.47
1:A:137:PRO:O	1:A:139:ASP:N	2.45	0.47
1:A:145:MET:CE	1:A:181:LEU:HD22	2.44	0.47
1:C:197:VAL:HG22	1:C:208:LEU:HD12	1.96	0.47
1:A:193:LEU:HD23	1:A:194:GLN:N	2.30	0.47
2:D:5:LEU:HD22	2:D:29:VAL:CG2	2.39	0.47
1:A:42:GLU:O	1:A:49:LEU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:LYS:HB2	2:B:177:LEU:HD13	1.95	0.47
1:A:77:GLY:O	1:A:80:LEU:HB2	2.13	0.47
1:A:359:LEU:O	1:A:363:LEU:HG	2.13	0.47
1:C:267:SER:H	1:C:442:ARG:NH2	2.12	0.47
1:C:399:LEU:HA	1:C:399:LEU:HD23	1.79	0.47
1:C:456:PHE:HB3	1:C:462:LEU:HD12	1.97	0.47
1:A:127:LEU:HD11	1:A:173:PHE:CE2	2.49	0.47
1:C:64:LEU:HD12	1:C:64:LEU:HA	1.73	0.47
1:A:498:GLU:HA	1:A:501:ASN:HD22	1.79	0.47
2:D:107:HIS:O	2:D:109:LYS:HG3	2.14	0.47
1:A:423:MET:HG2	1:A:452:ARG:NH1	2.29	0.47
1:A:75:ALA:O	1:A:78:PRO:HG2	2.14	0.47
1:A:211:ARG:O	1:A:215:LEU:HB2	2.15	0.47
2:D:170:GLN:CG	2:D:170:GLN:O	2.55	0.47
1:C:226:ILE:CD1	1:C:226:ILE:H	2.28	0.47
2:D:17:LEU:CD2	2:D:174:GLU:HB3	2.45	0.47
1:A:499:THR:OG1	1:A:500:ARG:N	2.47	0.47
1:C:459:VAL:O	1:C:460:ARG:HB2	2.15	0.47
2:B:37:ALA:O	2:B:41:ILE:HG12	2.15	0.47
1:A:413:VAL:O	1:A:416:ALA:HB3	2.14	0.47
1:C:469:ARG:CG	1:C:469:ARG:HH11	2.28	0.47
1:C:249:VAL:O	1:C:253:GLN:HG3	2.14	0.47
2:B:20:GLN:HE22	2:B:174:GLU:HA	1.80	0.47
1:A:216:GLN:C	1:A:218:GLU:H	2.17	0.46
1:C:426:LEU:HD22	1:C:468:ILE:HG23	1.97	0.46
2:D:52:VAL:HG22	2:D:80:PRO:HG2	1.97	0.46
1:C:272:LEU:HG	1:C:510:ILE:CD1	2.45	0.46
2:D:116:ASP:OD2	2:D:149:ASN:CB	2.64	0.46
2:D:105:ILE:HG22	2:D:106:LEU:N	2.26	0.46
2:D:106:LEU:HB3	2:D:107:HIS:H	1.40	0.46
1:A:218:GLU:C	1:A:220:GLN:H	2.17	0.46
1:A:331:PRO:HA	1:A:395:PHE:O	2.15	0.46
1:C:262:PHE:HD1	1:C:364:MET:HE2	1.80	0.46
1:C:221:GLN:O	1:C:223:PRO:CD	2.58	0.46
2:B:2:ALA:HB2	2:B:193:LEU:CD1	2.45	0.46
1:C:413:VAL:CG2	1:C:462:LEU:HD13	2.45	0.46
1:C:8:LEU:HD23	1:C:8:LEU:C	2.34	0.46
1:A:309:GLU:HG3	1:A:310:SER:N	2.31	0.46
1:A:383:TYR:CD2	1:C:342:LEU:HD13	2.51	0.46
1:A:501:ASN:OD1	1:A:504:ARG:NH2	2.39	0.46
1:A:8:LEU:HD23	1:A:9:THR:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:GLY:N	2:B:137:VAL:CG2	2.78	0.46
1:A:469:ARG:HH11	1:A:469:ARG:HG3	1.78	0.46
1:C:230:LYS:C	1:C:232:GLU:H	2.18	0.46
1:C:276:ALA:O	1:C:280:PRO:HD2	2.16	0.46
1:C:412:ASP:N	1:C:415:HIS:HD2	2.12	0.46
1:A:170:CYS:HB2	1:A:472:TYR:OH	2.15	0.46
2:D:10:VAL:HG22	2:D:32:ARG:HD2	1.97	0.46
1:C:316:ALA:HB1	1:C:460:ARG:HB2	1.97	0.46
1:C:52:LEU:HG	1:C:183:VAL:HG22	1.98	0.46
1:C:158:PHE:CD1	1:C:421:MET:HE1	2.51	0.46
1:C:294:PHE:O	1:C:304:PHE:HA	2.16	0.46
1:A:308:PRO:CD	1:A:468:ILE:HD11	2.46	0.46
1:C:76:ASN:N	1:C:204:GLU:OE1	2.48	0.46
2:D:149:ASN:ND2	2:D:160:ARG:NE	2.64	0.46
2:D:54:MET:HA	2:D:82:ILE:O	2.15	0.46
1:A:293:MET:HG2	1:A:306:ALA:CB	2.45	0.46
1:A:75:ALA:HA	1:A:78:PRO:CG	2.44	0.45
2:B:2:ALA:CB	2:B:193:LEU:HD11	2.46	0.45
1:A:318:ASN:HD22	1:A:318:ASN:C	2.19	0.45
1:C:426:LEU:HD23	1:C:450:GLY:CA	2.46	0.45
2:D:80:PRO:HB2	2:D:192:ALA:HB1	1.96	0.45
2:B:21:LEU:HD21	2:B:185:LEU:HD13	1.98	0.45
1:A:355:ASP:OD2	1:A:357:LYS:CD	2.63	0.45
1:C:234:MET:CG	1:C:516:ALA:HB2	2.46	0.45
1:C:478:ARG:NE	1:C:510:ILE:HG13	2.28	0.45
1:A:193:LEU:HD23	1:A:194:GLN:H	1.81	0.45
2:D:115:HIS:CE1	2:D:126:ASN:HB2	2.52	0.45
1:A:279:GLY:N	1:A:280:PRO:CD	2.79	0.45
1:C:245:TYR:O	1:C:248:VAL:HB	2.17	0.45
1:A:278:LEU:HD23	1:A:295:PHE:CE2	2.51	0.45
1:C:142:GLU:H	1:C:142:GLU:CD	2.16	0.45
1:A:343:ASP:OD1	1:A:347:ARG:HD3	2.16	0.45
2:B:107:HIS:O	2:B:109:LYS:N	2.46	0.45
2:B:100:GLY:CA	2:B:137:VAL:HG22	2.46	0.45
1:C:280:PRO:HB3	1:C:510:ILE:HA	1.97	0.45
1:C:226:ILE:HA	1:C:227:PRO:HD3	1.79	0.45
2:D:142:PRO:CD	2:D:146:LEU:HD23	2.47	0.45
1:C:29:CYS:O	1:C:30:GLY:C	2.55	0.45
2:D:112:ALA:HB1	2:D:127:PRO:HB2	1.98	0.45
2:D:100:GLY:N	2:D:137:VAL:CG2	2.79	0.45
1:A:507:LEU:HA	1:A:510:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:THR:OG1	1:A:398:HIS:CD2	2.62	0.45
2:B:172:HIS:HB3	2:B:174:GLU:OE1	2.17	0.45
1:C:111:VAL:HG12	1:C:111:VAL:O	2.16	0.45
1:C:262:PHE:CE2	2:D:133:TYR:HB3	2.52	0.45
1:A:423:MET:HG3	1:A:466:ILE:HD11	1.98	0.45
1:A:438:ILE:HG23	1:A:442:ARG:CZ	2.46	0.45
1:A:254:GLU:OE1	1:A:257:ARG:HD3	2.17	0.45
2:B:74:ARG:HH11	2:B:74:ARG:HG3	1.82	0.45
1:C:462:LEU:HD21	1:C:464:THR:HG23	1.98	0.45
1:A:279:GLY:H	1:A:280:PRO:HD2	1.79	0.45
2:D:61:THR:CB	2:D:62:PRO:HD2	2.46	0.45
1:C:250:SER:HA	1:C:253:GLN:HE21	1.81	0.45
1:A:478:ARG:NH2	1:A:510:ILE:HG23	2.31	0.45
1:C:119:ARG:CZ	1:C:411:LEU:HD21	2.47	0.45
1:A:364:MET:CE	1:A:429:ALA:HB1	2.47	0.45
2:D:105:ILE:CD1	2:D:133:TYR:O	2.65	0.45
1:C:362:HIS:O	1:C:366:VAL:HG23	2.17	0.45
1:C:170:CYS:HB2	1:C:472:TYR:OH	2.17	0.45
2:D:80:PRO:HB3	2:D:165:ARG:HB3	1.99	0.45
1:C:119:ARG:HH22	1:C:408:ARG:HH21	1.65	0.44
1:A:162:PRO:HD2	1:A:439:ALA:HB3	1.98	0.44
2:B:136:LEU:O	2:B:137:VAL:CG2	2.60	0.44
1:C:145:MET:HE1	1:C:181:LEU:CD1	2.47	0.44
2:B:112:ALA:HB1	2:B:127:PRO:HB2	1.99	0.44
2:B:99:VAL:HA	2:B:139:SER:HB2	1.99	0.44
2:B:5:LEU:HD22	2:B:29:VAL:CG2	2.43	0.44
1:A:302:THR:OG1	1:A:473:VAL:HB	2.18	0.44
1:A:252:LEU:O	1:A:255:ALA:N	2.47	0.44
1:A:275:PRO:O	1:A:277:PRO:HD3	2.18	0.44
1:A:437:LEU:HD23	1:A:437:LEU:HA	1.72	0.44
2:D:137:VAL:HG11	2:D:139:SER:HB2	2.00	0.44
1:A:316:ALA:HB3	1:A:461:ASN:ND2	2.31	0.44
1:A:462:LEU:C	1:A:462:LEU:HD23	2.37	0.44
1:C:115:ASP:O	1:C:119:ARG:HD2	2.17	0.44
2:D:142:PRO:O	2:D:146:LEU:CB	2.65	0.44
1:C:518:GLU:O	1:C:519:VAL:C	2.56	0.44
1:C:206:GLN:OE1	1:C:210:HIS:CE1	2.70	0.44
2:D:26:HIS:NE2	2:D:189:LEU:HD12	2.33	0.44
1:C:274:CYS:SG	1:C:510:ILE:CG2	3.05	0.44
2:D:95:TYR:CZ	2:D:164:ARG:HD3	2.53	0.44
1:C:210:HIS:O	1:C:213:GLU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:HD12	1:A:271:SER:O	2.18	0.44
2:B:105:ILE:HG22	2:B:106:LEU:N	2.31	0.44
2:B:106:LEU:HB3	2:B:107:HIS:H	1.38	0.44
2:D:38:GLU:O	2:D:42:GLU:HG3	2.17	0.44
2:B:30:ILE:HD12	2:B:30:ILE:N	2.33	0.44
2:D:75:LEU:HA	2:D:78:GLN:HG3	1.99	0.44
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.84	0.44
1:C:279:GLY:N	1:C:280:PRO:HD2	2.33	0.44
1:C:478:ARG:HE	1:C:510:ILE:HG13	1.83	0.44
1:C:411:LEU:HA	1:C:415:HIS:CD2	2.53	0.44
1:A:165:ARG:HH12	1:A:167:ASP:CG	2.21	0.44
1:C:231:LEU:O	1:C:232:GLU:C	2.56	0.44
1:A:25:PHE:CD1	1:A:37:LEU:HB2	2.53	0.44
1:C:314:TYR:CE1	1:C:319:ARG:HA	2.52	0.44
1:C:145:MET:HE1	1:C:181:LEU:HD13	2.00	0.44
2:B:100:GLY:N	2:B:137:VAL:HG21	2.23	0.43
2:D:98:GLN:HB3	2:D:99:VAL:H	1.53	0.43
2:D:115:HIS:CD2	2:D:117:GLY:H	2.36	0.43
2:D:174:GLU:N	2:D:174:GLU:OE1	2.43	0.43
1:C:311:ALA:HB2	1:C:466:ILE:HG13	2.00	0.43
1:C:90:PRO:HG2	1:C:91:GLU:OE2	2.18	0.43
1:A:199:SER:HB3	1:A:200:GLU:H	1.46	0.43
1:A:478:ARG:HD2	1:A:510:ILE:HG12	1.98	0.43
1:C:192:ARG:HG2	1:C:192:ARG:NH2	2.32	0.43
1:A:93:ARG:CB	1:A:104:THR:HB	2.48	0.43
1:A:158:PHE:N	1:A:158:PHE:CD1	2.85	0.43
1:C:200:GLU:O	1:C:201:GLN:C	2.56	0.43
1:A:253:GLN:O	1:A:257:ARG:HG3	2.19	0.43
2:B:70:GLU:HG2	2:B:74:ARG:CZ	2.48	0.43
1:C:411:LEU:HA	1:C:415:HIS:HD2	1.83	0.43
1:A:50:GLN:HA	1:A:184:LEU:O	2.18	0.43
1:C:66:HIS:HA	1:C:123:VAL:HG11	1.99	0.43
1:C:423:MET:HG3	1:C:466:ILE:HG12	2.00	0.43
1:A:481:GLN:HE21	1:A:481:GLN:HB2	1.46	0.43
1:A:375:ARG:HD3	1:A:419:ALA:HB1	2.00	0.43
2:D:109:LYS:HB2	2:D:177:LEU:CD1	2.48	0.43
1:C:422:ASN:OD1	1:C:452:ARG:NH2	2.51	0.43
1:C:308:PRO:O	1:C:309:GLU:HB2	2.19	0.43
1:C:144:VAL:CG2	1:C:458:ALA:HB3	2.48	0.43
1:C:492:PRO:O	1:C:495:GLU:HB2	2.18	0.43
2:B:142:PRO:O	2:B:146:LEU:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:SER:OG	1:A:137:PRO:HD2	2.19	0.43
1:A:145:MET:HE1	1:A:181:LEU:CD1	2.49	0.43
1:C:146:LEU:O	1:C:455:TYR:HA	2.17	0.43
1:A:315:ASP:OD1	1:A:317:GLY:N	2.51	0.43
1:C:231:LEU:O	1:C:231:LEU:HG	2.17	0.43
1:C:218:GLU:O	1:C:220:GLN:N	2.51	0.43
1:A:279:GLY:O	1:A:282:GLN:HB3	2.19	0.43
1:C:91:GLU:H	1:C:91:GLU:CD	2.21	0.43
1:A:262:PHE:CZ	2:B:133:TYR:HB3	2.53	0.43
1:A:355:ASP:OD2	1:A:355:ASP:C	2.57	0.43
1:C:78:PRO:O	1:C:82:PRO:CD	2.65	0.43
1:A:426:LEU:CD2	1:A:468:ILE:CG2	2.97	0.43
2:B:57:PRO:HD3	2:B:84:ILE:HB	2.01	0.43
2:B:9:ASN:OD1	2:B:33:ASN:ND2	2.51	0.43
1:A:386:ASP:HB3	1:A:389:LYS:HG2	2.00	0.43
1:A:91:GLU:H	1:A:91:GLU:CD	2.21	0.43
2:D:102:ALA:O	2:D:104:GLU:HG2	2.18	0.43
1:A:267:SER:HA	1:A:483:GLY:HA2	2.00	0.43
1:C:478:ARG:NH1	1:C:510:ILE:HG23	2.33	0.43
1:A:292:TYR:OH	1:A:310:SER:HB2	2.19	0.43
1:A:138:ALA:O	1:A:139:ASP:HB3	2.19	0.43
2:D:33:ASN:HD22	2:D:33:ASN:HA	1.44	0.43
1:A:336:ALA:C	1:A:338:GLY:H	2.21	0.43
1:A:274:CYS:SG	1:A:280:PRO:HG3	2.58	0.43
2:D:165:ARG:HA	2:D:165:ARG:HD2	1.81	0.43
1:C:156:ALA:HA	1:C:161:LEU:HD23	2.00	0.43
1:A:350:LEU:HD13	1:C:387:LEU:HD21	2.01	0.43
1:A:61:ILE:HD13	1:A:130:ILE:CD1	2.48	0.43
1:C:59:LEU:HD23	1:C:72:ALA:HA	2.00	0.42
1:A:373:LEU:HD23	1:A:373:LEU:HA	1.76	0.42
1:C:471:ALA:HB2	1:C:506:VAL:HG11	2.01	0.42
2:B:98:GLN:HB3	2:B:99:VAL:H	1.64	0.42
1:C:72:ALA:HB1	1:C:78:PRO:HD3	2.01	0.42
1:A:462:LEU:HD23	1:A:463:ASP:N	2.34	0.42
1:C:165:ARG:HH12	1:C:167:ASP:CG	2.22	0.42
1:A:200:GLU:O	1:A:201:GLN:C	2.57	0.42
1:C:392:ARG:O	1:C:393:TYR:HD2	2.02	0.42
2:B:109:LYS:O	2:B:110:ALA:CB	2.67	0.42
2:B:137:VAL:HG12	2:B:138:GLY:N	2.33	0.42
1:A:17:TYR:CE1	1:A:189:GLY:HA2	2.55	0.42
1:A:510:ILE:O	1:A:514:HIS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:142:PRO:HG2	2:D:146:LEU:HD23	2.00	0.42
1:A:382:ARG:HA	1:A:404:VAL:O	2.19	0.42
1:A:314:TYR:CD2	1:A:413:VAL:HB	2.54	0.42
1:A:360:ALA:CB	2:B:108:GLY:HA2	2.47	0.42
1:A:230:LYS:C	1:A:232:GLU:N	2.69	0.42
1:A:208:LEU:O	1:A:209:GLN:C	2.58	0.42
2:D:185:LEU:HA	2:D:185:LEU:HD23	1.91	0.42
1:C:438:ILE:O	1:C:442:ARG:HD2	2.20	0.42
1:C:280:PRO:HA	1:C:513:ALA:HB2	2.02	0.42
1:C:19:GLY:O	1:C:20:ASP:HB3	2.19	0.42
1:C:328:GLY:O	1:C:398:HIS:HA	2.19	0.42
1:A:431:LYS:N	2:B:12:SER:OG	2.43	0.42
1:C:149:LEU:HD12	1:C:452:ARG:O	2.20	0.42
1:A:329:THR:C	1:A:330:ARG:HG2	2.39	0.42
1:C:288:ASN:N	1:C:289:PRO:CD	2.83	0.42
2:B:105:ILE:CD1	2:B:133:TYR:O	2.67	0.42
1:A:78:PRO:O	1:A:81:LEU:HB2	2.18	0.42
2:B:29:VAL:HG11	2:B:43:ARG:HH21	1.84	0.42
1:A:280:PRO:HB2	1:A:478:ARG:HH22	1.85	0.42
1:C:248:VAL:CG1	1:C:441:LEU:HG	2.47	0.42
1:C:408:ARG:HG3	1:C:408:ARG:HH11	1.84	0.42
1:A:308:PRO:HD3	1:A:468:ILE:HD11	2.02	0.42
1:C:201:GLN:HA	1:C:201:GLN:OE1	2.20	0.42
2:D:104:GLU:C	2:D:105:ILE:HG13	2.39	0.42
2:D:99:VAL:HG12	2:D:100:GLY:N	2.31	0.42
1:C:274:CYS:SG	1:C:280:PRO:HG3	2.60	0.42
1:A:478:ARG:HE	1:A:510:ILE:CG1	2.31	0.42
1:C:226:ILE:HD13	1:C:228:HIS:CE1	2.45	0.42
2:B:185:LEU:HD23	2:B:185:LEU:HA	1.83	0.42
2:B:4:ILE:HD11	2:B:189:LEU:HD11	2.02	0.42
2:D:109:LYS:O	2:D:110:ALA:CB	2.68	0.42
2:D:42:GLU:HA	2:D:45:GLN:CD	2.39	0.42
1:A:216:GLN:O	1:A:218:GLU:N	2.53	0.42
1:A:280:PRO:CG	1:A:281:TYR:N	2.83	0.42
1:C:318:ASN:HD22	1:C:318:ASN:C	2.22	0.42
1:A:231:LEU:O	1:A:232:GLU:C	2.56	0.42
1:C:204:GLU:O	1:C:205:ALA:C	2.58	0.42
1:C:34:ALA:HA	1:C:176:TYR:CZ	2.55	0.42
2:B:98:GLN:C	2:B:99:VAL:HG23	2.40	0.42
2:D:99:VAL:HG12	2:D:137:VAL:HG21	2.01	0.42
1:C:17:TYR:CD2	1:C:18:ARG:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ILE:HG12	1:A:282:GLN:HE22	1.84	0.42
2:B:17:LEU:HD23	2:B:174:GLU:HB3	2.02	0.42
2:B:170:GLN:O	2:B:170:GLN:CG	2.48	0.41
1:A:75:ALA:HB3	1:A:204:GLU:CD	2.40	0.41
1:A:274:CYS:HB2	1:A:510:ILE:HG21	2.02	0.41
2:B:20:GLN:NE2	1:C:347:ARG:HH12	2.17	0.41
1:A:332:ARG:NH1	1:A:345:ASP:OD1	2.53	0.41
2:D:70:GLU:HG2	2:D:74:ARG:CZ	2.50	0.41
1:C:17:TYR:CE2	1:C:19:GLY:N	2.88	0.41
1:A:230:LYS:O	1:A:232:GLU:N	2.53	0.41
2:D:33:ASN:HB3	2:D:34:GLN:HE21	1.85	0.41
1:C:13:VAL:HG12	1:C:14:GLN:N	2.36	0.41
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.64	0.41
1:C:37:LEU:O	1:C:294:PHE:HA	2.20	0.41
1:A:294:PHE:O	1:A:304:PHE:HA	2.20	0.41
1:A:330:ARG:O	1:A:397:MET:N	2.41	0.41
2:D:3:ASP:O	2:D:51:PRO:HA	2.21	0.41
2:D:50:GLN:N	2:D:51:PRO:CD	2.82	0.41
1:A:8:LEU:HD23	1:A:9:THR:C	2.40	0.41
2:D:100:GLY:N	2:D:137:VAL:HG21	2.31	0.41
1:A:459:VAL:O	1:A:460:ARG:CB	2.67	0.41
1:A:459:VAL:O	1:A:460:ARG:HB2	2.20	0.41
1:C:39:GLU:OE1	1:C:285:LYS:HE3	2.21	0.41
1:C:329:THR:HA	1:C:397:MET:O	2.20	0.41
1:A:19:GLY:O	1:A:20:ASP:HB3	2.21	0.41
1:C:67:THR:HG23	1:C:102:GLU:OE2	2.20	0.41
1:C:334:ARG:NH1	1:C:338:GLY:O	2.53	0.41
1:A:74:THR:HG21	1:A:179:GLU:OE2	2.21	0.41
1:C:309:GLU:CG	1:C:310:SER:N	2.84	0.41
1:C:373:LEU:HD12	1:C:403:VAL:CG2	2.50	0.41
1:C:125:ASP:HA	1:C:128:ARG:HB3	2.02	0.41
2:B:137:VAL:CG1	2:B:139:SER:HB2	2.51	0.41
1:C:383:TYR:N	1:C:383:TYR:CD2	2.89	0.41
1:A:319:ARG:NH1	1:A:408:ARG:O	2.44	0.41
1:C:417:TYR:HE1	1:C:452:ARG:HG2	1.86	0.41
1:C:82:PRO:HA	1:C:85:ASP:OD2	2.21	0.41
2:B:38:GLU:O	2:B:42:GLU:CG	2.63	0.41
1:A:146:LEU:HA	1:A:146:LEU:HD23	1.97	0.41
2:B:132:ARG:HD3	2:B:132:ARG:HH21	1.72	0.41
2:D:107:HIS:C	2:D:109:LYS:N	2.74	0.41
2:D:136:LEU:C	2:D:137:VAL:HG23	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:189:LEU:O	2:D:190:ALA:C	2.58	0.41
1:A:77:GLY:N	1:A:78:PRO:CD	2.81	0.41
1:C:272:LEU:CG	1:C:510:ILE:HD13	2.51	0.41
1:C:152:TYR:CD1	1:C:422:ASN:ND2	2.89	0.41
1:A:218:GLU:C	1:A:220:GLN:N	2.73	0.41
1:C:18:ARG:HG3	1:C:219:LEU:HD22	2.02	0.41
1:C:21:PRO:HB2	1:C:39:GLU:OE1	2.21	0.41
1:A:226:ILE:H	1:A:226:ILE:CD1	2.33	0.41
2:B:141:ILE:HA	2:B:142:PRO:HD3	1.79	0.41
1:A:298:ASP:CG	1:A:299:ASP:H	2.24	0.41
1:C:331:PRO:HA	1:C:395:PHE:O	2.21	0.41
1:C:66:HIS:H	1:C:66:HIS:HD2	1.68	0.41
1:A:491:ILE:O	1:A:492:PRO:C	2.58	0.41
2:D:137:VAL:HG12	2:D:138:GLY:N	2.36	0.41
1:A:269:ARG:NH1	1:A:444:THR:OG1	2.50	0.41
2:D:71:LEU:HD12	2:D:71:LEU:HA	1.88	0.41
1:C:373:LEU:HD23	1:C:373:LEU:HA	1.76	0.41
1:A:499:THR:O	1:A:502:LYS:N	2.54	0.41
1:A:76:ASN:OD1	1:A:197:VAL:HA	2.21	0.41
1:C:459:VAL:O	1:C:460:ARG:CB	2.69	0.40
1:C:267:SER:HA	1:C:482:ALA:O	2.21	0.40
1:A:215:LEU:O	1:A:218:GLU:HB2	2.22	0.40
1:A:226:ILE:HG12	1:A:282:GLN:NE2	2.36	0.40
1:C:248:VAL:HG13	1:C:441:LEU:CD2	2.51	0.40
1:C:129:THR:O	1:C:130:ILE:C	2.59	0.40
1:A:84:LEU:HD13	1:A:88:LEU:CD1	2.51	0.40
1:A:365:LEU:HA	1:A:365:LEU:HD23	1.71	0.40
1:C:449:TYR:CD1	1:C:481:GLN:HB3	2.56	0.40
1:C:485:GLY:O	1:C:486:VAL:HB	2.22	0.40
1:C:145:MET:HE1	1:C:181:LEU:CD2	2.52	0.40
1:C:61:ILE:CD1	1:C:130:ILE:HD12	2.49	0.40
1:C:491:ILE:O	1:C:492:PRO:C	2.60	0.40
2:B:85:CYS:O	2:B:88:HIS:HB3	2.22	0.40
1:A:318:ASN:ND2	1:A:318:ASN:C	2.74	0.40
1:C:364:MET:CE	2:D:13:PHE:CZ	3.04	0.40
2:D:110:ALA:HB2	2:D:177:LEU:HD22	2.03	0.40
1:A:510:ILE:HG13	1:A:510:ILE:H	1.60	0.40
1:A:34:ALA:HA	1:A:176:TYR:CE1	2.56	0.40
1:C:138:ALA:O	1:C:139:ASP:CB	2.69	0.40
2:B:6:LEU:HD21	2:B:14:THR:HG23	2.03	0.40
1:A:245:TYR:CD2	1:A:496:ALA:HA	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	507/519 (98%)	449 (89%)	36 (7%)	22 (4%)	3	2
1	C	507/519 (98%)	449 (89%)	39 (8%)	19 (4%)	4	3
2	B	190/193 (98%)	162 (85%)	18 (10%)	10 (5%)	2	1
2	D	190/193 (98%)	158 (83%)	20 (10%)	12 (6%)	2	0
All	All	1394/1424 (98%)	1218 (87%)	113 (8%)	63 (4%)	3	2

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ASP
1	A	21	PRO
1	A	139	ASP
1	A	201	GLN
1	A	221	GLN
1	A	443	SER
1	A	519	VAL
2	B	99	VAL
2	B	105	ILE
2	B	107	HIS
2	B	109	LYS
2	B	110	ALA
1	C	20	ASP
1	C	21	PRO
1	C	139	ASP
1	C	187	GLN
1	C	221	GLN
1	C	519	VAL
2	D	99	VAL
2	D	105	ILE

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Mol	Chain	Res	Type
2	D	106	LEU
2	D	107	HIS
2	D	109	LYS
2	D	110	ALA
1	A	17	TYR
2	B	106	LEU
2	B	136	LEU
2	B	137	VAL
1	C	201	GLN
1	C	219	LEU
2	D	104	GLU
2	D	108	GLY
2	D	137	VAL
2	D	139	SER
1	A	187	GLN
1	A	231	LEU
1	A	232	GLU
1	A	337	ASP
1	A	395	PHE
2	B	104	GLU
2	B	108	GLY
1	C	232	GLU
1	C	443	SER
2	D	97	GLY
2	D	136	LEU
1	A	486	VAL
1	C	233	ASN
1	C	356	HIS
1	C	388	THR
1	A	50	GLN
1	A	138	ALA
1	A	233	ASN
1	A	356	HIS
1	A	422	ASN
1	C	50	GLN
1	C	486	VAL
1	A	98	PRO
1	C	98	PRO
1	C	138	ALA
1	C	492	PRO
1	A	225	PRO
1	A	492	PRO

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Mol	Chain	Res	Type
1	C	485	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	A	422/434 (97%)	374 (89%)	48 (11%)	7	9
1	C	422/434 (97%)	372 (88%)	50 (12%)	6	8
2	B	152/153 (99%)	132 (87%)	20 (13%)	5	6
2	D	152/153 (99%)	134 (88%)	18 (12%)	6	8
All	All	1148/1174 (98%)	1012 (88%)	136 (12%)	6	8

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	14	GLN
1	A	16	SER
1	A	23	THR
1	A	28	LEU
1	A	42	GLU
1	A	49	LEU
1	A	51	SER
1	A	66	HIS
1	A	70	VAL
1	A	83	LEU
1	A	93	ARG
1	A	94	ASN
1	A	95	GLN
1	A	139	ASP
1	A	142	GLU
1	A	144	VAL
1	A	173	PHE
1	A	177	LEU
1	A	193	LEU

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Mol	Chain	Res	Type
1	A	199	SER
1	A	200	GLU
1	A	212	LEU
1	A	213	GLU
1	A	226	ILE
1	A	237	SER
1	A	242	ASP
1	A	278	LEU
1	A	302	THR
1	A	303	LEU
1	A	318	ASN
1	A	347	ARG
1	A	357	LYS
1	A	368	LEU
1	A	382	ARG
1	A	389	LYS
1	A	399	LEU
1	A	403	VAL
1	A	426	LEU
1	A	442	ARG
1	A	444	THR
1	A	452	ARG
1	A	457	THR
1	A	468	ILE
1	A	469	ARG
1	A	478	ARG
1	A	488	GLN
1	A	520	PHE
2	B	5	LEU
2	B	7	LEU
2	B	33	ASN
2	B	34	GLN
2	B	42	GLU
2	B	44	LEU
2	B	47	MET
2	B	74	ARG
2	B	101	GLN
2	B	105	ILE
2	B	109	LYS
2	B	120	MET
2	B	140	ASN
2	B	145	ASP

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Mol	Chain	Res	Type
2	B	159	VAL
2	B	163	ARG
2	B	165	ARG
2	B	184	LEU
2	B	185	LEU
2	B	195	LYS
1	C	14	GLN
1	C	21	PRO
1	C	23	THR
1	C	28	LEU
1	C	42	GLU
1	C	51	SER
1	C	66	HIS
1	C	70	VAL
1	C	83	LEU
1	C	84	LEU
1	C	93	ARG
1	C	94	ASN
1	C	95	GLN
1	C	139	ASP
1	C	142	GLU
1	C	144	VAL
1	C	173	PHE
1	C	177	LEU
1	C	193	LEU
1	C	199	SER
1	C	200	GLU
1	C	212	LEU
1	C	213	GLU
1	C	215	LEU
1	C	226	ILE
1	C	234	MET
1	C	237	SER
1	C	273	PRO
1	C	278	LEU
1	C	303	LEU
1	C	310	SER
1	C	313	LYS
1	C	318	ASN
1	C	346	SER
1	C	347	ARG
1	C	357	LYS

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Mol	Chain	Res	Type
1	C	368	LEU
1	C	382	ARG
1	C	389	LYS
1	C	394	SER
1	C	399	LEU
1	C	426	LEU
1	C	442	ARG
1	C	452	ARG
1	C	468	ILE
1	C	469	ARG
1	C	478	ARG
1	C	487	VAL
1	C	488	GLN
1	C	520	PHE
2	D	7	LEU
2	D	27	GLN
2	D	33	ASN
2	D	34	GLN
2	D	42	GLU
2	D	74	ARG
2	D	99	VAL
2	D	101	GLN
2	D	105	ILE
2	D	109	LYS
2	D	120	MET
2	D	145	ASP
2	D	163	ARG
2	D	165	ARG
2	D	170	GLN
2	D	184	LEU
2	D	185	LEU
2	D	195	LYS

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

Mol	Chain	Res	Type
1	A	27	GLN
1	A	66	HIS
1	A	71	GLN
1	A	166	GLN
1	A	186	HIS
1	A	187	GLN

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Mol	Chain	Res	Type
1	A	229	GLN
1	A	253	GLN
1	A	263	GLN
1	A	287	ASN
1	A	288	ASN
1	A	297	GLN
1	A	318	ASN
1	A	371	ASN
1	A	378	GLN
1	A	398	HIS
1	A	415	HIS
1	A	461	ASN
1	A	481	GLN
1	A	488	GLN
1	A	514	HIS
2	B	20	GLN
2	B	27	GLN
2	B	33	ASN
2	B	34	GLN
2	B	101	GLN
2	B	115	HIS
2	B	140	ASN
1	C	27	GLN
1	C	66	HIS
1	C	166	GLN
1	C	168	GLN
1	C	186	HIS
1	C	210	HIS
1	C	228	HIS
1	C	229	GLN
1	C	253	GLN
1	C	263	GLN
1	C	287	ASN
1	C	288	ASN
1	C	297	GLN
1	C	318	ASN
1	C	371	ASN
1	C	398	HIS
1	C	415	HIS
1	C	481	GLN
1	C	488	GLN
1	C	514	HIS

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Mol	Chain	Res	Type
2	D	33	ASN
2	D	34	GLN
2	D	88	HIS
2	D	89	GLN
2	D	101	GLN
2	D	115	HIS
2	D	140	ASN
2	D	170	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TRP	A	601	-	12,16,16	1.12	1 (8%)	7,22,22	0.99	0
3	TRP	C	701	-	12,16,16	1.20	2 (16%)	7,22,22	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRP	A	601	-	-	0/3/8/8	0/2/2/2
3	TRP	C	701	-	-	0/3/8/8	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	701	TRP	CD1-NE1	2.07	1.40	1.36
3	C	701	TRP	CZ3-CE3	2.50	1.42	1.36
3	A	601	TRP	CZ3-CE3	2.68	1.42	1.36

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	TRP	1	0
3	C	701	TRP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.