Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 01:52 PM EDT

PDB ID	:	2IBM
Title	:	A novel dimer interface and conformational changes revealed by an X-ray structure of B. subtilis SecA
Authors	:	Zimmer, J.; Li, W.; Rapoport, T.A.
Deposited on	:	2006-09-11
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

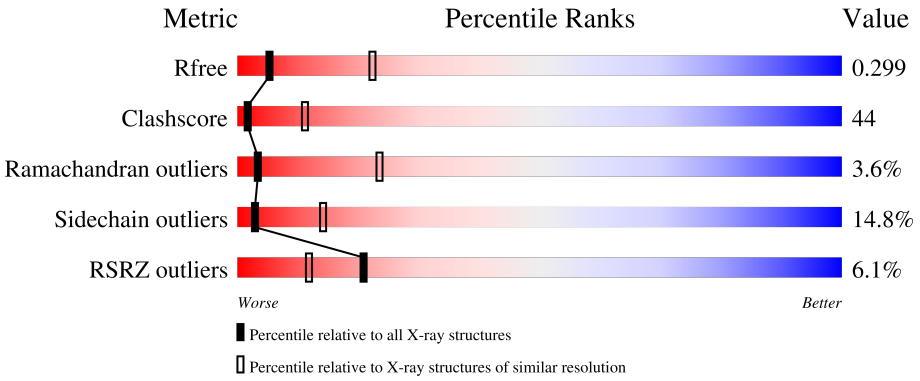
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	780	7%, 44%, 45%, 11%
1	B	780	5%, 44%, 45%, 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	A	781	-	-	-	X

2 Entry composition (i)

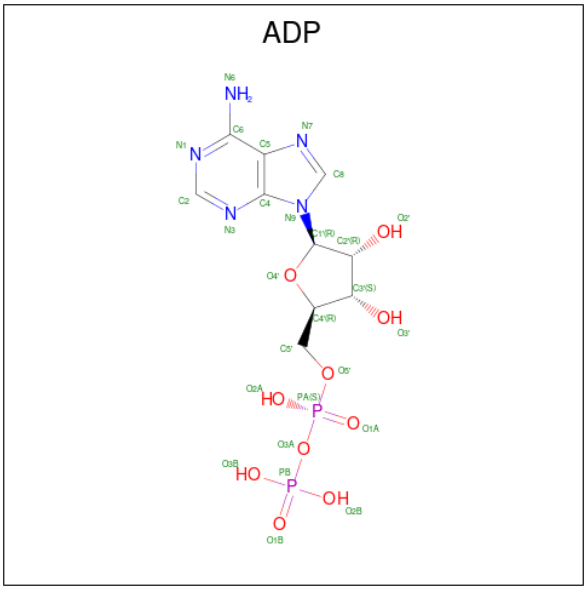
There are 2 unique types of molecules in this entry. The entry contains 12403 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Preprotein translocase secA subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	780	Total	C	N	O	S	0	0	0
			6228	3899	1084	1210	35			
1	B	770	Total	C	N	O	S	0	0	0
			6148	3846	1072	1197	33			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



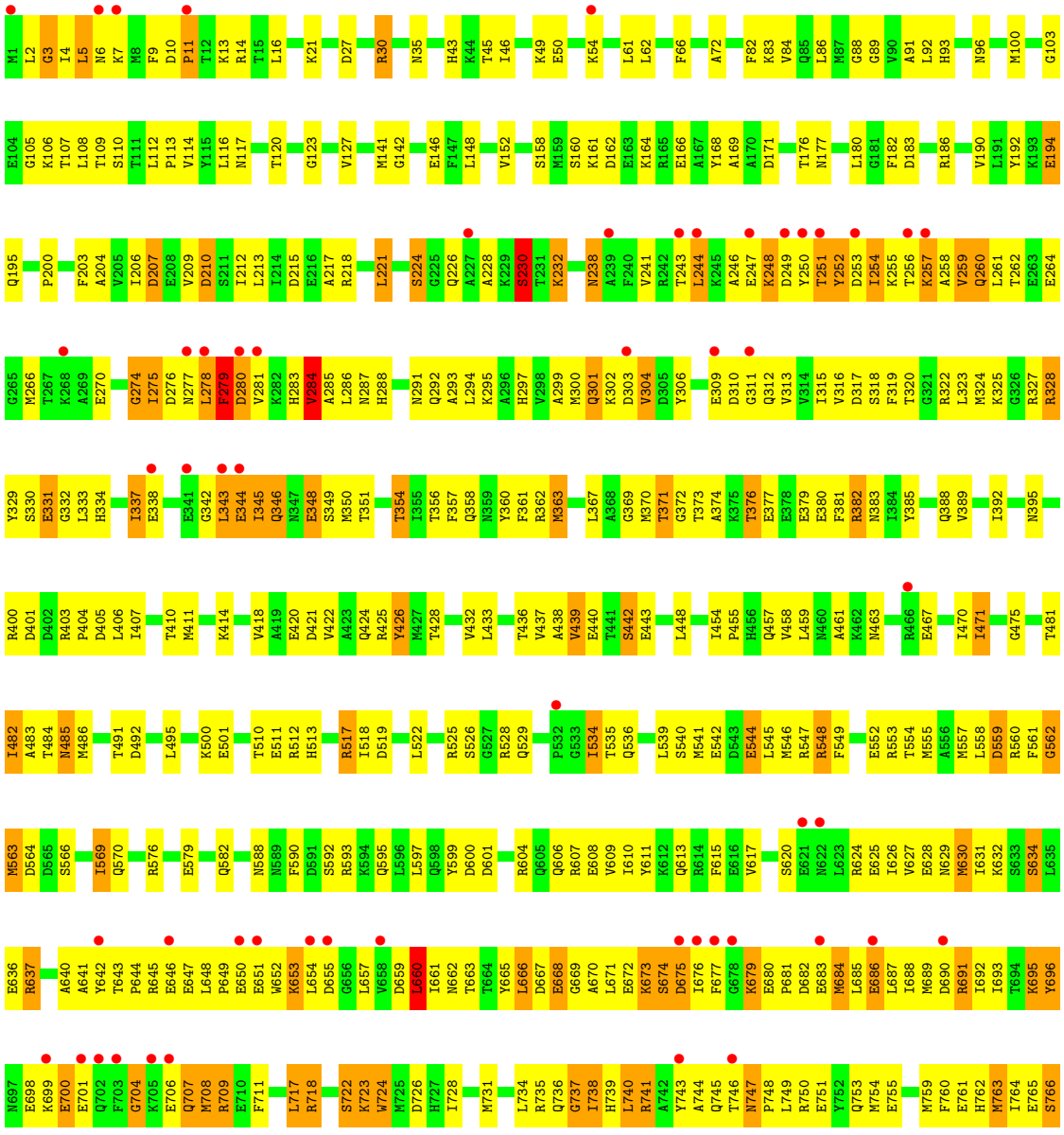
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

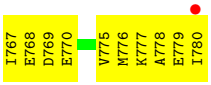
3 Residue-property plots (i)

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

• Molecule 1: Preprotein translocase secA subunit

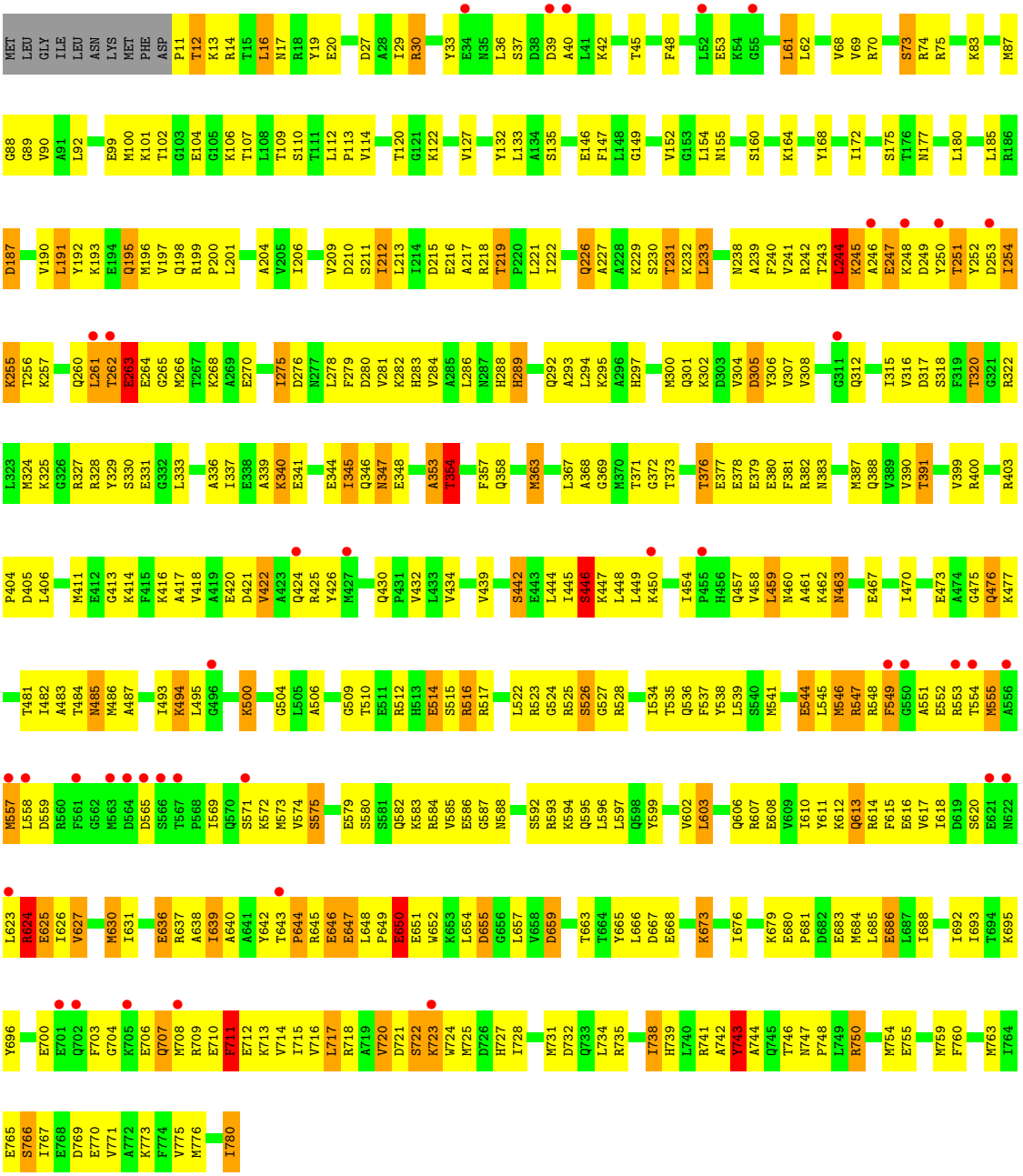
Chain A:





• Molecule 1: Preprotein translocase secA subunit

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	125.83Å 166.83Å 211.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.53 – 3.20 40.53 – 3.10	Depositor EDS
% Data completeness (in resolution range)	92.7 (40.53-3.20) 90.9 (40.53-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.321 , 0.323 0.293 , 0.299	Depositor DCC
R_{free} test set	3431 reflections (8.64%)	wwPDB-VP
Wilson B-factor (Å^2)	69.9	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	12403	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	2/6316 (0.0%)	0.88	9/8492 (0.1%)
1	B	0.68	1/6235 (0.0%)	0.90	19/8384 (0.2%)
All	All	0.65	3/12551 (0.0%)	0.89	28/16876 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	354	THR	CB-OG1	-13.18	1.16	1.43
1	A	279	PHE	C-N	6.88	1.49	1.34
1	A	701	GLU	N-CA	5.04	1.56	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	244	LEU	C-N-CA	10.24	147.31	121.70
1	B	247	GLU	CA-C-N	-9.45	96.40	117.20
1	B	353	ALA	N-CA-CB	8.80	122.42	110.10
1	B	244	LEU	CA-C-N	-8.14	99.29	117.20
1	A	11	PRO	N-CA-C	7.27	130.99	112.10
1	B	354	THR	CA-CB-OG1	6.79	123.26	109.00
1	A	14	ARG	N-CA-C	-6.36	93.82	111.00
1	B	711	PHE	CB-CG-CD1	-6.33	116.37	120.80
1	B	650	GLU	N-CA-CB	-6.24	99.36	110.60
1	B	247	GLU	O-C-N	6.21	132.64	122.70
1	B	353	ALA	CB-CA-C	-6.14	100.89	110.10
1	B	704	GLY	N-CA-C	5.99	128.08	113.10
1	B	244	LEU	N-CA-C	5.94	127.04	111.00
1	A	252	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	B	623	LEU	CA-C-N	-5.94	104.14	117.20
1	B	624	ARG	CA-CB-CG	5.90	126.39	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	624	ARG	CB-CA-C	5.85	122.10	110.40
1	B	244	LEU	O-C-N	5.75	131.90	122.70
1	A	704	GLY	N-CA-C	5.61	127.12	113.10
1	A	280	ASP	C-N-CA	5.54	135.54	121.70
1	A	230	SER	N-CA-C	5.43	125.67	111.00
1	A	280	ASP	N-CA-CB	5.20	119.96	110.60
1	B	711	PHE	CB-CA-C	-5.18	100.04	110.40
1	B	247	GLU	CA-C-O	5.17	130.95	120.10
1	A	620	SER	N-CA-C	5.07	124.69	111.00
1	B	717	LEU	C-N-CA	-5.05	109.08	121.70
1	A	280	ASP	CA-C-N	-5.01	106.18	117.20
1	B	650	GLU	CB-CA-C	5.00	120.41	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6228	0	6227	545	0
1	B	6148	0	6139	578	0
2	A	27	0	12	3	0
All	All	12403	0	12378	1092	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 44.

All (1092) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:SER:HB3	1:B:625:GLU:CG	1.49	1.39
1:A:723:LYS:HD3	1:A:763:MET:SD	1.67	1.35
1:A:747:ASN:H	1:A:748:PRO:CD	1.39	1.31
1:A:10:ASP:HB3	1:A:11:PRO:CD	1.61	1.29
1:A:303:ASP:O	1:A:304:VAL:HG23	1.10	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:ASN:N	1:A:748:PRO:HD2	1.34	1.27
1:B:723:LYS:CE	1:B:767:ILE:HD11	1.66	1.25
1:A:10:ASP:CB	1:A:11:PRO:HD2	1.57	1.25
1:B:620:SER:HB3	1:B:625:GLU:CB	1.67	1.25
1:B:723:LYS:HE3	1:B:767:ILE:CD1	1.65	1.25
1:B:650:GLU:C	1:B:650:GLU:OE1	1.78	1.22
1:A:723:LYS:CD	1:A:763:MET:SD	2.31	1.18
1:A:303:ASP:O	1:A:304:VAL:CG2	1.93	1.16
1:B:245:LYS:HE3	1:B:247:GLU:OE1	1.40	1.16
1:B:624:ARG:HH21	1:B:707:GLN:CB	1.57	1.16
1:B:248:LYS:HB2	1:B:265:GLY:CA	1.76	1.15
1:B:650:GLU:OE1	1:B:650:GLU:O	1.63	1.14
1:B:248:LYS:HB2	1:B:265:GLY:HA3	1.15	1.14
1:B:718:ARG:HG3	1:B:770:GLU:OE2	1.48	1.13
1:B:624:ARG:HH21	1:B:707:GLN:HB3	0.96	1.13
1:A:278:LEU:HB3	1:A:283:HIS:CG	1.83	1.11
1:A:281:VAL:HB	1:A:283:HIS:CD2	1.86	1.11
1:A:661:ILE:HG22	1:A:666:LEU:HD21	1.23	1.10
1:B:750:ARG:HG2	1:B:750:ARG:HH11	1.07	1.09
1:B:620:SER:HB3	1:B:625:GLU:HG2	1.13	1.08
1:B:630:MET:SD	1:B:775:VAL:HG21	1.93	1.07
1:B:620:SER:CB	1:B:625:GLU:HG2	1.85	1.06
1:A:661:ILE:HG22	1:A:666:LEU:CD2	1.85	1.06
1:A:349:SER:HB3	1:B:557:MET:HG3	1.37	1.05
1:B:620:SER:CB	1:B:625:GLU:CG	2.33	1.05
1:A:207:ASP:HB2	1:A:370:MET:HE1	1.34	1.05
1:A:349:SER:CB	1:B:557:MET:HG3	1.86	1.05
1:A:558:LEU:HG	1:A:563:MET:CE	1.87	1.04
1:A:558:LEU:HG	1:A:563:MET:HE1	1.35	1.04
1:B:516:ARG:CZ	1:B:582:GLN:HG2	1.86	1.04
1:B:723:LYS:HB2	1:B:763:MET:CG	1.87	1.04
1:B:647:GLU:CB	1:B:652:TRP:CZ3	2.42	1.03
1:B:647:GLU:C	1:B:652:TRP:HH2	1.61	1.03
1:A:254:ILE:HG22	1:A:255:LYS:H	0.86	1.03
1:A:284:VAL:HG21	1:A:717:LEU:HD21	1.35	1.01
1:A:279:PHE:HA	1:A:778:ALA:HB1	1.42	1.01
1:B:637:ARG:HH21	1:B:769:ASP:HB3	1.21	1.01
1:B:620:SER:CB	1:B:625:GLU:HB3	1.89	1.01
1:A:254:ILE:HG22	1:A:255:LYS:N	1.66	1.00
1:A:708:MET:SD	1:A:711:PHE:HE1	1.84	1.00
1:A:254:ILE:CG2	1:A:255:LYS:H	1.72	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:MET:O	1:A:564:ASP:OD1	1.80	0.99
1:A:723:LYS:HD3	1:A:763:MET:CE	1.92	0.99
1:B:275:ILE:HD11	1:B:283:HIS:CD2	1.98	0.99
1:A:553:ARG:HH21	1:A:560:ARG:HH21	1.02	0.99
1:A:661:ILE:CG2	1:A:666:LEU:HD21	1.93	0.99
1:B:295:LYS:HE2	1:B:333:LEU:HD22	1.39	0.99
1:A:226:GLN:HE21	1:A:228:ALA:H	1.11	0.98
1:B:248:LYS:CB	1:B:265:GLY:CA	2.41	0.98
1:B:718:ARG:HG3	1:B:770:GLU:CD	1.82	0.98
1:B:218:ARG:HD3	1:B:592:SER:HB3	1.44	0.98
1:A:485:ASN:O	1:A:486:MET:HG2	1.63	0.98
1:B:620:SER:HB3	1:B:625:GLU:HB3	1.39	0.97
1:A:457:GLN:HE21	1:A:470:ILE:HD12	1.27	0.97
1:B:243:THR:C	1:B:244:LEU:HD23	1.85	0.97
1:B:624:ARG:NH2	1:B:707:GLN:HB3	1.79	0.97
1:B:647:GLU:HB3	1:B:652:TRP:CZ3	1.98	0.97
1:B:637:ARG:HE	1:B:769:ASP:CB	1.77	0.96
1:B:12:THR:O	1:B:16:LEU:HD22	1.63	0.96
1:B:647:GLU:CA	1:B:652:TRP:CH2	2.48	0.96
1:A:278:LEU:HB3	1:A:283:HIS:CB	1.95	0.96
1:A:746:THR:HG22	1:A:746:THR:O	1.64	0.96
1:B:637:ARG:NH2	1:B:769:ASP:HB3	1.80	0.96
1:A:337:ILE:HD12	1:A:346:GLN:NE2	1.79	0.96
1:A:275:ILE:CG2	1:A:276:ASP:H	1.78	0.96
1:A:221:LEU:HD11	1:A:357:PHE:CZ	2.01	0.96
1:B:418:VAL:O	1:B:422:VAL:HG23	1.66	0.95
1:B:625:GLU:O	1:B:625:GLU:HG3	1.65	0.95
1:B:603:LEU:HD11	1:B:731:MET:HG2	1.47	0.95
1:A:666:LEU:CD1	1:A:691:ARG:HB3	1.96	0.95
1:A:708:MET:SD	1:A:711:PHE:CE1	2.59	0.95
1:B:647:GLU:HB3	1:B:652:TRP:HZ3	1.31	0.94
1:A:275:ILE:HG23	1:A:276:ASP:H	1.31	0.94
1:A:610:ILE:HG13	1:A:723:LYS:HE3	1.47	0.94
1:B:626:ILE:HD12	1:B:715:ILE:HD12	1.49	0.94
1:A:627:VAL:O	1:A:631:ILE:HG12	1.66	0.94
1:B:248:LYS:HZ3	1:B:268:LYS:HB2	1.33	0.94
1:A:278:LEU:HB3	1:A:283:HIS:HB3	1.48	0.93
1:A:5:LEU:HB3	1:A:383:ASN:OD1	1.69	0.93
1:B:647:GLU:N	1:B:652:TRP:CH2	2.37	0.92
1:B:331:GLU:OE2	1:B:722:SER:HB2	1.69	0.92
1:B:245:LYS:HE3	1:B:247:GLU:CD	1.90	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:647:GLU:C	1:B:652:TRP:CH2	2.43	0.92
1:B:620:SER:CB	1:B:625:GLU:CB	2.48	0.92
1:A:278:LEU:CB	1:A:283:HIS:HB3	2.00	0.91
1:B:647:GLU:O	1:B:652:TRP:CH2	2.23	0.91
1:B:614:ARG:HH12	1:B:720:VAL:CG2	1.84	0.90
1:A:182:PHE:HB3	1:A:186:ARG:HH21	1.36	0.90
1:A:275:ILE:CG2	1:A:276:ASP:N	2.34	0.90
1:B:336:ALA:O	1:B:340:LYS:HD3	1.72	0.90
1:A:660:LEU:HD23	1:A:661:ILE:HG13	1.52	0.90
1:B:248:LYS:CD	1:B:265:GLY:HA2	2.02	0.90
1:B:636:GLU:HA	1:B:636:GLU:OE1	1.69	0.89
1:B:647:GLU:O	1:B:652:TRP:HH2	1.52	0.89
1:A:232:LYS:H	1:A:232:LYS:HD2	1.37	0.89
1:B:324:MET:HA	1:B:741:ARG:HD2	1.53	0.89
1:A:244:LEU:O	1:A:248:LYS:HB2	1.72	0.89
1:A:749:LEU:O	1:A:753:GLN:HG2	1.73	0.89
1:B:750:ARG:HG2	1:B:750:ARG:NH1	1.82	0.89
1:B:750:ARG:HH11	1:B:750:ARG:CG	1.86	0.88
1:A:228:ALA:HB3	1:A:230:SER:OG	1.74	0.88
1:A:317:ASP:HB3	1:A:320:THR:HG22	1.55	0.88
1:A:313:VAL:HG22	1:A:337:ILE:HD13	1.56	0.88
1:A:338:GLU:HG2	1:A:345:ILE:HG13	1.55	0.87
1:A:666:LEU:HD12	1:A:691:ARG:HB3	1.55	0.87
1:B:713:LYS:O	1:B:717:LEU:HB2	1.72	0.87
1:A:485:ASN:O	1:A:486:MET:CG	2.23	0.87
1:A:640:ALA:O	1:A:644:PRO:HD3	1.74	0.87
1:A:647:GLU:HG3	1:A:649:PRO:CD	2.05	0.87
1:A:226:GLN:HB2	1:A:350:MET:HB2	1.54	0.87
1:A:673:LYS:HB2	1:A:677:PHE:HB3	1.54	0.86
1:A:722:SER:O	1:A:726:ASP:HB2	1.74	0.86
1:A:561:PHE:O	1:A:569:ILE:HG13	1.76	0.85
1:B:248:LYS:CB	1:B:265:GLY:HA2	2.05	0.85
1:A:281:VAL:HG12	1:A:281:VAL:O	1.74	0.85
1:B:522:LEU:O	1:B:525:ARG:HG3	1.76	0.85
1:A:647:GLU:HG3	1:A:649:PRO:HD3	1.59	0.85
1:A:755:GLU:O	1:A:759:MET:HG3	1.75	0.84
1:B:229:LYS:HB3	1:B:289:HIS:NE2	1.92	0.84
1:B:718:ARG:CG	1:B:770:GLU:OE2	2.24	0.84
1:B:152:VAL:HG13	1:B:172:ILE:HG22	1.58	0.84
1:B:614:ARG:HH12	1:B:720:VAL:HG23	1.43	0.84
1:A:576:ARG:HH22	1:B:346:GLN:CD	1.80	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:LYS:HD2	1:A:763:MET:SD	2.16	0.83
1:A:657:LEU:HD12	1:A:660:LEU:HD22	1.59	0.83
1:A:700:GLU:O	1:A:704:GLY:HA3	1.78	0.83
1:B:12:THR:O	1:B:16:LEU:CD2	2.26	0.83
1:B:703:PHE:CE1	1:B:707:GLN:NE2	2.45	0.83
1:A:249:ASP:OD2	1:A:294:LEU:HD21	1.78	0.83
1:A:741:ARG:HH22	1:B:376:THR:HG22	1.43	0.83
1:B:723:LYS:HB2	1:B:763:MET:HG3	1.61	0.83
1:A:673:LYS:HB2	1:A:677:PHE:CB	2.08	0.82
1:B:459:LEU:HD22	1:B:487:ALA:HB1	1.61	0.82
1:B:626:ILE:CG2	1:B:715:ILE:HD11	2.09	0.82
1:B:706:GLU:O	1:B:709:ARG:HB2	1.79	0.82
1:A:338:GLU:HG2	1:A:345:ILE:HA	1.61	0.82
1:B:514:GLU:HA	1:B:514:GLU:OE1	1.79	0.82
1:B:637:ARG:HE	1:B:769:ASP:HB3	1.45	0.82
1:A:630:MET:HE3	1:A:775:VAL:HG11	1.58	0.82
1:B:295:LYS:HE2	1:B:333:LEU:CD2	2.10	0.82
1:A:599:TYR:HD2	1:A:735:ARG:HG3	1.45	0.81
1:B:637:ARG:HE	1:B:769:ASP:CA	1.92	0.81
1:A:351:THR:HG22	1:A:728:ILE:HG22	1.62	0.81
1:A:255:LYS:CD	1:A:762:HIS:HE1	1.93	0.81
1:B:217:ALA:HB1	1:B:358:GLN:HE22	1.45	0.81
1:A:348:GLU:OE2	1:B:573:MET:CB	2.29	0.81
1:B:624:ARG:NH2	1:B:707:GLN:CB	2.41	0.81
1:B:348:GLU:OE1	1:B:348:GLU:HA	1.81	0.81
1:B:647:GLU:CB	1:B:652:TRP:HZ3	1.88	0.81
1:A:253:ASP:OD2	1:A:645:ARG:HG2	1.81	0.80
1:A:611:TYR:O	1:A:615:PHE:HD1	1.65	0.80
1:A:5:LEU:H	1:A:5:LEU:CD2	1.94	0.80
1:B:248:LYS:CB	1:B:265:GLY:HA3	2.01	0.80
1:A:221:LEU:HD11	1:A:357:PHE:CE2	2.17	0.80
1:B:248:LYS:HD2	1:B:265:GLY:HA2	1.62	0.80
1:B:256:THR:HG21	1:B:295:LYS:HD2	1.63	0.79
1:B:720:VAL:O	1:B:725:MET:HG3	1.82	0.79
1:A:557:MET:HG2	1:B:226:GLN:NE2	1.97	0.79
1:A:255:LYS:HD3	1:A:762:HIS:CE1	2.18	0.79
1:A:610:ILE:HG13	1:A:723:LYS:CE	2.12	0.79
1:A:218:ARG:O	1:B:549:PHE:HB3	1.83	0.79
1:A:744:ALA:O	1:A:748:PRO:HD3	1.83	0.79
1:B:368:ALA:HA	1:B:387:MET:CE	2.12	0.79
1:B:637:ARG:HB3	1:B:665:TYR:OH	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ILE:HD11	1:B:283:HIS:NE2	1.98	0.79
1:A:626:ILE:HG23	1:A:711:PHE:CD1	2.18	0.79
1:A:110:SER:O	1:A:114:VAL:HG23	1.82	0.78
1:A:243:THR:HG22	1:A:243:THR:O	1.84	0.78
1:A:400:ARG:HD2	1:A:526:SER:HB3	1.65	0.78
1:B:248:LYS:HZ3	1:B:268:LYS:CB	1.97	0.78
1:B:626:ILE:HG21	1:B:715:ILE:HD11	1.64	0.78
1:B:626:ILE:HD12	1:B:715:ILE:CD1	2.13	0.78
1:A:275:ILE:HG22	1:A:276:ASP:N	1.99	0.78
1:A:553:ARG:HH21	1:A:560:ARG:NH2	1.81	0.78
1:B:695:LYS:HD3	1:B:776:MET:CE	2.12	0.78
1:B:703:PHE:O	1:B:703:PHE:CD1	2.37	0.78
1:A:278:LEU:N	1:A:278:LEU:HD23	1.99	0.78
1:B:582:GLN:HE21	1:B:586:GLU:HG3	1.48	0.78
1:A:226:GLN:HE21	1:A:228:ALA:N	1.81	0.77
1:A:740:LEU:H	1:A:740:LEU:HD23	1.49	0.77
1:B:301:GLN:HB3	1:B:304:VAL:HB	1.66	0.77
1:B:448:LEU:HD12	1:B:449:LEU:N	1.98	0.77
1:B:637:ARG:NE	1:B:769:ASP:HB3	1.99	0.77
1:A:284:VAL:HG21	1:A:717:LEU:CD2	2.14	0.77
1:A:279:PHE:CA	1:A:778:ALA:HB1	2.14	0.77
1:A:279:PHE:CD1	1:A:778:ALA:O	2.37	0.77
1:A:278:LEU:HD11	1:A:286:LEU:HB2	1.67	0.76
1:A:10:ASP:CB	1:A:11:PRO:CD	2.36	0.76
1:B:245:LYS:CE	1:B:247:GLU:OE1	2.28	0.76
1:B:650:GLU:O	1:B:650:GLU:CD	2.24	0.76
1:B:241:VAL:O	1:B:244:LEU:HG	1.86	0.76
1:B:463:ASN:O	1:B:467:GLU:HG3	1.85	0.76
1:A:210:ASP:OD2	1:A:371:THR:HG21	1.84	0.76
1:B:425:ARG:HD2	1:B:430:GLN:OE1	1.85	0.76
1:B:711:PHE:O	1:B:715:ILE:HG13	1.86	0.76
1:A:9:PHE:CD2	1:A:10:ASP:N	2.53	0.75
1:A:217:ALA:HB1	1:A:358:GLN:NE2	2.01	0.75
1:B:250:TYR:HE2	1:B:659:ASP:HB3	1.49	0.75
1:B:516:ARG:NE	1:B:582:GLN:HG2	2.00	0.75
1:B:647:GLU:HB2	1:B:652:TRP:CZ3	2.20	0.75
1:B:552:GLU:HA	1:B:555:MET:HG3	1.67	0.75
1:A:654:LEU:HD12	1:A:657:LEU:HB3	1.68	0.75
1:B:307:VAL:HG12	1:B:308:VAL:N	2.01	0.75
1:B:637:ARG:HE	1:B:769:ASP:HA	1.51	0.74
1:A:276:ASP:O	1:A:278:LEU:HD23	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:HG21	1:B:209:VAL:HG23	1.70	0.74
1:A:626:ILE:CG2	1:A:711:PHE:HD1	2.00	0.74
1:B:354:THR:CG2	1:B:735:ARG:HH22	2.00	0.74
1:B:723:LYS:HB2	1:B:763:MET:HG2	1.70	0.74
1:B:637:ARG:CZ	1:B:769:ASP:HB3	2.17	0.74
1:A:194:GLU:HG3	1:A:195:GLN:N	2.02	0.73
1:A:654:LEU:HB3	1:A:675:ASP:HB2	1.69	0.73
1:B:655:ASP:O	1:B:659:ASP:HB2	1.86	0.73
1:B:414:LYS:O	1:B:418:VAL:HG23	1.88	0.73
1:B:650:GLU:C	1:B:650:GLU:CD	2.46	0.73
1:A:654:LEU:HD22	1:A:677:PHE:HE2	1.53	0.73
1:A:182:PHE:HB3	1:A:186:ARG:NH2	2.03	0.73
1:A:747:ASN:N	1:A:748:PRO:CD	2.10	0.73
1:B:199:ARG:HB3	1:B:200:PRO:CD	2.18	0.73
1:B:514:GLU:OE1	1:B:585:VAL:HG11	1.88	0.73
1:A:351:THR:HG22	1:A:728:ILE:CG2	2.17	0.73
1:B:610:ILE:CD1	1:B:723:LYS:HZ3	2.01	0.73
1:A:666:LEU:HD11	1:A:691:ARG:HB3	1.70	0.73
1:A:207:ASP:HB2	1:A:370:MET:CE	2.18	0.73
1:A:291:ASN:O	1:A:295:LYS:HG3	1.89	0.73
1:A:382:ARG:CZ	1:A:388:GLN:HG2	2.18	0.72
1:A:654:LEU:HD23	1:A:675:ASP:HA	1.71	0.72
1:A:255:LYS:HD3	1:A:762:HIS:HE1	1.49	0.72
1:A:349:SER:HB2	1:B:557:MET:HG3	1.69	0.72
1:A:315:ILE:HD12	1:A:327:ARG:HB3	1.71	0.72
1:A:142:GLY:HA2	1:A:152:VAL:HG21	1.72	0.72
1:B:295:LYS:CE	1:B:333:LEU:HD22	2.18	0.72
1:A:562:GLY:CA	1:A:569:ILE:HG13	2.19	0.72
1:B:722:SER:OG	1:B:723:LYS:N	2.12	0.72
1:A:348:GLU:OE2	1:B:573:MET:HB2	1.89	0.71
1:B:288:HIS:CD2	1:B:718:ARG:HH12	2.06	0.71
1:B:190:VAL:HG22	1:B:195:GLN:HG3	1.72	0.71
1:B:198:GLN:O	1:B:199:ARG:HD2	1.91	0.71
1:B:243:THR:O	1:B:243:THR:HG22	1.90	0.71
1:B:636:GLU:OE1	1:B:636:GLU:CA	2.38	0.71
1:A:348:GLU:OE2	1:B:573:MET:HB3	1.90	0.71
1:A:246:ALA:HB1	1:A:264:GLU:HB3	1.73	0.71
1:B:39:ASP:HA	1:B:42:LYS:HB3	1.73	0.71
1:A:213:LEU:HD22	1:A:385:TYR:CZ	2.27	0.70
1:B:368:ALA:HA	1:B:387:MET:HE1	1.73	0.70
1:B:459:LEU:HD21	1:B:467:GLU:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:LEU:O	1:B:657:LEU:N	2.23	0.70
1:B:354:THR:HG21	1:B:735:ARG:HH22	1.54	0.70
1:A:279:PHE:HD1	1:A:779:GLU:CA	2.03	0.70
1:A:706:GLU:O	1:A:709:ARG:HB3	1.92	0.70
1:B:642:TYR:HE1	1:B:685:LEU:HA	1.56	0.70
1:A:66:PHE:CE2	1:A:112:LEU:HB3	2.26	0.70
1:A:426:TYR:HE1	1:A:455:PRO:HG2	1.56	0.70
1:A:662:ASN:HA	1:A:666:LEU:O	1.90	0.70
1:A:662:ASN:HB3	1:A:670:ALA:HB3	1.72	0.70
1:A:279:PHE:HA	1:A:778:ALA:CB	2.20	0.70
1:A:627:VAL:O	1:A:631:ILE:CG1	2.38	0.69
1:B:626:ILE:CG2	1:B:715:ILE:CD1	2.70	0.69
1:A:258:ALA:HB3	1:A:295:LYS:HG2	1.74	0.69
1:A:647:GLU:HG3	1:A:649:PRO:HD2	1.74	0.69
1:B:626:ILE:HG21	1:B:715:ILE:CD1	2.22	0.69
1:A:744:ALA:O	1:A:748:PRO:CD	2.40	0.69
1:A:677:PHE:HZ	1:A:684:MET:HE2	1.57	0.69
1:A:562:GLY:HA2	1:A:569:ILE:HG13	1.75	0.69
1:B:233:LEU:HB3	1:B:289:HIS:HD1	1.58	0.69
1:B:246:ALA:HB3	1:B:248:LYS:HG2	1.73	0.69
1:A:426:TYR:CD1	1:A:454:ILE:HG23	2.27	0.68
1:A:746:THR:O	1:A:746:THR:CG2	2.37	0.68
1:B:325:LYS:H	1:B:741:ARG:HD3	1.57	0.68
1:A:627:VAL:HG11	1:A:696:TYR:OH	1.93	0.68
1:B:36:LEU:H	1:B:75:ARG:HH22	1.42	0.68
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.59	0.68
1:B:246:ALA:HB1	1:B:268:LYS:NZ	2.08	0.68
1:A:279:PHE:O	1:A:778:ALA:HB1	1.94	0.68
1:A:254:ILE:CG2	1:A:255:LYS:N	2.42	0.68
1:B:626:ILE:HB	1:B:711:PHE:CD1	2.29	0.68
1:A:278:LEU:HD23	1:A:278:LEU:H	1.58	0.68
1:A:528:ARG:HH11	1:A:528:ARG:HG3	1.59	0.68
1:A:553:ARG:NH2	1:A:560:ARG:HH21	1.85	0.68
1:A:300:MET:SD	1:A:306:TYR:CE2	2.87	0.67
1:B:380:GLU:OE2	1:B:593:ARG:NH1	2.27	0.67
1:A:255:LYS:CD	1:A:762:HIS:CE1	2.75	0.67
1:A:303:ASP:C	1:A:304:VAL:HG23	2.10	0.67
1:A:406:LEU:CD2	1:A:570:GLN:HE21	2.07	0.67
1:B:206:ILE:O	1:B:369:GLY:HA2	1.94	0.67
1:B:301:GLN:HA	1:B:301:GLN:OE1	1.94	0.67
1:A:337:ILE:HD12	1:A:346:GLN:HE22	1.55	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:647:GLU:CB	1:B:652:TRP:CH2	2.78	0.67
1:A:249:ASP:OD2	1:A:294:LEU:CD2	2.42	0.67
1:A:182:PHE:CB	1:A:186:ARG:HH21	2.06	0.67
1:A:717:LEU:HG	1:A:718:ARG:N	2.09	0.67
1:B:218:ARG:CD	1:B:592:SER:HB3	2.23	0.67
1:B:610:ILE:CD1	1:B:723:LYS:NZ	2.57	0.67
1:A:677:PHE:CZ	1:A:684:MET:HE2	2.30	0.67
1:B:627:VAL:HG22	1:B:711:PHE:CZ	2.30	0.67
1:B:769:ASP:OD1	1:B:770:GLU:N	2.28	0.67
1:A:544:GLU:O	1:A:545:LEU:HB2	1.95	0.66
1:B:307:VAL:CG1	1:B:308:VAL:N	2.57	0.66
1:B:476:GLN:HE22	1:B:494:LYS:HZ3	1.43	0.66
1:A:599:TYR:CD2	1:A:735:ARG:HG3	2.28	0.66
1:B:206:ILE:HG23	1:B:212:ILE:HD12	1.77	0.66
1:B:261:LEU:HD12	1:B:262:THR:HB	1.75	0.66
1:A:458:VAL:HA	1:A:482:ILE:HG23	1.77	0.66
1:B:248:LYS:NZ	1:B:268:LYS:HB2	2.08	0.66
1:B:400:ARG:HD2	1:B:535:THR:HG23	1.76	0.66
1:A:246:ALA:O	1:A:262:THR:HB	1.96	0.66
1:A:611:TYR:O	1:A:615:PHE:CD1	2.49	0.66
1:B:248:LYS:HA	1:B:261:LEU:HB3	1.78	0.66
1:B:302:LYS:O	1:B:302:LYS:CG	2.43	0.66
1:A:561:PHE:O	1:A:561:PHE:HD1	1.78	0.66
1:A:421:ASP:O	1:A:425:ARG:HG2	1.95	0.66
1:B:16:LEU:CD2	1:B:16:LEU:H	2.07	0.66
1:B:344:GLU:O	1:B:346:GLN:N	2.29	0.66
1:A:313:VAL:HG22	1:A:337:ILE:CD1	2.25	0.66
1:A:361:PHE:HB3	1:A:367:LEU:HD21	1.78	0.66
1:B:206:ILE:CG2	1:B:209:VAL:HG23	2.25	0.66
1:A:485:ASN:OD1	1:A:485:ASN:C	2.34	0.66
1:A:576:ARG:HH12	1:B:346:GLN:HE22	1.44	0.65
1:B:720:VAL:HG12	1:B:721:ASP:N	2.09	0.65
1:B:582:GLN:NE2	1:B:586:GLU:HG3	2.11	0.65
1:B:368:ALA:HA	1:B:387:MET:HE3	1.77	0.65
1:A:206:ILE:HG23	1:A:212:ILE:HD12	1.78	0.65
1:A:724:TRP:HA	1:A:724:TRP:CE3	2.31	0.65
1:A:761:GLU:O	1:A:765:GLU:HG3	1.97	0.65
1:B:516:ARG:N	1:B:516:ARG:HH11	1.94	0.65
1:A:433:LEU:HD21	1:A:525:ARG:HD3	1.78	0.65
1:A:274:GLY:O	1:A:275:ILE:HG13	1.96	0.65
1:A:317:ASP:HB3	1:A:320:THR:CG2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:LEU:HD22	1:A:677:PHE:CE2	2.33	0.64
1:B:554:THR:O	1:B:558:LEU:HG	1.98	0.64
1:A:278:LEU:HB2	1:A:283:HIS:HB3	1.79	0.64
1:A:279:PHE:HD1	1:A:779:GLU:HA	1.61	0.64
1:A:637:ARG:NE	1:A:769:ASP:HB2	2.13	0.64
1:A:680:GLU:HB2	1:A:683:GLU:HB2	1.80	0.64
1:B:439:VAL:HA	1:B:442:SER:HB2	1.79	0.64
1:B:620:SER:HB2	1:B:625:GLU:HB3	1.75	0.64
1:B:248:LYS:HB3	1:B:265:GLY:CA	2.28	0.64
1:B:637:ARG:HH21	1:B:769:ASP:CB	2.05	0.64
1:A:426:TYR:CE1	1:A:455:PRO:HG2	2.32	0.64
1:B:630:MET:SD	1:B:775:VAL:CG2	2.79	0.64
1:B:649:PRO:O	1:B:652:TRP:CH2	2.50	0.64
1:A:667:ASP:OD1	1:A:777:LYS:HE2	1.97	0.64
1:B:135:SER:OG	1:B:154:LEU:HD21	1.98	0.64
1:B:254:ILE:HG23	1:B:255:LYS:H	1.61	0.64
1:B:110:SER:O	1:B:114:VAL:HG23	1.97	0.64
1:B:270:GLU:HA	1:B:275:ILE:HG22	1.79	0.64
1:B:233:LEU:HB2	1:B:289:HIS:CE1	2.34	0.63
1:B:379:GLU:HG2	1:B:383:ASN:HD22	1.63	0.63
1:A:471:ILE:HG21	1:A:491:THR:HB	1.81	0.63
1:B:246:ALA:HB1	1:B:268:LYS:HZ1	1.63	0.63
1:A:637:ARG:HE	1:A:769:ASP:HB2	1.63	0.63
1:A:654:LEU:CD1	1:A:657:LEU:HB3	2.28	0.63
1:B:325:LYS:N	1:B:741:ARG:HD3	2.13	0.63
1:B:377:GLU:HG2	1:B:517:ARG:HD3	1.81	0.63
1:B:380:GLU:CD	1:B:593:ARG:HH12	2.02	0.63
1:A:249:ASP:HB2	1:A:260:GLN:HG2	1.78	0.63
1:A:645:ARG:O	1:A:646:GLU:HG3	1.98	0.63
1:B:238:ASN:HD21	1:B:340:LYS:HA	1.63	0.63
1:A:410:THR:HG21	1:B:462:LYS:HE3	1.81	0.63
1:A:5:LEU:H	1:A:5:LEU:HD22	1.63	0.63
1:A:206:ILE:H	1:A:206:ILE:HD12	1.61	0.63
1:A:627:VAL:HA	1:A:630:MET:SD	2.39	0.63
1:B:723:LYS:HE2	1:B:763:MET:HG2	1.80	0.63
1:A:626:ILE:HG23	1:A:711:PHE:HD1	1.59	0.63
1:A:645:ARG:HG3	1:A:657:LEU:HD13	1.80	0.63
1:B:238:ASN:OD1	1:B:297:HIS:HE1	1.81	0.63
1:B:307:VAL:HG21	1:B:316:VAL:HG21	1.81	0.63
1:A:106:LYS:HD3	1:A:370:MET:HB3	1.81	0.62
1:A:640:ALA:O	1:A:644:PRO:CD	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ILE:HG23	1:B:255:LYS:N	2.14	0.62
1:A:547:ARG:O	1:B:219:THR:HG22	1.99	0.62
1:A:261:LEU:HD23	1:A:266:MET:HG2	1.82	0.62
1:B:261:LEU:C	1:B:261:LEU:CD1	2.67	0.62
1:B:421:ASP:OD1	1:B:425:ARG:NH1	2.32	0.62
1:B:627:VAL:O	1:B:631:ILE:N	2.28	0.62
1:A:255:LYS:NZ	1:A:762:HIS:HE1	1.98	0.62
1:A:420:GLU:O	1:A:424:GLN:HG3	2.00	0.62
1:B:354:THR:HG21	1:B:735:ARG:HH12	1.65	0.62
1:B:185:LEU:HD22	1:B:353:ALA:HB1	1.80	0.62
1:B:190:VAL:HG22	1:B:195:GLN:CG	2.29	0.62
1:B:512:ARG:HG2	1:B:539:LEU:HD21	1.80	0.62
1:B:676:ILE:HG12	1:B:684:MET:HG2	1.80	0.62
1:B:354:THR:HG21	1:B:735:ARG:NH2	2.13	0.62
1:A:324:MET:HA	1:A:740:LEU:HD13	1.82	0.62
1:B:723:LYS:CB	1:B:763:MET:HG3	2.30	0.62
1:B:250:TYR:O	1:B:251:THR:HB	1.99	0.61
1:B:213:LEU:O	1:B:217:ALA:HB2	2.00	0.61
1:A:558:LEU:HG	1:A:563:MET:HE3	1.75	0.61
1:B:74:ARG:HG3	1:B:74:ARG:HH11	1.64	0.61
1:B:624:ARG:CZ	1:B:700:GLU:HG2	2.30	0.61
1:A:281:VAL:O	1:A:281:VAL:CG1	2.49	0.61
1:B:640:ALA:O	1:B:644:PRO:HD3	2.01	0.61
1:A:686:GLU:HG2	1:A:687:LEU:N	2.14	0.61
1:B:732:ASP:O	1:B:735:ARG:HB3	2.01	0.61
1:B:191:LEU:HD21	1:B:716:VAL:HG11	1.82	0.61
1:B:723:LYS:HG2	1:B:767:ILE:HG12	1.83	0.61
1:A:406:LEU:HG	1:A:536:GLN:NE2	2.15	0.61
1:A:426:TYR:C	1:A:426:TYR:CD2	2.73	0.61
1:B:711:PHE:O	1:B:715:ILE:CG1	2.49	0.61
1:A:254:ILE:HG22	1:A:255:LYS:HG3	1.81	0.61
1:A:255:LYS:O	1:A:256:THR:HB	2.00	0.61
1:B:317:ASP:HB3	1:B:320:THR:HG23	1.83	0.61
1:B:760:PHE:CD1	1:B:763:MET:HE1	2.36	0.61
1:B:238:ASN:ND2	1:B:340:LYS:HD2	2.15	0.60
1:A:288:HIS:O	1:A:292:GLN:HG2	2.00	0.60
1:A:404:PRO:O	1:A:536:GLN:NE2	2.34	0.60
1:A:541:MET:SD	1:A:561:PHE:HZ	2.25	0.60
1:A:217:ALA:HB1	1:A:358:GLN:HE21	1.66	0.60
1:A:259:VAL:HG21	1:A:769:ASP:OD2	1.99	0.60
1:A:312:GLN:NE2	1:B:572:LYS:HD3	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:ILE:HD12	1:A:723:LYS:NZ	2.17	0.60
1:B:718:ARG:HG3	1:B:770:GLU:OE1	2.01	0.60
1:A:270:GLU:O	1:A:274:GLY:N	2.33	0.60
1:A:418:VAL:O	1:A:422:VAL:HG23	2.02	0.60
1:A:700:GLU:O	1:A:704:GLY:CA	2.48	0.60
1:A:724:TRP:HA	1:A:724:TRP:HE3	1.66	0.60
1:B:645:ARG:HG3	1:B:657:LEU:HB2	1.84	0.60
1:B:102:THR:HB	1:B:524:GLY:O	2.02	0.60
1:B:243:THR:O	1:B:244:LEU:HD23	2.01	0.60
1:B:218:ARG:HD3	1:B:592:SER:CB	2.26	0.60
1:B:494:LYS:H	1:B:494:LYS:HD3	1.65	0.60
1:B:713:LYS:O	1:B:717:LEU:CB	2.49	0.60
1:B:288:HIS:O	1:B:292:GLN:HG2	2.01	0.60
1:A:661:ILE:CG2	1:A:666:LEU:CD2	2.65	0.60
1:A:723:LYS:HG2	1:A:767:ILE:HD11	1.84	0.60
1:A:142:GLY:O	1:A:146:GLU:HG3	2.02	0.60
1:A:646:GLU:HA	1:A:651:GLU:HA	1.84	0.60
1:A:747:ASN:H	1:A:748:PRO:HD2	0.51	0.60
1:B:627:VAL:HG22	1:B:711:PHE:HZ	1.66	0.60
1:B:627:VAL:HG12	1:B:631:ILE:HG13	1.84	0.60
1:A:325:LYS:HB2	1:A:740:LEU:HB3	1.82	0.59
1:A:401:ASP:OD2	1:A:403:ARG:HD3	2.02	0.59
1:A:255:LYS:NZ	1:A:762:HIS:CE1	2.69	0.59
1:A:284:VAL:HG13	1:A:718:ARG:HH21	1.67	0.59
1:A:560:ARG:O	1:A:561:PHE:CG	2.55	0.59
1:B:19:TYR:HE1	1:B:390:VAL:HG11	1.68	0.59
1:B:297:HIS:CE1	1:B:340:LYS:HB3	2.37	0.59
1:B:463:ASN:C	1:B:463:ASN:HD22	2.05	0.59
1:B:248:LYS:NZ	1:B:268:LYS:HD2	2.17	0.59
1:B:617:VAL:O	1:B:617:VAL:HG12	2.02	0.59
1:B:624:ARG:HH21	1:B:707:GLN:HB2	1.59	0.59
1:A:249:ASP:HB3	1:A:260:GLN:O	2.02	0.59
1:A:529:GLN:OE1	1:A:529:GLN:HA	2.00	0.59
1:A:358:GLN:HG3	1:A:385:TYR:OH	2.02	0.59
1:A:406:LEU:HD23	1:A:570:GLN:HE21	1.66	0.59
1:A:554:THR:HG21	1:A:557:MET:O	2.02	0.59
1:A:374:ALA:O	1:A:389:VAL:HG21	2.02	0.59
1:B:187:ASP:OD1	1:B:196:MET:HA	2.02	0.59
1:B:300:MET:HG3	1:B:337:ILE:HD11	1.84	0.59
1:B:417:ALA:HA	1:B:420:GLU:HB3	1.84	0.59
1:B:442:SER:O	1:B:446:SER:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:CD1	1:A:286:LEU:HB2	2.32	0.59
1:A:592:SER:O	1:A:595:GLN:HG2	2.03	0.59
1:A:684:MET:SD	1:A:684:MET:N	2.75	0.59
1:A:83:LYS:HA	1:A:86:LEU:HD12	1.85	0.59
1:B:614:ARG:NH1	1:B:720:VAL:HG23	2.14	0.59
1:B:686:GLU:HA	1:B:686:GLU:OE1	2.02	0.59
1:A:328:ARG:HG2	1:A:328:ARG:NH1	2.14	0.58
1:B:244:LEU:HD22	1:B:248:LYS:HE3	1.84	0.58
1:A:626:ILE:O	1:A:630:MET:HB3	2.04	0.58
1:A:647:GLU:HG3	1:A:648:LEU:N	2.18	0.58
1:B:206:ILE:CG2	1:B:209:VAL:HA	2.34	0.58
1:B:483:ALA:HB1	1:B:487:ALA:HB3	1.84	0.58
1:B:695:LYS:HD3	1:B:776:MET:HE3	1.83	0.58
1:A:279:PHE:HD1	1:A:778:ALA:O	1.83	0.58
1:B:88:GLY:HA3	1:B:109:THR:HG21	1.86	0.58
1:B:245:LYS:CE	1:B:247:GLU:CD	2.69	0.58
1:A:764:ILE:O	1:A:768:GLU:HG3	2.03	0.58
1:B:476:GLN:HE22	1:B:494:LYS:NZ	2.00	0.58
1:B:703:PHE:CZ	1:B:707:GLN:NE2	2.71	0.58
1:B:87:MET:HA	1:B:90:VAL:HG12	1.86	0.58
1:B:100:MET:O	1:B:372:GLY:HA2	2.04	0.58
1:B:676:ILE:CG1	1:B:684:MET:HG2	2.34	0.58
1:A:257:LYS:NZ	1:A:660:LEU:HD12	2.18	0.58
1:A:510:THR:O	1:A:511:GLU:HB3	2.04	0.58
1:A:626:ILE:CG2	1:A:711:PHE:CD1	2.81	0.58
1:B:703:PHE:O	1:B:703:PHE:CG	2.57	0.58
1:B:741:ARG:HG3	1:B:742:ALA:N	2.17	0.58
1:B:302:LYS:O	1:B:302:LYS:HG3	2.04	0.57
1:B:460:ASN:ND2	1:B:462:LYS:HB2	2.19	0.57
1:A:279:PHE:HD1	1:A:778:ALA:C	2.07	0.57
1:A:426:TYR:C	1:A:426:TYR:HD2	2.08	0.57
1:A:610:ILE:HG21	1:A:723:LYS:HE2	1.85	0.57
1:A:5:LEU:CB	1:A:383:ASN:OD1	2.49	0.57
1:A:324:MET:HB3	1:A:327:ARG:HD2	1.86	0.57
1:A:561:PHE:CD1	1:A:561:PHE:C	2.77	0.57
1:B:718:ARG:HD2	1:B:722:SER:HB3	1.87	0.57
1:B:647:GLU:HB3	1:B:652:TRP:CH2	2.39	0.57
1:A:561:PHE:O	1:A:561:PHE:CD1	2.57	0.57
1:B:766:SER:O	1:B:769:ASP:OD1	2.21	0.57
1:A:649:PRO:O	1:A:650:GLU:HG3	2.04	0.57
1:A:723:LYS:HG3	1:A:724:TRP:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:VAL:CG2	1:B:316:VAL:HG21	2.35	0.57
1:A:301:GLN:O	1:A:306:TYR:HB2	2.05	0.56
1:A:329:TYR:HB3	1:A:333:LEU:HB2	1.86	0.56
1:B:152:VAL:HG13	1:B:172:ILE:CG2	2.34	0.56
1:B:168:TYR:CD1	1:B:197:VAL:HG12	2.39	0.56
1:A:300:MET:SD	1:A:306:TYR:HE2	2.28	0.56
1:A:637:ARG:NH2	1:A:769:ASP:HB2	2.20	0.56
1:B:102:THR:HA	1:B:106:LYS:HZ3	1.70	0.56
1:B:403:ARG:HB3	1:B:536:GLN:OE1	2.05	0.56
1:B:430:GLN:HG2	1:B:504:GLY:O	2.06	0.56
1:B:696:TYR:OH	1:B:711:PHE:CE2	2.58	0.56
1:A:190:VAL:CG1	1:A:192:TYR:O	2.53	0.56
1:A:668:GLU:C	1:A:670:ALA:H	2.09	0.56
1:A:358:GLN:CG	1:A:385:TYR:OH	2.54	0.56
1:A:747:ASN:O	1:A:750:ARG:HB2	2.05	0.56
1:B:27:ASP:O	1:B:30:ARG:HB3	2.04	0.56
1:B:249:ASP:H	1:B:261:LEU:HB2	1.70	0.56
1:A:610:ILE:CD1	1:A:723:LYS:HZ2	2.17	0.56
1:A:647:GLU:HG3	1:A:648:LEU:H	1.70	0.56
1:B:221:LEU:HD11	1:B:357:PHE:CE2	2.40	0.56
1:A:438:ALA:HB1	1:A:440:GLU:OE1	2.06	0.56
1:B:250:TYR:CE2	1:B:659:ASP:HB3	2.37	0.56
1:B:695:LYS:HD3	1:B:776:MET:HE1	1.86	0.56
1:A:348:GLU:OE1	1:B:573:MET:SD	2.63	0.56
1:A:512:ARG:HD2	1:A:519:ASP:OD1	2.05	0.56
1:B:233:LEU:HB3	1:B:289:HIS:ND1	2.19	0.56
1:B:626:ILE:O	1:B:627:VAL:C	2.44	0.56
1:B:723:LYS:HB2	1:B:763:MET:SD	2.46	0.56
1:A:426:TYR:HD1	1:A:454:ILE:HG23	1.68	0.56
1:B:642:TYR:O	1:B:646:GLU:HG3	2.06	0.56
1:A:279:PHE:CD1	1:A:778:ALA:C	2.80	0.55
1:B:17:ASN:O	1:B:20:GLU:HB2	2.06	0.55
1:B:637:ARG:NE	1:B:769:ASP:HA	2.19	0.55
1:A:373:THR:O	1:A:517:ARG:HD2	2.06	0.55
1:A:734:LEU:O	1:A:738:ILE:HB	2.06	0.55
1:A:270:GLU:OE2	1:A:278:LEU:HD21	2.07	0.55
1:B:252:TYR:HE2	1:B:254:ILE:HG22	1.71	0.55
1:B:626:ILE:HG23	1:B:715:ILE:CD1	2.36	0.55
1:A:300:MET:SD	1:A:306:TYR:CD2	2.99	0.55
1:A:641:ALA:HB1	1:A:660:LEU:HD11	1.87	0.55
1:B:16:LEU:HD22	1:B:16:LEU:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:HIS:HA	1:A:46:ILE:HD12	1.89	0.55
1:A:541:MET:SD	1:A:561:PHE:CZ	3.00	0.55
1:A:626:ILE:HG21	1:A:711:PHE:HD1	1.71	0.55
1:A:337:ILE:HD12	1:A:346:GLN:CD	2.27	0.55
1:A:552:GLU:H	1:A:560:ARG:HH12	1.54	0.55
1:A:672:GLU:O	1:A:673:LYS:C	2.45	0.55
1:B:315:ILE:HG13	1:B:327:ARG:HB2	1.88	0.55
1:B:720:VAL:CG1	1:B:721:ASP:N	2.69	0.55
1:A:561:PHE:O	1:A:569:ILE:CG1	2.53	0.55
1:B:354:THR:HG21	1:B:735:ARG:NH1	2.21	0.55
1:A:356:THR:HB	1:A:358:GLN:OE1	2.07	0.55
1:A:606:GLN:NE2	1:A:760:PHE:HB2	2.21	0.55
1:A:736:GLN:O	1:A:737:GLY:C	2.43	0.55
1:A:160:SER:C	1:A:162:ASP:H	2.09	0.54
1:A:301:GLN:O	1:A:306:TYR:CB	2.55	0.54
1:B:624:ARG:NH1	1:B:700:GLU:HG2	2.22	0.54
1:B:711:PHE:O	1:B:715:ILE:CD1	2.55	0.54
1:A:337:ILE:HG22	1:A:344:GLU:O	2.07	0.54
1:A:440:GLU:HB3	1:B:411:MET:HE1	1.88	0.54
1:A:650:GLU:HB3	1:A:652:TRP:HB2	1.89	0.54
1:B:647:GLU:O	1:B:652:TRP:CZ2	2.59	0.54
1:B:230:SER:C	1:B:232:LYS:H	2.10	0.54
1:B:646:GLU:OE1	1:B:681:PRO:HG3	2.08	0.54
1:B:706:GLU:O	1:B:709:ARG:CB	2.55	0.54
1:B:92:LEU:HB2	1:B:113:PRO:HG3	1.89	0.54
1:B:344:GLU:O	1:B:344:GLU:CG	2.56	0.54
1:B:614:ARG:HH12	1:B:720:VAL:HG22	1.69	0.54
1:A:279:PHE:CD1	1:A:779:GLU:HA	2.40	0.54
1:A:606:GLN:HG2	1:A:760:PHE:CE1	2.43	0.54
1:A:625:GLU:O	1:A:629:ASN:ND2	2.40	0.54
1:B:595:GLN:HE22	1:B:739:HIS:CE1	2.25	0.54
1:B:610:ILE:HG13	1:B:724:TRP:CZ3	2.42	0.54
1:A:50:GLU:O	1:A:54:LYS:HG3	2.07	0.54
1:B:325:LYS:H	1:B:741:ARG:CD	2.20	0.54
1:B:650:GLU:OE1	1:B:651:GLU:N	2.37	0.54
1:B:217:ALA:HB1	1:B:358:GLN:NE2	2.20	0.54
1:B:723:LYS:O	1:B:727:HIS:HB2	2.07	0.54
1:A:606:GLN:HE21	1:A:760:PHE:HB2	1.72	0.54
1:A:676:ILE:O	1:A:676:ILE:HG22	2.08	0.54
1:A:723:LYS:CG	1:A:767:ILE:HD11	2.38	0.54
1:B:177:ASN:HD22	1:B:212:ILE:HG23	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:THR:HB	1:B:348:GLU:HG3	1.88	0.54
1:B:476:GLN:NE2	1:B:494:LYS:NZ	2.56	0.54
1:B:595:GLN:HE22	1:B:739:HIS:HE1	1.56	0.54
1:B:642:TYR:N	1:B:642:TYR:CD2	2.73	0.54
1:B:718:ARG:NH1	1:B:770:GLU:OE1	2.35	0.54
1:A:604:ARG:O	1:A:608:GLU:HG2	2.08	0.54
1:B:238:ASN:HD21	1:B:340:LYS:CA	2.21	0.54
1:B:447:LYS:HD3	1:B:450:LYS:HE3	1.90	0.54
1:B:718:ARG:HD2	1:B:722:SER:CB	2.38	0.54
1:B:760:PHE:CE1	1:B:763:MET:HE1	2.43	0.54
1:A:322:ARG:NH1	1:A:743:TYR:HE1	2.06	0.54
1:B:209:VAL:HG13	1:B:210:ASP:N	2.22	0.54
1:A:671:LEU:HD11	1:A:674:SER:HA	1.90	0.53
1:A:695:LYS:O	1:A:698:GLU:HG2	2.08	0.53
1:B:523:ARG:HB3	1:B:535:THR:HG21	1.90	0.53
1:B:541:MET:HE1	1:B:559:ASP:OD2	2.07	0.53
1:B:652:TRP:HB2	1:B:654:LEU:HG	1.89	0.53
1:A:459:LEU:HD22	1:A:467:GLU:HB3	1.89	0.53
1:A:548:ARG:HH12	1:B:735:ARG:HD3	1.73	0.53
1:B:494:LYS:HD3	1:B:494:LYS:N	2.21	0.53
1:A:105:GLY:HA2	2:A:781:ADP:PA	2.48	0.53
1:A:284:VAL:CG1	1:A:718:ARG:HH21	2.21	0.53
1:B:610:ILE:HG13	1:B:724:TRP:CE3	2.44	0.53
1:A:252:TYR:CD2	1:A:257:LYS:O	2.62	0.53
1:A:259:VAL:HA	1:A:291:ASN:OD1	2.08	0.53
1:A:302:LYS:HG2	1:A:303:ASP:N	2.23	0.53
1:A:610:ILE:CD1	1:A:723:LYS:NZ	2.71	0.53
1:B:244:LEU:HD22	1:B:248:LYS:CE	2.39	0.53
1:B:248:LYS:NZ	1:B:268:LYS:CB	2.70	0.53
1:B:336:ALA:O	1:B:340:LYS:CD	2.53	0.53
1:A:127:VAL:HB	1:A:206:ILE:HA	1.91	0.53
1:B:647:GLU:OE1	1:B:647:GLU:HA	2.09	0.53
1:B:199:ARG:HB3	1:B:200:PRO:HD3	1.90	0.53
1:B:206:ILE:HG22	1:B:209:VAL:HA	1.91	0.53
1:B:210:ASP:OD1	1:B:371:THR:HG21	2.09	0.53
1:A:206:ILE:CG2	1:A:212:ILE:HD12	2.39	0.52
1:A:630:MET:O	1:A:634:SER:OG	2.25	0.52
1:B:447:LYS:HB3	1:B:450:LYS:HG3	1.90	0.52
1:A:93:HIS:CD2	1:A:116:LEU:HD23	2.45	0.52
1:A:279:PHE:CD1	1:A:779:GLU:CA	2.89	0.52
1:B:221:LEU:O	1:B:354:THR:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ASP:OD2	1:A:371:THR:CG2	2.57	0.52
1:A:576:ARG:HE	1:B:312:GLN:HE21	1.56	0.52
1:B:434:VAL:HB	1:B:482:ILE:HG13	1.92	0.52
1:A:27:ASP:O	1:A:30:ARG:HB3	2.10	0.52
1:A:317:ASP:CB	1:A:320:THR:HG22	2.34	0.52
1:A:637:ARG:HH21	1:A:769:ASP:HB2	1.75	0.52
1:A:644:PRO:C	1:A:646:GLU:H	2.13	0.52
1:A:686:GLU:OE2	1:A:687:LEU:HG	2.10	0.52
1:B:522:LEU:O	1:B:525:ARG:CG	2.55	0.52
1:A:5:LEU:H	1:A:5:LEU:HD23	1.75	0.52
1:A:91:ALA:O	1:A:96:ASN:HB2	2.10	0.52
1:A:407:ILE:HB	1:A:569:ILE:HG22	1.92	0.52
1:A:637:ARG:CZ	1:A:769:ASP:HB2	2.40	0.52
1:B:322:ARG:HG3	1:B:742:ALA:HB3	1.92	0.52
1:A:457:GLN:NE2	1:A:470:ILE:HD12	2.10	0.51
1:A:643:THR:N	1:A:644:PRO:CD	2.74	0.51
1:B:612:LYS:O	1:B:613:GLN:C	2.48	0.51
1:A:283:HIS:O	1:A:284:VAL:C	2.48	0.51
1:B:418:VAL:O	1:B:422:VAL:CG2	2.51	0.51
1:B:625:GLU:CG	1:B:625:GLU:O	2.42	0.51
1:A:206:ILE:HD12	1:A:206:ILE:N	2.24	0.51
1:A:221:LEU:O	1:A:354:THR:HA	2.10	0.51
1:A:436:THR:HG22	1:A:438:ALA:H	1.75	0.51
1:B:13:LYS:HA	1:B:16:LEU:HD21	1.93	0.51
1:B:39:ASP:HA	1:B:42:LYS:CB	2.39	0.51
1:B:246:ALA:CB	1:B:268:LYS:HZ2	2.24	0.51
1:B:539:LEU:HD13	1:B:546:MET:HE1	1.93	0.51
1:A:654:LEU:CD2	1:A:677:PHE:CE2	2.94	0.51
1:B:233:LEU:HB2	1:B:289:HIS:HE1	1.73	0.51
1:B:325:LYS:O	1:B:741:ARG:NH1	2.43	0.51
1:B:371:THR:HG22	1:B:372:GLY:N	2.26	0.51
1:B:642:TYR:CE1	1:B:685:LEU:HA	2.42	0.51
1:B:718:ARG:HG3	1:B:718:ARG:HH11	1.76	0.51
1:A:411:MET:HG2	1:A:542:GLU:OE2	2.10	0.51
1:A:741:ARG:NH2	1:B:376:THR:HG22	2.21	0.51
1:B:199:ARG:CB	1:B:200:PRO:CD	2.88	0.51
1:B:239:ALA:HA	1:B:242:ARG:NH1	2.25	0.51
1:B:512:ARG:HG2	1:B:539:LEU:CD2	2.41	0.51
1:B:710:GLU:O	1:B:714:VAL:HG23	2.11	0.51
1:A:327:ARG:HH21	1:A:755:GLU:HG2	1.76	0.51
1:A:522:LEU:O	1:A:525:ARG:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLU:O	1:B:345:ILE:C	2.48	0.51
1:B:718:ARG:CD	1:B:722:SER:HB3	2.39	0.51
1:A:255:LYS:HZ2	1:A:762:HIS:CE1	2.29	0.51
1:A:278:LEU:HB3	1:A:283:HIS:CD2	2.41	0.51
1:A:279:PHE:HD1	1:A:779:GLU:N	2.09	0.51
1:A:680:GLU:O	1:A:684:MET:SD	2.69	0.51
1:B:400:ARG:HD3	1:B:526:SER:O	2.10	0.51
1:B:639:ILE:HG22	1:B:640:ALA:N	2.26	0.51
1:B:42:LYS:HE3	1:B:149:GLY:HA3	1.92	0.50
1:B:250:TYR:CE1	1:B:261:LEU:HA	2.45	0.50
1:B:344:GLU:O	1:B:344:GLU:HG2	2.11	0.50
1:A:247:GLU:O	1:A:249:ASP:N	2.44	0.50
1:A:562:GLY:HA2	1:A:569:ILE:CG1	2.39	0.50
1:B:647:GLU:N	1:B:652:TRP:CZ2	2.78	0.50
1:A:251:THR:OG1	1:A:252:TYR:N	2.45	0.50
1:B:69:VAL:O	1:B:73:SER:HB2	2.12	0.50
1:B:101:LYS:O	1:B:104:GLU:HB2	2.10	0.50
1:B:193:LYS:O	1:B:196:MET:HG3	2.11	0.50
1:B:610:ILE:HD12	1:B:723:LYS:NZ	2.26	0.50
1:B:549:PHE:N	1:B:549:PHE:CD2	2.79	0.50
1:B:637:ARG:HB3	1:B:665:TYR:HH	1.74	0.50
1:B:666:LEU:HD21	1:B:692:ILE:HG13	1.94	0.50
1:A:100:MET:HG2	1:A:392:ILE:HB	1.92	0.50
1:A:548:ARG:NH1	1:B:735:ARG:HD3	2.26	0.50
1:A:689:MET:O	1:A:693:ILE:HG22	2.12	0.50
1:B:48:PHE:HE1	1:B:68:VAL:HG21	1.75	0.50
1:B:190:VAL:CG2	1:B:195:GLN:HG3	2.38	0.50
1:B:215:ASP:OD1	1:B:517:ARG:NH2	2.45	0.50
1:B:249:ASP:N	1:B:261:LEU:HB2	2.27	0.50
1:A:475:GLY:O	1:A:495:LEU:HA	2.11	0.50
1:A:559:ASP:O	1:A:563:MET:HE2	2.11	0.50
1:A:588:ASN:OD1	1:B:588:ASN:HB3	2.12	0.50
1:B:240:PHE:O	1:B:244:LEU:HD21	2.12	0.50
1:B:380:GLU:CD	1:B:593:ARG:NH1	2.64	0.50
1:A:442:SER:HA	1:A:482:ILE:HD11	1.93	0.50
1:B:642:TYR:HE1	1:B:685:LEU:CA	2.23	0.50
1:A:3:GLY:O	1:A:4:ILE:HG13	2.12	0.49
1:A:107:THR:HG22	1:A:141:MET:SD	2.52	0.49
1:A:210:ASP:OD2	1:A:210:ASP:N	2.40	0.49
1:A:769:ASP:O	1:A:770:GLU:C	2.50	0.49
1:B:371:THR:HG22	1:B:373:THR:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:MET:O	1:A:486:MET:HG3	2.12	0.49
1:B:432:VAL:HG13	1:B:506:ALA:HB3	1.93	0.49
1:B:261:LEU:HD13	1:B:261:LEU:O	2.13	0.49
1:B:484:THR:O	1:B:486:MET:N	2.45	0.49
1:A:232:LYS:H	1:A:232:LYS:CD	2.19	0.49
1:A:190:VAL:HG13	1:A:195:GLN:HB2	1.94	0.49
1:B:647:GLU:N	1:B:652:TRP:CZ3	2.76	0.49
1:A:243:THR:O	1:A:243:THR:CG2	2.55	0.49
1:B:248:LYS:HG3	1:B:248:LYS:O	2.13	0.49
1:B:233:LEU:CB	1:B:289:HIS:CE1	2.95	0.49
1:B:275:ILE:CD1	1:B:283:HIS:CD2	2.83	0.49
1:B:347:ASN:O	1:B:348:GLU:CD	2.51	0.49
1:B:637:ARG:NE	1:B:769:ASP:CB	2.55	0.49
1:A:301:GLN:HB2	1:A:306:TYR:CE1	2.48	0.49
1:B:637:ARG:NE	1:B:769:ASP:CA	2.70	0.49
1:A:7:LYS:O	1:B:743:TYR:CD2	2.66	0.49
1:A:279:PHE:C	1:A:778:ALA:HB1	2.33	0.49
1:A:324:MET:CB	1:A:327:ARG:HD2	2.43	0.49
1:A:647:GLU:CG	1:A:649:PRO:HD2	2.42	0.49
1:B:199:ARG:CB	1:B:200:PRO:HD3	2.42	0.49
1:B:445:ILE:O	1:B:447:LYS:N	2.45	0.48
1:B:620:SER:OG	1:B:625:GLU:HG2	2.14	0.48
1:B:48:PHE:CE1	1:B:68:VAL:HG21	2.49	0.48
1:B:284:VAL:HG12	1:B:718:ARG:NH2	2.28	0.48
1:B:400:ARG:HD2	1:B:535:THR:CG2	2.42	0.48
1:B:673:LYS:HA	1:B:676:ILE:HG22	1.94	0.48
1:A:89:GLY:HA2	1:A:92:LEU:HD12	1.95	0.48
1:A:177:ASN:OD1	1:A:177:ASN:N	2.46	0.48
1:A:379:GLU:O	1:A:383:ASN:HB3	2.13	0.48
1:B:246:ALA:CB	1:B:268:LYS:NZ	2.75	0.48
1:B:261:LEU:C	1:B:261:LEU:HD13	2.34	0.48
1:B:185:LEU:HD22	1:B:353:ALA:CB	2.44	0.48
1:A:257:LYS:HZ3	1:A:660:LEU:HD12	1.78	0.48
1:A:624:ARG:HG2	1:A:627:VAL:HB	1.95	0.48
1:B:539:LEU:HD13	1:B:546:MET:CE	2.42	0.48
1:B:708:MET:HA	1:B:711:PHE:HB2	1.96	0.48
1:A:637:ARG:HG2	1:A:769:ASP:HA	1.94	0.48
1:A:82:PHE:CE1	2:A:781:ADP:N6	2.82	0.48
1:A:513:HIS:CE1	1:A:518:ILE:HG22	2.49	0.48
1:A:688:ILE:HG12	1:A:692:ILE:HD12	1.96	0.48
1:A:249:ASP:CB	1:A:260:GLN:O	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLU:CD	1:A:278:LEU:HD21	2.33	0.48
1:A:645:ARG:O	1:A:646:GLU:CG	2.62	0.48
1:B:616:GLU:OE1	1:B:616:GLU:HA	2.14	0.48
1:B:624:ARG:NH2	1:B:707:GLN:HB2	2.23	0.48
1:B:340:LYS:CD	1:B:340:LYS:N	2.77	0.48
1:B:649:PRO:O	1:B:652:TRP:CZ3	2.67	0.48
1:A:284:VAL:HG11	1:A:717:LEU:HD11	1.95	0.48
1:A:414:LYS:HD3	1:A:540:SER:N	2.28	0.48
1:A:576:ARG:HH22	1:B:346:GLN:NE2	2.11	0.48
1:A:610:ILE:HD12	1:A:723:LYS:HZ1	1.78	0.48
1:B:626:ILE:HG23	1:B:715:ILE:HD11	1.93	0.48
1:B:637:ARG:O	1:B:638:ALA:C	2.52	0.48
1:A:322:ARG:NH1	1:A:743:TYR:CE1	2.81	0.47
1:A:662:ASN:HB3	1:A:670:ALA:CB	2.42	0.47
1:B:500:LYS:HE2	1:B:500:LYS:H	1.78	0.47
1:B:572:LYS:O	1:B:575:SER:HB3	2.13	0.47
1:A:279:PHE:HB2	1:A:779:GLU:N	2.30	0.47
1:A:380:GLU:OE1	1:A:593:ARG:NH1	2.46	0.47
1:B:245:LYS:C	1:B:247:GLU:H	2.17	0.47
1:B:617:VAL:HG11	1:B:716:VAL:CG2	2.45	0.47
1:B:624:ARG:NH2	1:B:700:GLU:HG2	2.29	0.47
1:A:10:ASP:HB3	1:A:11:PRO:HD2	0.68	0.47
1:A:203:PHE:CD2	1:A:204:ALA:N	2.82	0.47
1:A:209:VAL:HG12	1:A:371:THR:HG22	1.95	0.47
1:A:324:MET:HG3	1:A:327:ARG:NH1	2.29	0.47
1:A:549:PHE:CD2	1:A:561:PHE:HE2	2.32	0.47
1:A:382:ARG:O	1:A:382:ARG:HG3	2.14	0.47
1:B:248:LYS:HD2	1:B:265:GLY:CA	2.39	0.47
1:B:484:THR:HG22	1:B:485:ASN:OD1	2.14	0.47
1:B:627:VAL:HG13	1:B:696:TYR:CZ	2.49	0.47
1:B:750:ARG:NH1	1:B:750:ARG:CG	2.56	0.47
1:B:262:THR:O	1:B:264:GLU:N	2.48	0.47
1:B:548:ARG:HG3	1:B:549:PHE:H	1.80	0.47
1:B:679:LYS:HB3	1:B:683:GLU:HG3	1.97	0.47
1:B:770:GLU:O	1:B:771:VAL:C	2.52	0.47
1:A:194:GLU:HG3	1:A:195:GLN:H	1.77	0.47
1:A:738:ILE:HD11	1:A:743:TYR:HE2	1.80	0.47
1:A:293:ALA:O	1:A:297:HIS:HD2	1.97	0.47
1:A:360:TYR:O	1:A:363:MET:HG3	2.14	0.47
1:A:554:THR:CG2	1:A:555:MET:N	2.78	0.47
1:B:248:LYS:HA	1:B:261:LEU:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:THR:OG1	1:B:668:GLU:CD	2.53	0.47
1:A:226:GLN:NE2	1:A:228:ALA:HB2	2.30	0.47
1:A:647:GLU:CG	1:A:648:LEU:H	2.28	0.47
1:B:248:LYS:HZ3	1:B:268:LYS:HD2	1.79	0.47
1:B:485:ASN:OD1	1:B:486:MET:HG2	2.14	0.47
1:A:662:ASN:O	1:A:777:LYS:NZ	2.47	0.46
1:B:74:ARG:HG3	1:B:74:ARG:NH1	2.29	0.46
1:B:88:GLY:HA3	1:B:109:THR:CG2	2.45	0.46
1:B:708:MET:HA	1:B:711:PHE:CD1	2.50	0.46
1:A:302:LYS:HG2	1:A:303:ASP:HB2	1.98	0.46
1:A:338:GLU:CG	1:A:345:ILE:HG13	2.35	0.46
1:A:672:GLU:C	1:A:673:LYS:HG2	2.35	0.46
1:B:229:LYS:HD3	1:B:289:HIS:CD2	2.50	0.46
1:B:302:LYS:HD3	1:B:341:GLU:CD	2.35	0.46
1:B:307:VAL:CG1	1:B:308:VAL:H	2.28	0.46
1:B:554:THR:HG21	1:B:574:VAL:HA	1.97	0.46
1:A:706:GLU:O	1:A:709:ARG:N	2.49	0.46
1:B:256:THR:CG2	1:B:295:LYS:HD2	2.42	0.46
1:B:39:ASP:OD2	1:B:42:LYS:HB3	2.15	0.46
1:A:328:ARG:HH11	1:A:328:ARG:CG	2.25	0.46
1:A:600:ASP:O	1:A:604:ARG:N	2.36	0.46
1:B:611:TYR:O	1:B:614:ARG:HG2	2.16	0.46
1:A:9:PHE:HD2	1:A:10:ASP:N	2.09	0.46
1:A:84:VAL:HG21	1:A:395:ASN:HB2	1.97	0.46
1:A:123:GLY:HA2	1:A:171:ASP:O	2.16	0.46
1:B:238:ASN:HD21	1:B:340:LYS:HD2	1.79	0.46
1:B:279:PHE:HZ	1:B:773:LYS:HE2	1.80	0.46
1:B:403:ARG:HG2	1:B:404:PRO:HD2	1.96	0.46
1:A:160:SER:C	1:A:162:ASP:N	2.69	0.46
1:A:164:LYS:NZ	1:A:183:ASP:OD1	2.48	0.46
1:A:439:VAL:HG23	1:B:411:MET:CE	2.46	0.46
1:A:463:ASN:O	1:A:467:GLU:HG3	2.15	0.46
1:A:513:HIS:ND1	1:A:519:ASP:OD2	2.49	0.46
1:A:739:HIS:HB3	1:B:583:LYS:HD2	1.98	0.46
1:A:745:GLN:NE2	1:B:584:ARG:HA	2.31	0.46
1:B:324:MET:HA	1:B:741:ARG:CD	2.37	0.46
1:B:376:THR:C	1:B:378:GLU:H	2.19	0.46
1:B:406:LEU:HD12	1:B:538:TYR:CE1	2.51	0.46
1:B:414:LYS:NZ	1:B:510:THR:O	2.29	0.46
1:A:112:LEU:HB2	1:A:113:PRO:HD3	1.98	0.46
1:A:226:GLN:NE2	1:A:228:ALA:CB	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LEU:HD22	1:A:248:LYS:HG3	1.98	0.46
1:A:512:ARG:HH11	1:A:582:GLN:NE2	2.14	0.46
1:A:552:GLU:O	1:A:560:ARG:NH1	2.48	0.46
1:B:686:GLU:OE1	1:B:686:GLU:CA	2.63	0.46
1:B:711:PHE:O	1:B:715:ILE:HD12	2.15	0.46
1:A:255:LYS:CE	1:A:762:HIS:HE1	2.29	0.46
1:A:609:VAL:HG12	1:A:610:ILE:HD13	1.97	0.46
1:B:155:ASN:HB3	1:B:175:SER:HB2	1.98	0.46
1:A:226:GLN:HE22	1:A:228:ALA:HB2	1.80	0.45
1:A:410:THR:HA	1:A:542:GLU:HB2	1.98	0.45
1:B:425:ARG:CD	1:B:430:GLN:OE1	2.61	0.45
1:A:740:LEU:H	1:A:740:LEU:CD2	2.24	0.45
1:B:602:VAL:O	1:B:606:GLN:HG3	2.16	0.45
1:B:611:TYR:O	1:B:615:PHE:HD1	2.00	0.45
1:B:37:SER:N	1:B:40:ALA:HB3	2.30	0.45
1:B:218:ARG:O	1:B:218:ARG:HG2	2.16	0.45
1:B:231:THR:HB	1:B:348:GLU:CG	2.46	0.45
1:B:248:LYS:HD3	1:B:265:GLY:HA2	1.94	0.45
1:B:426:TYR:CD2	1:B:454:ILE:HG23	2.50	0.45
1:B:617:VAL:O	1:B:617:VAL:CG1	2.65	0.45
1:A:330:SER:C	1:A:331:GLU:HG3	2.36	0.45
1:A:442:SER:O	1:A:482:ILE:HD11	2.15	0.45
1:A:528:ARG:HG3	1:A:528:ARG:NH1	2.27	0.45
1:A:5:LEU:HG	1:A:590:PHE:HZ	1.82	0.45
1:A:45:THR:O	1:A:49:LYS:HG3	2.16	0.45
1:A:88:GLY:HA2	1:A:392:ILE:CD1	2.46	0.45
1:A:283:HIS:O	1:A:285:ALA:N	2.50	0.45
1:A:659:ASP:O	1:A:660:LEU:C	2.55	0.45
1:A:682:ASP:HA	1:A:685:LEU:HG	1.99	0.45
1:A:741:ARG:NH2	1:B:376:THR:O	2.50	0.45
1:B:191:LEU:HD13	1:B:191:LEU:O	2.16	0.45
1:B:252:TYR:CE2	1:B:254:ILE:HG22	2.50	0.45
1:B:376:THR:HB	1:B:377:GLU:OE2	2.16	0.45
1:B:738:ILE:HD12	1:B:748:PRO:HB2	1.98	0.45
1:A:203:PHE:HD2	1:A:204:ALA:N	2.14	0.45
1:A:258:ALA:CB	1:A:295:LYS:HG2	2.45	0.45
1:A:642:TYR:CE1	1:A:684:MET:HB3	2.52	0.45
1:A:707:GLN:HB3	1:A:708:MET:HE1	1.98	0.45
1:B:89:GLY:HA2	1:B:113:PRO:HD3	1.98	0.45
1:B:639:ILE:HG13	1:B:685:LEU:HD22	1.98	0.45
1:A:279:PHE:O	1:A:778:ALA:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LYS:HB3	1:B:265:GLY:HA2	1.89	0.45
1:B:506:ALA:HA	1:B:534:ILE:HG23	1.99	0.45
1:A:5:LEU:O	1:A:6:ASN:HB2	2.16	0.45
1:A:206:ILE:O	1:A:369:GLY:HA2	2.17	0.45
1:A:653:LYS:HE3	1:A:653:LYS:O	2.17	0.45
1:B:112:LEU:HB2	1:B:113:PRO:HD3	1.98	0.45
1:A:66:PHE:HE2	1:A:112:LEU:C	2.20	0.45
1:A:436:THR:HG22	1:A:437:VAL:N	2.31	0.45
1:A:643:THR:N	1:A:644:PRO:HD2	2.32	0.45
1:A:645:ARG:C	1:A:646:GLU:HG3	2.37	0.45
1:B:723:LYS:HG2	1:B:767:ILE:CG1	2.46	0.45
1:B:512:ARG:HD2	1:B:537:PHE:CD2	2.53	0.44
1:A:2:LEU:O	1:A:3:GLY:C	2.55	0.44
1:B:256:THR:O	1:B:257:LYS:HD3	2.16	0.44
1:B:283:HIS:HB3	1:B:286:LEU:HB3	1.98	0.44
1:B:596:LEU:HD12	1:B:596:LEU:HA	1.79	0.44
1:A:210:ASP:OD2	1:A:371:THR:CB	2.64	0.44
1:A:718:ARG:NH1	1:A:722:SER:HB3	2.32	0.44
1:A:737:GLY:C	1:A:739:HIS:H	2.21	0.44
1:B:13:LYS:O	1:B:16:LEU:HD23	2.18	0.44
1:B:222:ILE:HG12	1:B:354:THR:HG23	1.98	0.44
1:B:731:MET:O	1:B:735:ARG:HB2	2.17	0.44
1:A:238:ASN:O	1:A:241:VAL:HG23	2.17	0.44
1:A:362:ARG:HH21	1:A:597:LEU:HD11	1.82	0.44
1:A:718:ARG:HD3	1:A:770:GLU:HG2	1.98	0.44
1:B:354:THR:HG21	1:B:735:ARG:CZ	2.48	0.44
1:B:413:GLY:O	1:B:416:LYS:HB3	2.17	0.44
1:B:493:ILE:HD13	1:B:525:ARG:HB3	1.98	0.44
1:A:215:ASP:OD2	1:A:517:ARG:NH2	2.43	0.44
1:A:753:GLN:HG3	1:A:754:MET:H	1.83	0.44
1:B:238:ASN:CG	1:B:340:LYS:HD2	2.37	0.44
1:B:322:ARG:NH2	1:B:742:ALA:O	2.51	0.44
1:B:516:ARG:N	1:B:516:ARG:HD2	2.33	0.44
1:B:243:THR:O	1:B:243:THR:CG2	2.62	0.44
1:B:554:THR:CG2	1:B:574:VAL:HG22	2.48	0.44
1:B:755:GLU:O	1:B:759:MET:HG3	2.18	0.44
1:A:558:LEU:HD12	1:A:558:LEU:HA	1.76	0.44
1:A:637:ARG:HE	1:A:769:ASP:CA	2.31	0.44
1:A:718:ARG:HD3	1:A:770:GLU:CG	2.48	0.44
1:B:102:THR:HA	1:B:106:LYS:NZ	2.32	0.44
1:B:379:GLU:HG2	1:B:383:ASN:ND2	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ALA:HA	1:B:467:GLU:OE2	2.18	0.44
1:A:641:ALA:HB1	1:A:660:LEU:CD1	2.48	0.44
1:B:99:GLU:OE2	1:B:391:THR:HG23	2.18	0.44
1:B:337:ILE:HA	1:B:340:LYS:HG2	1.98	0.44
1:B:614:ARG:NH1	1:B:720:VAL:CG2	2.67	0.44
1:A:266:MET:HB3	1:A:277:ASN:OD1	2.18	0.43
1:A:457:GLN:HE21	1:A:470:ILE:CD1	2.15	0.43
1:A:667:ASP:O	1:A:669:GLY:N	2.51	0.43
1:B:16:LEU:CD2	1:B:16:LEU:N	2.77	0.43
1:B:262:THR:O	1:B:263:GLU:C	2.55	0.43
1:B:457:GLN:HE21	1:B:470:ILE:HG23	1.82	0.43
1:B:630:MET:HB3	1:B:630:MET:HE2	1.59	0.43
1:A:105:GLY:N	2:A:781:ADP:O3A	2.49	0.43
1:A:723:LYS:HB2	1:A:763:MET:HG2	2.00	0.43
1:B:238:ASN:HD21	1:B:340:LYS:N	2.15	0.43
1:A:723:LYS:CD	1:A:763:MET:CE	2.82	0.43
1:B:250:TYR:CD1	1:B:261:LEU:HA	2.52	0.43
1:B:270:GLU:HB3	1:B:275:ILE:O	2.18	0.43
1:B:716:VAL:O	1:B:720:VAL:HB	2.18	0.43
1:B:760:PHE:O	1:B:763:MET:HB3	2.19	0.43
1:A:166:GLU:O	1:A:169:ALA:HB3	2.19	0.43
1:B:16:LEU:H	1:B:16:LEU:HD23	1.80	0.43
1:A:278:LEU:H	1:A:278:LEU:CD2	2.20	0.43
1:A:459:LEU:HB2	1:A:483:ALA:HA	1.99	0.43
1:A:647:GLU:CG	1:A:648:LEU:N	2.81	0.43
1:A:657:LEU:O	1:A:660:LEU:HD23	2.18	0.43
1:A:745:GLN:NE2	1:B:587:GLY:HA3	2.34	0.43
1:B:422:VAL:HG13	1:B:432:VAL:HG11	2.00	0.43
1:A:425:ARG:HB2	1:A:432:VAL:HG21	2.00	0.43
1:A:610:ILE:CG2	1:A:723:LYS:HE2	2.47	0.43
1:B:204:ALA:HB3	1:B:367:LEU:HD12	2.01	0.43
1:B:509:GLY:O	1:B:538:TYR:N	2.45	0.43
1:B:639:ILE:CG2	1:B:640:ALA:N	2.82	0.43
1:B:643:THR:HA	1:B:646:GLU:OE2	2.18	0.43
1:B:741:ARG:O	1:B:742:ALA:C	2.56	0.43
1:A:218:ARG:HB3	1:B:549:PHE:CD2	2.54	0.43
1:A:244:LEU:O	1:A:244:LEU:HD13	2.18	0.43
1:B:160:SER:O	1:B:164:LYS:HG3	2.19	0.43
1:B:227:ALA:HB3	1:B:348:GLU:OE1	2.19	0.43
1:B:354:THR:HG22	1:B:735:ARG:HH22	1.80	0.43
1:B:603:LEU:HD12	1:B:603:LEU:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LEU:HD12	1:A:108:LEU:HA	1.76	0.43
1:A:313:VAL:CG2	1:A:337:ILE:CD1	2.96	0.43
1:A:666:LEU:HD23	1:A:670:ALA:HB2	2.00	0.43
1:B:11:PRO:O	1:B:13:LYS:N	2.51	0.43
1:B:201:LEU:HD12	1:B:363:MET:HE2	2.01	0.43
1:B:262:THR:HG23	1:B:263:GLU:N	2.34	0.43
1:B:627:VAL:HG22	1:B:711:PHE:CE1	2.53	0.43
1:B:716:VAL:O	1:B:716:VAL:HG12	2.18	0.43
1:A:228:ALA:C	1:A:230:SER:N	2.69	0.43
1:A:604:ARG:HA	1:A:607:ARG:CZ	2.49	0.43
1:B:36:LEU:HD13	1:B:40:ALA:O	2.19	0.43
1:B:127:VAL:HG13	1:B:180:LEU:HD12	2.01	0.43
1:B:199:ARG:HB3	1:B:200:PRO:HD2	1.97	0.43
1:B:209:VAL:CG1	1:B:210:ASP:N	2.81	0.43
1:B:363:MET:HB3	1:B:363:MET:HE3	1.49	0.43
1:B:642:TYR:O	1:B:645:ARG:N	2.52	0.43
1:A:160:SER:O	1:A:162:ASP:N	2.52	0.42
1:A:576:ARG:HH12	1:B:346:GLN:NE2	2.14	0.42
1:B:718:ARG:CG	1:B:770:GLU:CD	2.71	0.42
1:A:182:PHE:CB	1:A:186:ARG:NH2	2.75	0.42
1:A:322:ARG:NE	1:A:324:MET:HE1	2.34	0.42
1:B:475:GLY:HA3	1:B:494:LYS:O	2.19	0.42
1:B:147:PHE:C	1:B:149:GLY:N	2.73	0.42
1:B:445:ILE:C	1:B:447:LYS:H	2.22	0.42
1:B:724:TRP:CZ2	1:B:728:ILE:HD11	2.54	0.42
1:A:334:HIS:HA	1:A:337:ILE:HG13	2.00	0.42
1:A:685:LEU:O	1:A:689:MET:HB2	2.19	0.42
1:B:29:ILE:HD12	1:B:33:TYR:HE1	1.83	0.42
1:B:70:ARG:O	1:B:70:ARG:HG2	2.19	0.42
1:B:256:THR:OG1	1:B:295:LYS:HE3	2.19	0.42
1:B:476:GLN:NE2	1:B:494:LYS:HZ1	2.16	0.42
1:A:426:TYR:CD2	1:A:426:TYR:O	2.71	0.42
1:A:484:THR:O	1:A:485:ASN:C	2.57	0.42
1:A:564:ASP:OD2	1:A:566:SER:HB2	2.20	0.42
1:A:637:ARG:HE	1:A:769:ASP:CB	2.28	0.42
1:A:708:MET:CE	1:A:711:PHE:CE1	3.03	0.42
1:B:61:LEU:O	1:B:62:LEU:C	2.58	0.42
1:B:107:THR:O	1:B:110:SER:OG	2.29	0.42
1:B:754:MET:HE3	1:B:754:MET:HB3	1.72	0.42
1:A:338:GLU:O	1:A:343:LEU:HA	2.19	0.42
1:B:241:VAL:HG21	1:B:293:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TYR:HB2	1:A:253:ASP:H	1.51	0.42
1:A:642:TYR:CD1	1:A:684:MET:HB3	2.55	0.42
1:B:539:LEU:HB3	1:B:546:MET:HE2	2.02	0.42
1:A:103:GLY:HA3	1:A:528:ARG:HB2	2.02	0.42
1:A:224:SER:HA	1:A:350:MET:O	2.19	0.42
1:B:617:VAL:HG11	1:B:716:VAL:HG23	2.02	0.42
1:A:648:LEU:N	1:A:649:PRO:CD	2.82	0.42
1:A:699:LYS:HD2	1:A:707:GLN:HE22	1.85	0.42
1:B:322:ARG:HG3	1:B:742:ALA:CB	2.50	0.42
1:A:93:HIS:HD2	1:A:117:ASN:HD21	1.68	0.42
1:A:288:HIS:HE2	1:A:331:GLU:HB2	1.85	0.42
1:A:331:GLU:OE2	1:A:766:SER:OG	2.31	0.42
1:A:425:ARG:NH1	1:A:534:ILE:HD11	2.34	0.42
1:A:553:ARG:HE	1:A:560:ARG:NH2	2.18	0.42
1:B:302:LYS:HD3	1:B:341:GLU:OE2	2.19	0.42
1:B:315:ILE:HD13	1:B:329:TYR:CZ	2.55	0.42
1:A:252:TYR:CE1	1:A:256:THR:HA	2.55	0.41
1:A:689:MET:SD	1:A:693:ILE:HB	2.60	0.41
1:B:39:ASP:CG	1:B:42:LYS:HB3	2.40	0.41
1:B:630:MET:HE3	1:B:630:MET:O	2.20	0.41
1:A:699:LYS:HE3	1:A:779:GLU:OE1	2.20	0.41
1:B:211:SER:O	1:B:216:GLU:HG3	2.20	0.41
1:B:254:ILE:CG2	1:B:255:LYS:N	2.83	0.41
1:B:460:ASN:O	1:B:461:ALA:HB3	2.19	0.41
1:A:109:THR:O	1:A:113:PRO:HD2	2.20	0.41
1:A:405:ASP:HB3	1:A:539:LEU:HD12	2.02	0.41
1:A:625:GLU:HA	1:A:628:GLU:HB3	2.02	0.41
1:B:301:GLN:H	1:B:305:ASP:HB2	1.84	0.41
1:B:331:GLU:OE2	1:B:722:SER:CB	2.55	0.41
1:B:780:ILE:HG22	1:B:780:ILE:OXT	2.20	0.41
1:A:226:GLN:HA	1:A:350:MET:HE3	2.01	0.41
1:A:258:ALA:H	1:A:295:LYS:HE2	1.85	0.41
1:B:190:VAL:HG13	1:B:192:TYR:H	1.85	0.41
1:B:708:MET:CA	1:B:711:PHE:HB2	2.50	0.41
1:B:754:MET:HE2	1:B:754:MET:HB2	1.73	0.41
1:A:257:LYS:HZ1	1:A:660:LEU:HD12	1.86	0.41
1:A:628:GLU:HG3	1:A:632:LYS:HZ2	1.86	0.41
1:A:728:ILE:HD13	1:A:728:ILE:HA	1.82	0.41
1:B:42:LYS:O	1:B:45:THR:HB	2.20	0.41
1:B:261:LEU:HD12	1:B:261:LEU:C	2.39	0.41
1:B:282:LYS:NZ	1:B:283:HIS:NE2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:GLN:C	1:B:426:TYR:H	2.24	0.41
1:B:461:ALA:HB2	1:B:487:ALA:HA	2.02	0.41
1:A:261:LEU:HD13	1:A:294:LEU:HD22	2.03	0.41
1:A:741:ARG:HH22	1:B:376:THR:CG2	2.22	0.41
1:B:19:TYR:C	1:B:87:MET:HE3	2.40	0.41
1:B:112:LEU:HB2	1:B:113:PRO:CD	2.51	0.41
1:B:458:VAL:O	1:B:458:VAL:HG12	2.20	0.41
1:B:484:THR:O	1:B:485:ASN:C	2.58	0.41
1:A:374:ALA:HB1	1:A:381:PHE:CE1	2.56	0.41
1:A:686:GLU:CG	1:A:687:LEU:N	2.83	0.41
1:B:168:TYR:HD1	1:B:197:VAL:HG12	1.86	0.41
1:B:217:ALA:HB3	1:B:593:ARG:CD	2.51	0.41
1:B:302:LYS:O	1:B:302:LYS:HG2	2.20	0.41
1:B:516:ARG:HD2	1:B:516:ARG:H	1.86	0.41
1:B:551:ALA:C	1:B:553:ARG:H	2.23	0.41
1:B:744:ALA:HB1	1:B:748:PRO:HG3	2.03	0.41
1:A:637:ARG:HA	1:A:637:ARG:HD3	1.58	0.41
1:B:708:MET:C	1:B:711:PHE:HB2	2.41	0.41
1:A:72:ALA:HB2	1:A:148:LEU:HD21	2.03	0.41
1:A:176:THR:O	1:A:177:ASN:C	2.59	0.41
1:A:247:GLU:HB2	1:A:261:LEU:HG	2.03	0.41
1:A:576:ARG:O	1:A:579:GLU:HB2	2.20	0.41
1:A:652:TRP:O	1:A:653:LYS:HG3	2.21	0.41
1:A:659:ASP:HA	1:A:662:ASN:OD1	2.21	0.41
1:B:218:ARG:HH11	1:B:592:SER:CB	2.33	0.41
1:B:263:GLU:N	1:B:263:GLU:OE2	2.50	0.41
1:B:339:ALA:HB2	1:B:345:ILE:HG12	2.03	0.41
1:B:599:TYR:HD1	1:B:599:TYR:N	2.18	0.41
1:A:332:GLY:HA2	1:A:334:HIS:NE2	2.36	0.41
1:A:624:ARG:HG2	1:A:624:ARG:O	2.21	0.41
1:A:685:LEU:O	1:A:689:MET:CB	2.69	0.40
1:B:607:ARG:O	1:B:608:GLU:C	2.58	0.40
1:B:637:ARG:NH2	1:B:765:GLU:O	2.54	0.40
1:A:206:ILE:H	1:A:206:ILE:CD1	2.33	0.40
1:A:279:PHE:CZ	1:A:780:ILE:HG23	2.56	0.40
1:A:613:GLN:O	1:A:617:VAL:HG23	2.20	0.40
1:B:358:GLN:HB3	1:B:597:LEU:HD13	2.03	0.40
1:B:642:TYR:OH	1:B:688:ILE:HD12	2.22	0.40
1:A:442:SER:O	1:A:482:ILE:CD1	2.69	0.40
1:A:747:ASN:HD22	1:A:747:ASN:HA	1.57	0.40
1:B:377:GLU:HB2	1:B:381:PHE:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:SER:C	1:B:516:ARG:HH11	2.25	0.40
1:A:100:MET:O	1:A:372:GLY:HA2	2.22	0.40
1:A:317:ASP:O	1:A:319:PHE:N	2.55	0.40
1:A:374:ALA:HB1	1:A:381:PHE:HE1	1.87	0.40
1:A:442:SER:CA	1:A:482:ILE:HD11	2.51	0.40
1:A:665:TYR:O	1:A:776:MET:HB3	2.21	0.40
1:A:671:LEU:CD1	1:A:674:SER:HA	2.52	0.40
1:A:763:MET:HE2	1:A:763:MET:HB3	1.88	0.40
1:B:400:ARG:HB2	1:B:527:GLY:HA3	2.04	0.40
1:B:512:ARG:CG	1:B:539:LEU:HD21	2.51	0.40
1:B:593:ARG:O	1:B:594:LYS:C	2.59	0.40
1:B:599:TYR:N	1:B:599:TYR:CD1	2.89	0.40
1:B:741:ARG:CG	1:B:742:ALA:N	2.83	0.40
1:A:168:TYR:OH	1:A:180:LEU:HD23	2.21	0.40
1:A:203:PHE:HD2	1:A:204:ALA:H	1.69	0.40
1:A:458:VAL:CG1	1:A:459:LEU:N	2.84	0.40
1:A:541:MET:HA	1:A:546:MET:HG2	2.04	0.40
1:A:641:ALA:CB	1:A:660:LEU:HD11	2.52	0.40
1:A:679:LYS:O	1:A:680:GLU:HG2	2.21	0.40
1:A:747:ASN:C	1:A:749:LEU:N	2.74	0.40
1:B:302:LYS:HA	1:B:306:TYR:CZ	2.56	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	778/780 (100%)	647 (83%)	99 (13%)	32 (4%)	3 21
1	B	768/780 (98%)	626 (82%)	118 (15%)	24 (3%)	4 26
All	All	1546/1560 (99%)	1273 (82%)	217 (14%)	56 (4%)	3 23

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	SER
1	A	259	VAL
1	A	275	ILE
1	A	280	ASP
1	A	304	VAL
1	A	544	GLU
1	A	563	MET
1	A	668	GLU
1	B	12	THR
1	B	120	THR
1	B	122	LYS
1	B	245	LYS
1	B	345	ILE
1	B	485	ASN
1	A	161	LYS
1	A	284	VAL
1	A	299	ALA
1	A	342	GLY
1	A	548	ARG
1	A	690	ASP
1	A	737	GLY
1	B	133	LEU
1	B	446	SER
1	B	655	ASP
1	A	248	LYS
1	A	254	ILE
1	A	257	LYS
1	A	311	GLY
1	A	318	SER
1	B	253	ASP
1	B	318	SER
1	B	625	GLU
1	B	743	TYR
1	A	310	ASP
1	A	679	LYS
1	B	263	GLU
1	B	544	GLU
1	A	3	GLY
1	A	376	THR
1	A	461	ALA
1	A	485	ASN
1	A	674	SER

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Mol	Chain	Res	Type
1	B	251	THR
1	B	575	SER
1	B	627	VAL
1	A	562	GLY
1	A	660	LEU
1	A	681	PRO
1	B	132	TYR
1	B	547	ARG
1	B	565	ASP
1	A	738	ILE
1	B	254	ILE
1	A	274	GLY
1	B	212	ILE
1	B	644	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	670/670 (100%)	576 (86%)	94 (14%)	3 16
1	B	661/670 (99%)	558 (84%)	103 (16%)	2 12
All	All	1331/1340 (99%)	1134 (85%)	197 (15%)	3 14

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	13	LYS
1	A	16	LEU
1	A	21	LYS
1	A	30	ARG
1	A	35	ASN
1	A	61	LEU
1	A	62	LEU
1	A	120	THR

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Mol	Chain	Res	Type
1	A	158	SER
1	A	194	GLU
1	A	200	PRO
1	A	207	ASP
1	A	210	ASP
1	A	221	LEU
1	A	224	SER
1	A	232	LYS
1	A	238	ASN
1	A	244	LEU
1	A	250	TYR
1	A	251	THR
1	A	260	GLN
1	A	278	LEU
1	A	279	PHE
1	A	284	VAL
1	A	287	ASN
1	A	301	GLN
1	A	309	GLU
1	A	316	VAL
1	A	323	LEU
1	A	328	ARG
1	A	331	GLU
1	A	337	ILE
1	A	343	LEU
1	A	344	GLU
1	A	345	ILE
1	A	346	GLN
1	A	348	GLU
1	A	354	THR
1	A	363	MET
1	A	371	THR
1	A	376	THR
1	A	377	GLU
1	A	382	ARG
1	A	426	TYR
1	A	428	THR
1	A	439	VAL
1	A	442	SER
1	A	443	GLU
1	A	448	LEU
1	A	471	ILE

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Mol	Chain	Res	Type
1	A	481	THR
1	A	482	ILE
1	A	492	ASP
1	A	500	LYS
1	A	501	GLU
1	A	517	ARG
1	A	534	ILE
1	A	535	THR
1	A	559	ASP
1	A	569	ILE
1	A	601	ASP
1	A	630	MET
1	A	634	SER
1	A	636	GLU
1	A	637	ARG
1	A	653	LYS
1	A	655	ASP
1	A	660	LEU
1	A	663	THR
1	A	666	LEU
1	A	673	LYS
1	A	675	ASP
1	A	684	MET
1	A	686	GLU
1	A	691	ARG
1	A	695	LYS
1	A	696	TYR
1	A	700	GLU
1	A	707	GLN
1	A	708	MET
1	A	709	ARG
1	A	717	LEU
1	A	718	ARG
1	A	722	SER
1	A	723	LYS
1	A	724	TRP
1	A	731	MET
1	A	740	LEU
1	A	741	ARG
1	A	747	ASN
1	A	751	GLU
1	A	763	MET

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Mol	Chain	Res	Type
1	A	766	SER
1	B	14	ARG
1	B	16	LEU
1	B	30	ARG
1	B	53	GLU
1	B	61	LEU
1	B	73	SER
1	B	83	LYS
1	B	146	GLU
1	B	187	ASP
1	B	191	LEU
1	B	195	GLN
1	B	219	THR
1	B	226	GLN
1	B	231	THR
1	B	233	LEU
1	B	244	LEU
1	B	255	LYS
1	B	260	GLN
1	B	261	LEU
1	B	262	THR
1	B	263	GLU
1	B	266	MET
1	B	275	ILE
1	B	276	ASP
1	B	278	LEU
1	B	280	ASP
1	B	281	VAL
1	B	289	HIS
1	B	294	LEU
1	B	305	ASP
1	B	320	THR
1	B	328	ARG
1	B	330	SER
1	B	340	LYS
1	B	347	ASN
1	B	354	THR
1	B	363	MET
1	B	376	THR
1	B	382	ARG
1	B	388	GLN
1	B	391	THR

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Mol	Chain	Res	Type
1	B	399	VAL
1	B	405	ASP
1	B	422	VAL
1	B	442	SER
1	B	444	LEU
1	B	446	SER
1	B	459	LEU
1	B	463	ASN
1	B	473	GLU
1	B	476	GLN
1	B	477	LYS
1	B	481	THR
1	B	494	LYS
1	B	495	LEU
1	B	500	LYS
1	B	514	GLU
1	B	516	ARG
1	B	526	SER
1	B	528	ARG
1	B	544	GLU
1	B	545	LEU
1	B	546	MET
1	B	547	ARG
1	B	549	PHE
1	B	555	MET
1	B	557	MET
1	B	569	ILE
1	B	571	SER
1	B	579	GLU
1	B	580	SER
1	B	603	LEU
1	B	613	GLN
1	B	618	ILE
1	B	624	ARG
1	B	630	MET
1	B	636	GLU
1	B	639	ILE
1	B	646	GLU
1	B	647	GLU
1	B	648	LEU
1	B	650	GLU
1	B	659	ASP

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Mol	Chain	Res	Type
1	B	663	THR
1	B	667	ASP
1	B	673	LYS
1	B	680	GLU
1	B	686	GLU
1	B	693	ILE
1	B	707	GLN
1	B	711	PHE
1	B	712	GLU
1	B	720	VAL
1	B	722	SER
1	B	723	LYS
1	B	734	LEU
1	B	738	ILE
1	B	743	TYR
1	B	746	THR
1	B	747	ASN
1	B	750	ARG
1	B	766	SER
1	B	780	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	93	HIS
1	A	125	HIS
1	A	226	GLN
1	A	238	ASN
1	A	297	HIS
1	A	312	GLN
1	A	457	GLN
1	A	570	GLN
1	A	598	GLN
1	A	629	ASN
1	A	697	ASN
1	A	727	HIS
1	A	745	GLN
1	A	747	ASN
1	A	762	HIS
1	B	17	ASN
1	B	202	HIS

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Mol	Chain	Res	Type
1	B	226	GLN
1	B	288	HIS
1	B	292	GLN
1	B	297	HIS
1	B	312	GLN
1	B	346	GLN
1	B	358	GLN
1	B	383	ASN
1	B	424	GLN
1	B	457	GLN
1	B	460	ASN
1	B	463	ASN
1	B	476	GLN
1	B	582	GLN
1	B	739	HIS
1	B	747	ASN
1	B	753	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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	$\#\|Z\|>2$
2	ADP	A	781	-	24,29,29	1.36	4 (16%)	29,45,45	1.56	6 (20%)

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
2	ADP	A	781	-	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	781	ADP	O3'-C3'	3.08	1.50	1.43
2	A	781	ADP	C5-C4	2.99	1.48	1.40
2	A	781	ADP	C2-N3	2.28	1.35	1.32
2	A	781	ADP	O4'-C1'	2.09	1.44	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	781	ADP	C3'-C2'-C1'	4.20	107.31	100.98
2	A	781	ADP	N3-C2-N1	-3.65	122.97	128.68
2	A	781	ADP	C4-C5-N7	-2.99	106.28	109.40
2	A	781	ADP	PA-O3A-PB	-2.37	124.70	132.83
2	A	781	ADP	O4'-C4'-C3'	2.35	109.76	105.11
2	A	781	ADP	C2-N1-C6	2.02	122.21	118.75

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	781	ADP	O4'-C4'-C5'-O5'
2	A	781	ADP	C3'-C4'-C5'-O5'

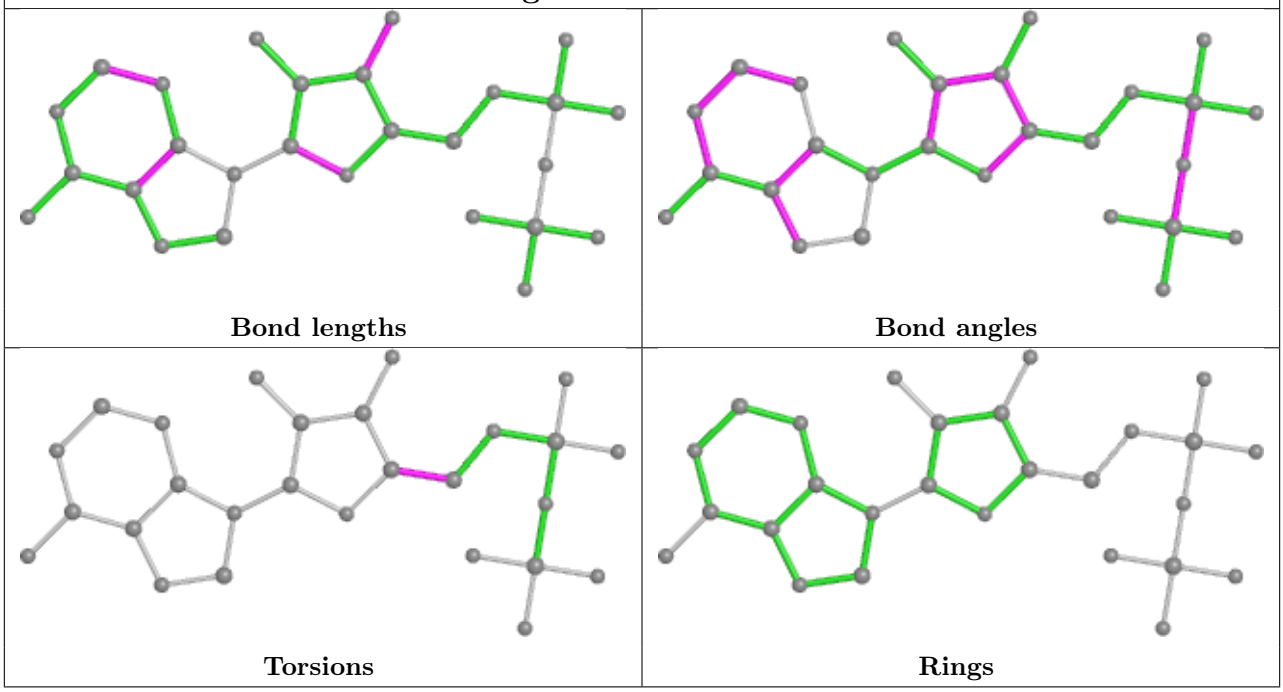
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	781	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP A 781



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	780/780 (100%)	0.35	55 (7%)	16	9	20, 45, 80, 187	0
1	B	770/780 (98%)	0.27	40 (5%)	27	15	18, 46, 61, 187	0
All	All	1550/1560 (99%)	0.31	95 (6%)	21	12	18, 46, 73, 187	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	622	ASN	7.7
1	A	622	ASN	7.3
1	B	623	LEU	5.6
1	A	654	LEU	5.2
1	B	261	LEU	5.1
1	A	675	ASP	5.1
1	B	549	PHE	4.9
1	A	651	GLU	4.7
1	A	646	GLU	4.7
1	B	621	GLU	4.6
1	A	690	ASP	4.2
1	A	676	ILE	4.2
1	B	563	MET	4.1
1	A	655	ASP	4.1
1	A	701	GLU	3.8
1	B	565	ASP	3.8
1	A	743	TYR	3.7
1	A	702	GLN	3.7
1	A	280	ASP	3.6
1	B	564	ASP	3.6
1	B	567	THR	3.4
1	A	256	THR	3.4
1	B	554	THR	3.3
1	B	262	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	250	TYR	3.3
1	A	642	TYR	3.2
1	B	571	SER	3.2
1	A	250	TYR	3.2
1	B	52	LEU	3.1
1	A	281	VAL	3.0
1	B	553	ARG	3.0
1	A	338	GLU	3.0
1	B	248	LYS	3.0
1	A	277	ASN	3.0
1	A	7	LYS	3.0
1	A	650	GLU	3.0
1	A	251	THR	2.9
1	A	677	PHE	2.9
1	B	701	GLU	2.9
1	A	699	LYS	2.9
1	A	746	THR	2.9
1	A	344	GLU	2.9
1	B	550	GLY	2.8
1	A	703	PHE	2.8
1	B	246	ALA	2.8
1	A	253	ASP	2.8
1	A	678	GLY	2.8
1	A	706	GLU	2.8
1	B	558	LEU	2.7
1	B	311	GLY	2.7
1	B	39	ASP	2.6
1	B	702	GLN	2.6
1	B	496	GLY	2.6
1	A	705	LYS	2.5
1	B	566	SER	2.5
1	A	227	ALA	2.5
1	A	239	ALA	2.4
1	B	643	THR	2.4
1	B	55	GLY	2.4
1	A	621	GLU	2.4
1	B	708	MET	2.4
1	A	268	LYS	2.4
1	B	427	MET	2.4
1	B	424	GLN	2.4
1	A	532	PRO	2.4
1	A	6	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	780	ILE	2.3
1	B	557	MET	2.3
1	A	244	LEU	2.3
1	B	723	LYS	2.3
1	A	686	GLU	2.3
1	B	561	PHE	2.3
1	A	247	GLU	2.3
1	B	34	GLU	2.3
1	B	556	ALA	2.3
1	A	343	LEU	2.2
1	A	466	ARG	2.2
1	A	243	THR	2.2
1	A	683	GLU	2.2
1	A	311	GLY	2.2
1	A	249	ASP	2.2
1	B	40	ALA	2.2
1	B	455	PRO	2.1
1	A	54	LYS	2.1
1	B	705	LYS	2.1
1	A	309	GLU	2.1
1	A	341	GLU	2.1
1	A	257	LYS	2.1
1	B	450	LYS	2.1
1	A	303	ASP	2.1
1	A	1	MET	2.1
1	A	658	VAL	2.0
1	A	11	PRO	2.0
1	A	278	LEU	2.0
1	B	253	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

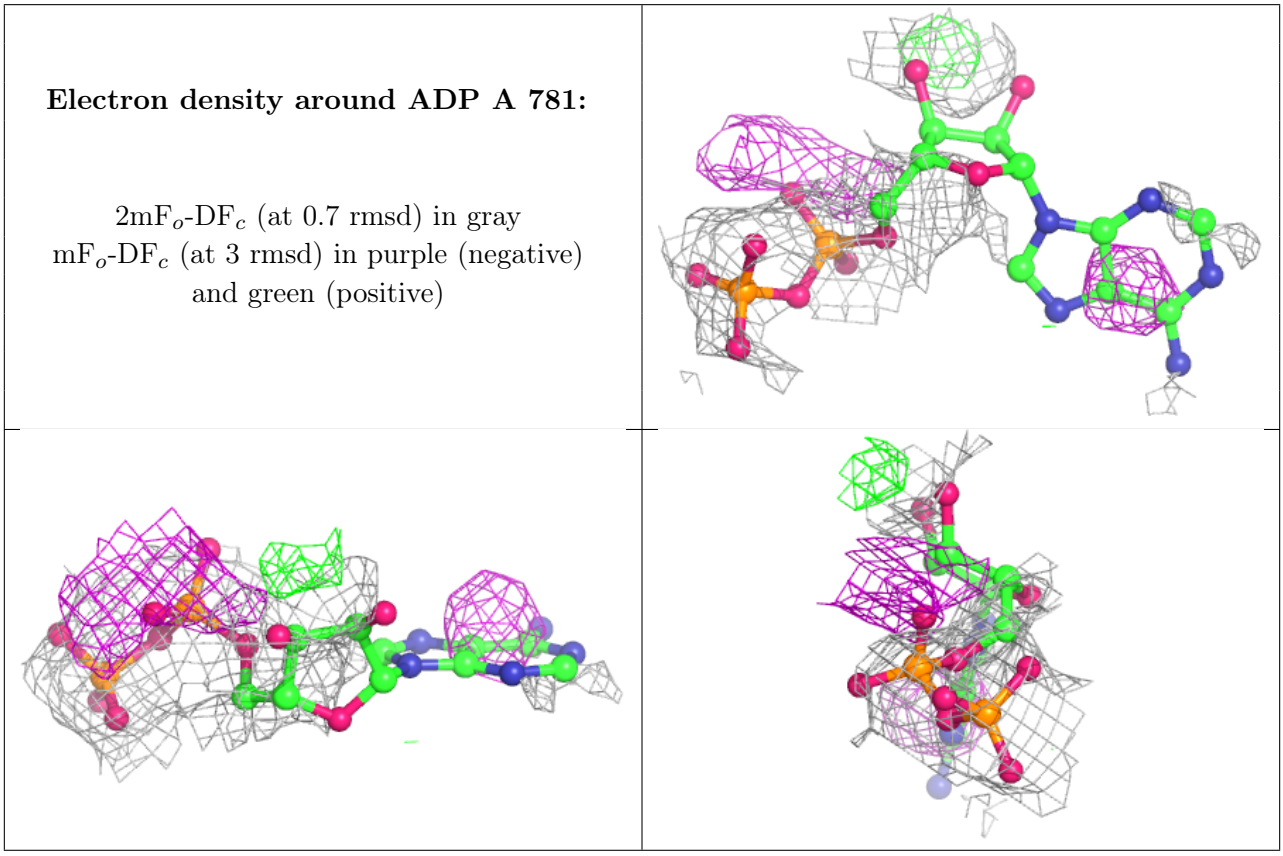
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	A	781	27/27	0.62	0.63	47,108,108,108	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP A 781:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.