



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:44 pm BST

PDB ID : 1ZM3  
Title : Structure of the apo eEF2-ETA complex  
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Deposited on : 2005-05-10  
Resolution : 3.07 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](mailto: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.

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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 : 2.11  
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) : 2.11

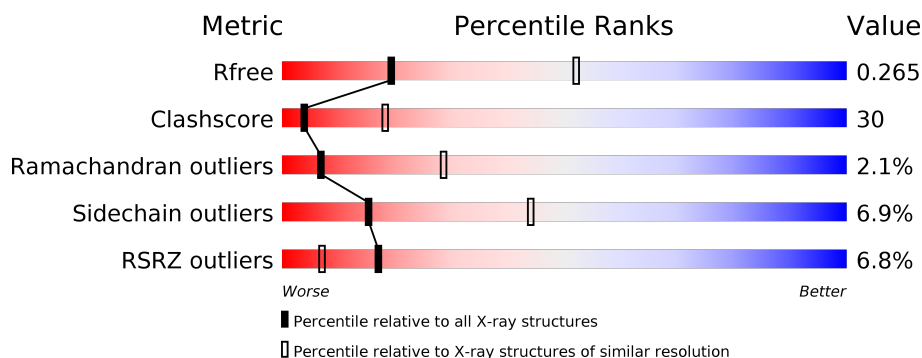
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.07 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	842	<div> <div>2%</div> <div> <div>54%</div> <div>40%</div> <div>• •</div> </div> </div>
1	C	842	<div> <div>5%</div> <div> <div>45%</div> <div>48%</div> <div>5%</div> <div>•</div> </div> </div>
1	E	842	<div> <div>18%</div> <div> <div>45%</div> <div>49%</div> <div>• •</div> </div> </div>
2	B	207	<div> <div>•</div> <div> <div>57%</div> <div>35%</div> <div>7%</div> </div> </div>
2	D	207	<div> <div>55%</div> <div>42%</div> <div>•</div> </div>
2	F	207	<div> <div>57%</div> <div>36%</div> <div>6%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23979 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 Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			
1	C	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			
1	E	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	699	DDE	HIS	MODIFIED RESIDUE	UNP P32324
C	699	DDE	HIS	MODIFIED RESIDUE	UNP P32324
E	699	DDE	HIS	MODIFIED RESIDUE	UNP P32324

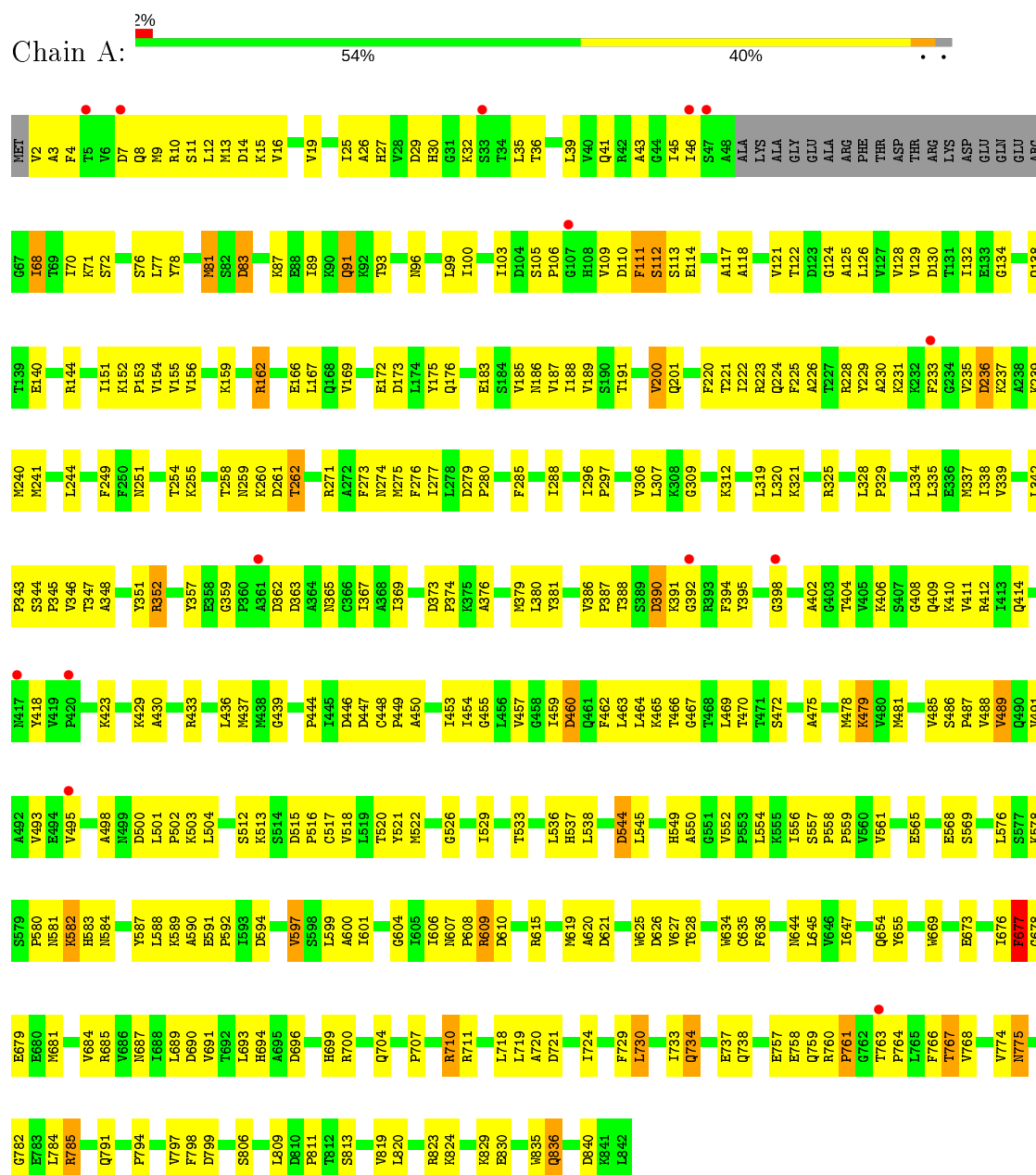
- Molecule 2 is a protein called exotoxin A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	0	0	0
			1588	1001	283	304			
2	D	207	Total	C	N	O	0	0	0
			1588	1001	283	304			
2	F	207	Total	C	N	O	0	0	0
			1588	1001	283	304			

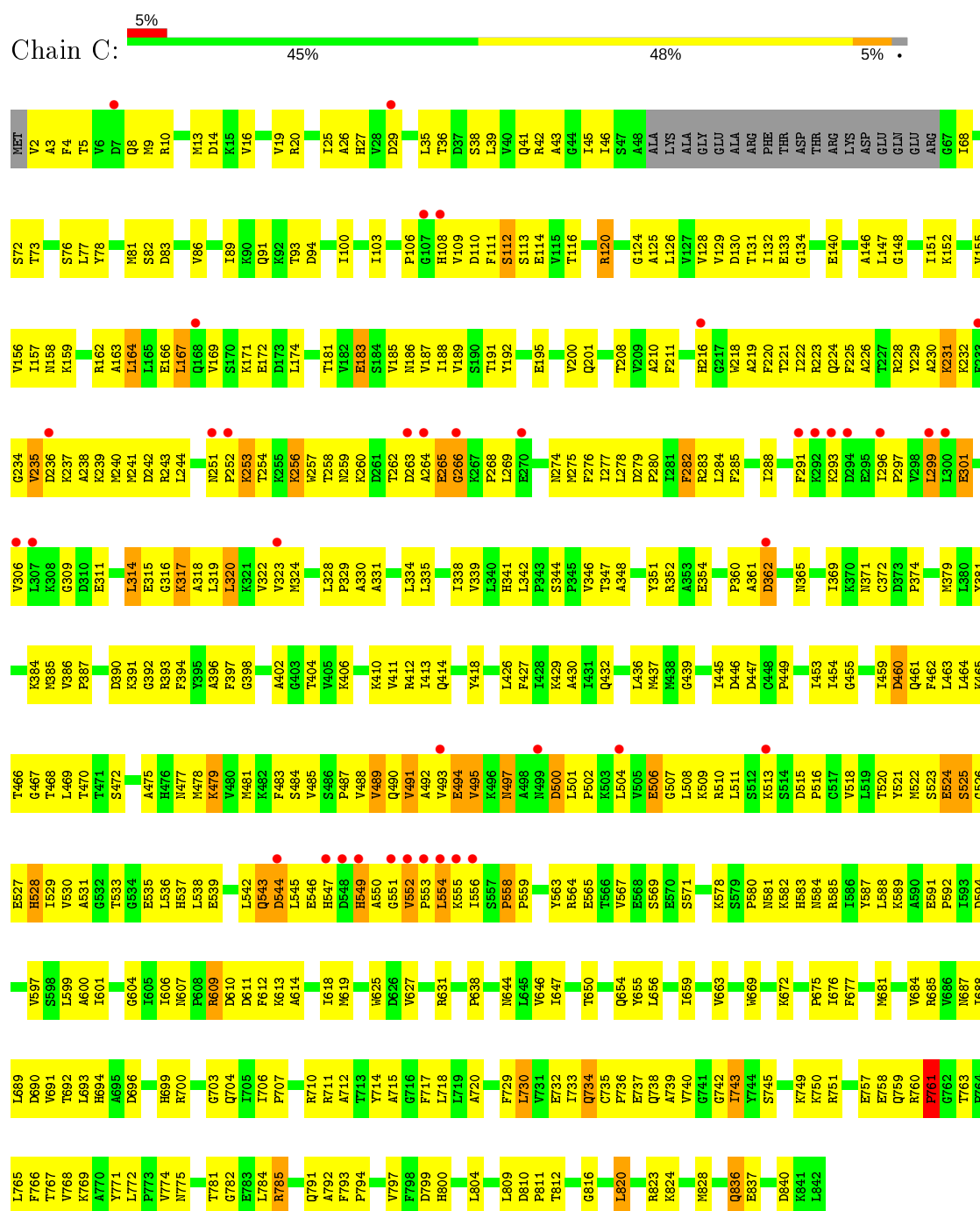
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

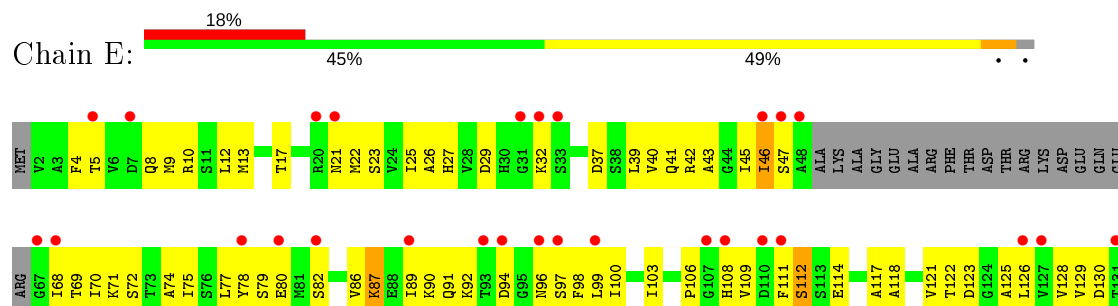
- Molecule 1: Elongation factor 2

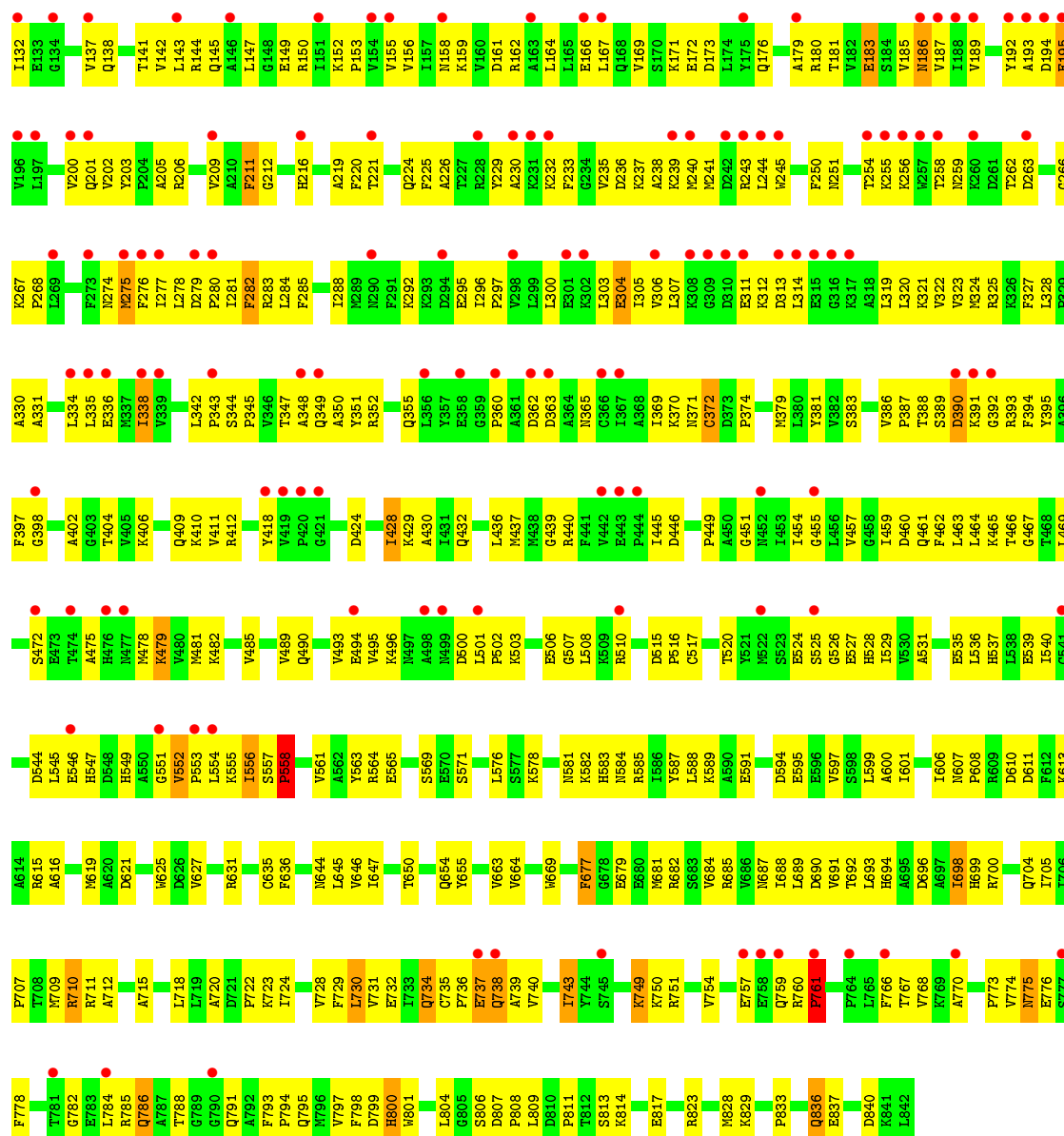


- Molecule 1: Elongation factor 2

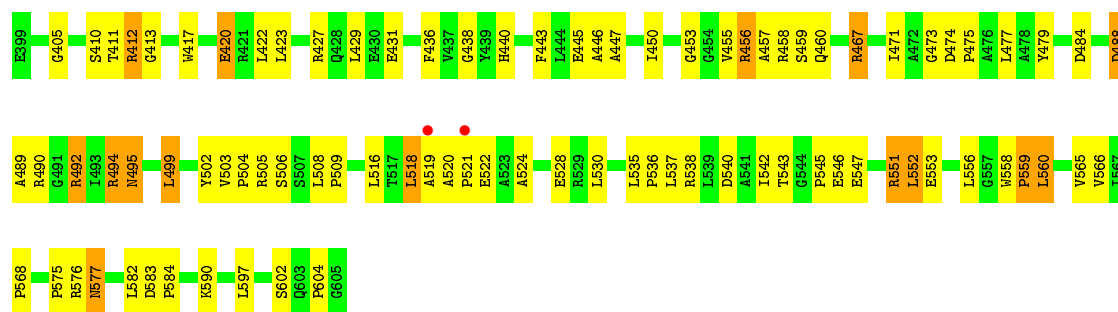


• Molecule 1: Elongation factor 2



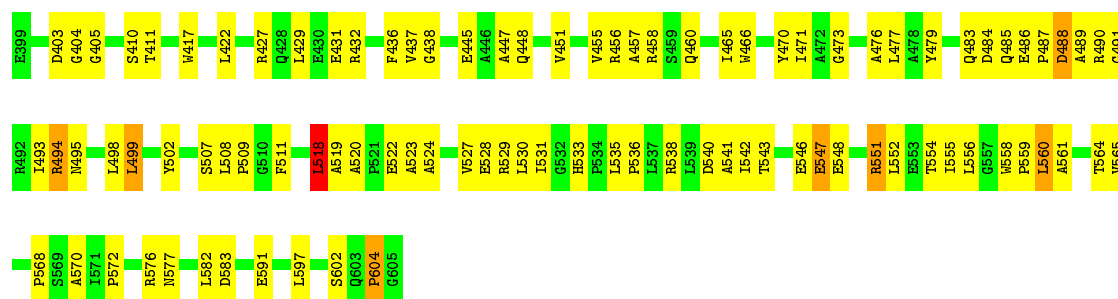


• Molecule 2: exotoxin A



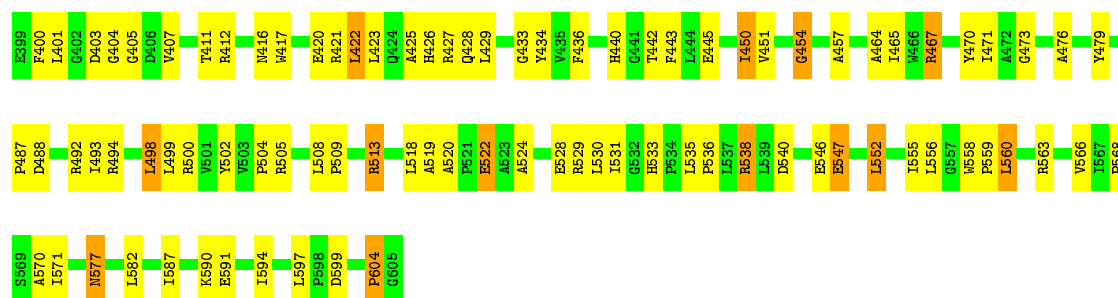
• Molecule 2: exotoxin A

Chain D:  55% 42%



• Molecule 2: exotoxin A

Chain F:  57% 36% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	329.43Å 69.09Å 190.80Å 90.00° 103.46° 90.00°	Depositor
Resolution (Å)	40.00 – 3.07 29.63 – 3.07	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.07) 97.9 (29.63-3.07)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 3.06Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.249 , 0.282 0.240 , 0.265	Depositor DCC
$R_{free}$ test set	1571 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.3	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 54.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	23979	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7793e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality

### 5.1 Standard geometry

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

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	0.47	0/6517	0.68	1/8823 (0.0%)
1	C	0.49	1/6517 (0.0%)	0.71	1/8823 (0.0%)
1	E	0.44	1/6517 (0.0%)	0.65	1/8823 (0.0%)
2	B	0.64	0/1627	0.85	0/2216
2	D	0.66	0/1627	0.83	1/2216 (0.0%)
2	F	0.58	0/1627	0.83	0/2216
All	All	0.50	2/24432 (0.0%)	0.71	4/33117 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	195	GLU	CD-OE1	6.84	1.33	1.25
1	C	543	GLN	CG-CD	6.52	1.66	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	195	GLU	CG-CD-OE2	-7.76	102.77	118.30
1	A	236	ASP	N-CA-C	-5.55	96.01	111.00
1	C	554	LEU	N-CA-C	5.20	125.04	111.00
2	D	518	LEU	N-CA-C	5.04	124.61	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	195	GLU	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	6405	0	6472	345	0
1	C	6405	0	6472	459	0
1	E	6405	0	6472	438	0
2	B	1588	0	1539	84	0
2	D	1588	0	1539	76	0
2	F	1588	0	1539	71	0
All	All	23979	0	24033	1462	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 30.

All (1462) 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:C:391:LYS:HG2	1:C:392:GLY:H	1.13	1.11
1:E:71:LYS:HE3	1:E:387:PRO:HD2	1.32	1.11
1:E:556:ILE:HG22	1:E:557:SER:H	1.10	1.10
1:A:16:VAL:HG13	1:A:345:PRO:HG2	1.33	1.09
1:C:253:LYS:HE3	1:C:253:LYS:HA	1.35	1.06
1:E:552:VAL:HG22	1:E:553:PRO:HD3	1.36	1.05
1:E:68:ILE:HD12	1:E:390:ASP:HB2	1.37	1.03
1:C:231:LYS:HE3	1:C:232:LYS:HG3	1.40	1.02
1:E:10:ARG:HH12	1:E:449:PRO:CD	1.75	0.99
1:C:820:LEU:O	1:C:824:LYS:HG3	1.63	0.98
2:F:546:GLU:HG3	2:F:547:GLU:HG3	1.43	0.97
1:A:16:VAL:CG1	1:A:345:PRO:HG2	1.92	0.97
1:C:404:THR:HG22	1:C:449:PRO:HA	1.43	0.96
1:E:552:VAL:HG22	1:E:553:PRO:CD	1.94	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:GLU:HG3	1:A:766:PHE:CE2	2.01	0.94
1:E:694:HIS:HD2	1:E:696:ASP:H	1.06	0.94
1:C:265:GLU:HG3	1:C:266:GLY:H	1.29	0.94
1:E:535:GLU:OE2	1:E:778:PHE:HA	1.68	0.94
1:C:42:ARG:HG3	1:C:331:ALA:CB	1.98	0.93
1:A:627:VAL:HG12	2:F:405:GLY:HA2	1.51	0.93
1:C:552:VAL:HG22	1:C:553:PRO:CD	1.99	0.93
1:C:784:LEU:HD23	1:C:794:PRO:HG3	1.50	0.92
1:A:533:THR:H	1:A:537:HIS:CD2	1.88	0.92
1:A:533:THR:H	1:A:537:HIS:HD2	1.16	0.91
1:C:578:LYS:HE2	1:C:840:ASP:OD1	1.70	0.91
2:D:546:GLU:HG3	2:D:547:GLU:HG3	1.52	0.91
1:C:256:LYS:HD3	1:C:257:TRP:H	1.36	0.90
1:C:256:LYS:HA	1:C:256:LYS:HE2	1.51	0.90
1:E:91:GLN:HE22	1:E:344:SER:H	1.16	0.90
2:D:520:ALA:HB3	2:D:522:GLU:OE2	1.71	0.90
1:C:836:GLN:HE21	1:C:836:GLN:H	1.20	0.88
1:A:578:LYS:HE3	1:A:840:ASP:OD1	1.73	0.88
1:C:694:HIS:HD2	1:C:696:ASP:H	1.18	0.88
1:E:27:HIS:HD2	1:E:29:ASP:H	1.16	0.88
1:E:45:ILE:HD11	1:E:78:TYR:CB	2.04	0.87
1:A:229:TYR:CE2	1:A:276:PHE:HB3	2.08	0.87
1:C:506:GLU:HG3	1:C:510:ARG:NE	1.88	0.87
1:C:391:LYS:HG2	1:C:392:GLY:N	1.88	0.87
1:C:315:GLU:HA	1:C:319:LEU:HB2	1.56	0.87
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.54	0.87
1:E:45:ILE:HD11	1:E:78:TYR:HB2	1.55	0.87
1:A:404:THR:HG22	1:A:449:PRO:HA	1.55	0.86
1:C:225:PHE:CD2	1:C:277:ILE:HG13	2.11	0.86
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.58	0.85
1:E:147:LEU:HD13	1:E:192:TYR:HB2	1.58	0.85
1:E:404:THR:HG22	1:E:449:PRO:HA	1.56	0.85
1:E:546:GLU:HB3	1:E:554:LEU:HD12	1.56	0.85
1:A:694:HIS:HD2	1:A:696:ASP:H	1.18	0.85
1:A:71:LYS:HB3	1:A:386:VAL:HG23	1.60	0.84
1:E:694:HIS:O	1:E:700:ARG:HD3	1.77	0.84
1:C:545:LEU:O	1:C:550:ALA:HB3	1.77	0.84
1:A:584:ASN:HD22	1:A:693:LEU:HA	1.40	0.84
2:B:552:LEU:HD12	2:B:552:LEU:H	1.43	0.84
2:B:520:ALA:HB3	2:B:522:GLU:OE2	1.77	0.83
1:E:10:ARG:HH12	1:E:449:PRO:HD2	1.40	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:556:ILE:HG22	1:E:557:SER:N	1.92	0.83
2:D:531:ILE:HD11	2:D:533:HIS:O	1.77	0.83
1:E:784:LEU:HD23	1:E:794:PRO:HG3	1.59	0.83
2:D:488:ASP:OD2	2:D:490:ARG:HG2	1.79	0.83
1:C:504:LEU:O	1:C:508:LEU:HG	1.79	0.82
1:E:503:LYS:HB3	1:E:551:GLY:HA3	1.60	0.82
1:E:482:LYS:HD3	1:E:797:VAL:HG11	1.62	0.82
1:C:296:ILE:HD13	1:C:319:LEU:HD21	1.61	0.82
1:E:71:LYS:HE3	1:E:387:PRO:CD	2.09	0.82
1:A:132:ILE:HD12	1:A:162:ARG:HH11	1.44	0.82
1:C:314:LEU:HD11	1:C:318:ALA:HB1	1.62	0.82
1:E:694:HIS:CD2	1:E:696:ASP:H	1.95	0.82
1:A:737:GLU:HG3	1:A:766:PHE:HE2	1.41	0.81
2:D:546:GLU:CG	2:D:547:GLU:HG3	2.09	0.81
1:C:552:VAL:HG22	1:C:553:PRO:HD2	1.61	0.81
1:E:237:LYS:HA	1:E:240:MET:HB3	1.61	0.81
1:E:155:VAL:HG23	1:E:202:VAL:HG11	1.62	0.81
1:C:229:TYR:CE2	1:C:276:PHE:HB3	2.16	0.81
1:E:26:ALA:HB2	1:E:128:VAL:HB	1.61	0.81
1:E:545:LEU:HD12	1:E:549:HIS:HB2	1.62	0.81
1:A:27:HIS:HD2	1:A:29:ASP:H	1.27	0.80
1:A:820:LEU:HD11	1:A:830:GLU:HG2	1.64	0.80
1:A:500:ASP:HB2	1:A:552:VAL:HG11	1.64	0.80
1:A:694:HIS:O	1:A:700:ARG:HD3	1.82	0.80
1:A:132:ILE:HD12	1:A:162:ARG:CD	2.12	0.80
2:D:531:ILE:HD12	2:D:533:HIS:CE1	2.17	0.80
1:C:391:LYS:CG	1:C:392:GLY:H	1.94	0.79
1:E:147:LEU:CD1	1:E:192:TYR:HB2	2.12	0.79
1:C:191:THR:O	1:C:763:THR:HG22	1.80	0.79
1:A:45:ILE:HD12	1:A:76:SER:HB3	1.62	0.79
2:D:417:TRP:CE2	2:D:568:PRO:HB2	2.17	0.79
1:A:140:GLU:HG3	1:A:188:ILE:CD1	2.12	0.79
1:C:591:GLU:O	1:C:685:ARG:HB3	1.81	0.79
1:E:27:HIS:CD2	1:E:29:ASP:H	2.01	0.79
1:E:71:LYS:HB3	1:E:386:VAL:HG23	1.64	0.79
1:E:459:ILE:HG21	1:E:463:LEU:HD12	1.65	0.79
2:B:417:TRP:CE2	2:B:568:PRO:HB2	2.17	0.78
2:D:527:VAL:O	2:D:531:ILE:HG23	1.84	0.78
2:B:552:LEU:HD12	2:B:552:LEU:N	1.97	0.78
1:C:836:GLN:NE2	1:C:836:GLN:H	1.81	0.78
1:E:10:ARG:HH12	1:E:449:PRO:HD3	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:GLN:HG2	1:A:655:TYR:CD2	2.18	0.78
2:D:527:VAL:HG13	2:D:542:ILE:HD12	1.65	0.78
1:C:157:ILE:CD1	1:C:181:THR:HG21	2.14	0.78
1:E:46:ILE:HG22	1:E:47:SER:H	1.49	0.78
2:D:458:ARG:H	2:D:460:GLN:HE21	1.28	0.77
2:F:488:ASP:OD2	2:F:492:ARG:HB2	1.84	0.77
1:A:647:ILE:HG13	1:A:685:ARG:HE	1.49	0.77
1:C:544:ASP:HB3	1:C:549:HIS:CD2	2.20	0.77
1:E:300:LEU:HG	1:E:305:ILE:HB	1.67	0.77
1:C:258:THR:HG22	1:C:260:LYS:H	1.47	0.77
2:F:417:TRP:CE2	2:F:568:PRO:HB2	2.19	0.77
2:F:513:ARG:HH11	2:F:513:ARG:HB2	1.47	0.76
1:C:265:GLU:HG3	1:C:266:GLY:N	1.96	0.76
1:C:659:ILE:O	1:C:663:VAL:HG23	1.84	0.76
1:A:16:VAL:HG13	1:A:345:PRO:CG	2.14	0.76
1:C:2:VAL:HG22	1:C:3:ALA:H	1.51	0.76
1:E:495:VAL:HG12	1:E:554:LEU:HD23	1.67	0.76
1:C:536:LEU:HD12	1:C:537:HIS:N	2.01	0.75
1:E:238:ALA:O	1:E:241:MET:HG2	1.86	0.75
1:E:694:HIS:HD2	1:E:696:ASP:N	1.83	0.75
1:A:465:LYS:HD2	1:A:517:CYS:SG	2.27	0.75
1:E:581:ASN:HD21	1:E:704:GLN:HG3	1.52	0.75
1:C:584:ASN:HD22	1:C:693:LEU:HA	1.52	0.75
1:C:552:VAL:HG22	1:C:553:PRO:HD3	1.65	0.74
1:E:334:LEU:O	1:E:338:ILE:HG12	1.86	0.74
1:C:229:TYR:CZ	1:C:276:PHE:HB3	2.22	0.74
1:E:152:LYS:HD2	1:E:200:VAL:CG2	2.17	0.74
1:E:152:LYS:HD2	1:E:200:VAL:HG23	1.69	0.74
1:A:454:ILE:HG13	1:A:455:GLY:H	1.53	0.74
1:A:533:THR:N	1:A:537:HIS:HD2	1.85	0.74
1:C:27:HIS:HD2	1:C:29:ASP:H	1.33	0.74
1:E:556:ILE:CG2	1:E:557:SER:H	1.94	0.74
1:A:140:GLU:HG3	1:A:188:ILE:HD13	1.68	0.74
1:A:321:LYS:O	1:A:325:ARG:HG3	1.86	0.74
1:C:251:ASN:HB2	1:C:254:THR:OG1	1.88	0.74
1:C:584:ASN:HD21	1:C:694:HIS:H	1.32	0.74
1:E:546:GLU:HG3	1:E:547:HIS:CD2	2.23	0.74
1:C:494:GLU:O	1:C:555:LYS:HB3	1.87	0.74
1:A:235:VAL:HG21	1:A:240:MET:HB2	1.69	0.74
1:C:810:ASP:OD1	1:C:812:THR:HG22	1.88	0.74
1:E:338:ILE:HG23	1:E:342:LEU:HD12	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ILE:HD12	1:A:162:ARG:HD3	1.70	0.74
1:C:316:GLY:N	1:C:319:LEU:HB2	2.02	0.74
1:C:533:THR:H	1:C:537:HIS:CD2	2.05	0.74
1:C:611:ASP:OD2	1:C:613:LYS:HB2	1.88	0.74
2:D:427:ARG:O	2:D:431:GLU:HG3	1.86	0.74
1:A:500:ASP:CB	1:A:552:VAL:HG11	2.18	0.73
1:E:734:GLN:N	1:E:734:GLN:HE21	1.86	0.73
1:E:26:ALA:CB	1:E:128:VAL:HB	2.17	0.73
1:A:561:VAL:HG21	1:A:775:ASN:HA	1.68	0.73
1:A:836:GLN:HE21	1:A:836:GLN:H	1.34	0.73
2:B:495:ASN:N	2:B:495:ASN:HD22	1.84	0.73
1:C:2:VAL:HG22	1:C:3:ALA:N	2.02	0.73
1:E:158:ASN:ND2	1:E:159:LYS:HG3	2.04	0.73
2:F:487:PRO:HA	2:F:492:ARG:O	1.89	0.73
2:B:427:ARG:O	2:B:431:GLU:HG3	1.88	0.73
1:E:500:ASP:OD2	1:E:552:VAL:HG21	1.87	0.73
1:C:472:SER:HB3	1:C:475:ALA:HB2	1.71	0.72
1:C:523:SER:OG	1:C:527:GLU:HB2	1.88	0.72
1:E:74:ALA:O	1:E:439:GLY:HA2	1.89	0.72
1:A:584:ASN:HD21	1:A:694:HIS:H	1.37	0.72
2:B:477:LEU:HD13	2:B:551:ARG:NH1	2.03	0.72
1:A:464:LEU:HD21	1:A:485:VAL:HB	1.72	0.72
1:C:243:ARG:NH1	1:C:257:TRP:CG	2.57	0.72
1:A:581:ASN:ND2	1:A:704:GLN:HG3	2.03	0.72
1:C:140:GLU:HG3	1:C:188:ILE:CD1	2.19	0.72
1:E:379:MET:HB2	1:E:402:ALA:HB3	1.72	0.72
1:C:25:ILE:HD12	1:C:125:ALA:HB1	1.71	0.72
1:E:69:THR:OG1	1:E:389:SER:HB3	1.90	0.72
1:E:236:ASP:OD1	1:E:238:ALA:HB3	1.90	0.71
1:E:581:ASN:ND2	1:E:704:GLN:HG3	2.05	0.71
1:A:627:VAL:CG1	2:F:405:GLY:HA2	2.20	0.71
1:A:27:HIS:CD2	1:A:29:ASP:H	2.09	0.71
2:B:455:VAL:O	2:B:456:ARG:HD2	1.91	0.71
1:E:288:ILE:HG23	1:E:319:LEU:HD23	1.72	0.71
1:E:87:LYS:CE	1:E:87:LYS:HA	2.20	0.71
1:C:454:ILE:HG13	1:C:455:GLY:H	1.54	0.71
1:C:694:HIS:O	1:C:700:ARG:HD3	1.91	0.71
1:A:32:LYS:NZ	1:A:105:SER:HB2	2.06	0.71
1:C:171:LYS:HG2	1:C:282:PHE:CD1	2.25	0.71
1:E:155:VAL:HG21	1:E:202:VAL:HG21	1.72	0.71
1:C:183:GLU:O	1:C:187:VAL:HG23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:552:VAL:CG2	1:E:553:PRO:HD3	2.19	0.70
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.71	0.70
1:E:279:ASP:HB3	1:E:280:PRO:HD3	1.73	0.70
1:E:503:LYS:HB3	1:E:551:GLY:CA	2.22	0.70
1:C:158:ASN:ND2	1:C:159:LYS:HG2	2.06	0.70
1:C:484:SER:HB3	1:C:797:VAL:CG2	2.21	0.70
2:B:455:VAL:C	2:B:456:ARG:HD2	2.12	0.70
1:E:338:ILE:O	1:E:342:LEU:HB2	1.92	0.70
2:D:556:LEU:HD22	2:D:560:LEU:HD13	1.74	0.70
1:A:25:ILE:HD12	1:A:125:ALA:HB1	1.74	0.69
1:A:607:ASN:OD1	1:A:609:ARG:HG3	1.91	0.69
1:A:410:LYS:HA	1:A:430:ALA:HA	1.73	0.69
1:E:87:LYS:HE2	1:E:87:LYS:HA	1.73	0.69
1:C:263:ASP:O	1:C:265:GLU:N	2.25	0.69
1:E:331:ALA:O	1:E:335:LEU:HG	1.92	0.69
1:C:584:ASN:ND2	1:C:694:HIS:H	1.90	0.69
1:C:694:HIS:CD2	1:C:696:ASP:H	2.08	0.69
1:E:77:LEU:HB2	1:E:100:ILE:HB	1.74	0.69
1:A:35:LEU:HD22	1:A:334:LEU:HD11	1.75	0.69
1:E:496:LYS:HD3	1:E:555:LYS:HE2	1.74	0.69
2:D:477:LEU:HB2	2:D:551:ARG:HD2	1.75	0.69
1:C:166:GLU:HB3	1:C:167:LEU:HD12	1.73	0.69
1:C:140:GLU:HG3	1:C:188:ILE:HD13	1.74	0.69
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.74	0.69
1:E:464:LEU:HD21	1:E:485:VAL:HB	1.75	0.69
1:A:565:GLU:HG2	1:A:676:ILE:HD12	1.75	0.69
1:E:607:ASN:HB3	1:E:610:ASP:OD2	1.93	0.69
1:E:737:GLU:HG3	1:E:766:PHE:CE1	2.28	0.68
1:E:141:THR:HA	1:E:144:ARG:NH2	2.08	0.68
1:A:433:ARG:HH21	1:A:444:PRO:HB3	1.58	0.68
1:E:185:VAL:O	1:E:189:VAL:HG23	1.93	0.68
1:E:465:LYS:HD2	1:E:517:CYS:SG	2.32	0.68
1:A:277:ILE:O	1:A:280:PRO:HD2	1.93	0.68
1:C:501:LEU:C	1:C:501:LEU:HD23	2.14	0.68
2:D:473:GLY:HA3	2:D:597:LEU:HD11	1.76	0.68
1:C:253:LYS:HE3	1:C:253:LYS:CA	2.20	0.68
1:C:506:GLU:HG3	1:C:510:ARG:CZ	2.23	0.68
1:C:533:THR:H	1:C:537:HIS:HD2	1.42	0.68
1:C:734:GLN:HE21	1:C:734:GLN:N	1.92	0.68
1:A:260:LYS:HE3	1:A:262:THR:O	1.93	0.67
1:A:459:ILE:HG21	1:A:463:LEU:HD12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ARG:HD3	1:C:445:ILE:HD11	1.76	0.67
1:E:836:GLN:NE2	1:E:836:GLN:H	1.91	0.67
1:A:836:GLN:NE2	1:A:836:GLN:H	1.92	0.67
1:E:578:LYS:HE2	1:E:840:ASP:OD1	1.95	0.67
2:F:552:LEU:HD12	2:F:552:LEU:N	2.09	0.67
1:A:169:VAL:HG22	1:A:173:ASP:HB2	1.76	0.67
1:C:189:VAL:CG1	1:C:200:VAL:HG12	2.24	0.67
1:E:589:LYS:HE3	1:E:689:LEU:HD11	1.76	0.67
1:E:75:ILE:HD13	1:E:439:GLY:CA	2.24	0.67
1:E:490:GLN:HB3	1:E:531:ALA:HB2	1.76	0.67
1:A:132:ILE:CD1	1:A:162:ARG:HD3	2.25	0.67
1:A:588:LEU:HD12	1:A:588:LEU:C	2.15	0.67
1:A:591:GLU:O	1:A:685:ARG:HB3	1.94	0.67
1:E:496:LYS:HB2	1:E:555:LYS:HZ3	1.60	0.67
1:C:110:ASP:OD1	1:C:781:THR:HG21	1.95	0.67
1:E:836:GLN:HE21	1:E:836:GLN:H	1.42	0.66
1:C:103:ILE:HD11	1:C:453:ILE:HG12	1.78	0.66
2:B:467:ARG:HG3	2:B:558:TRP:CD1	2.31	0.66
1:C:166:GLU:C	1:C:167:LEU:HD12	2.14	0.66
1:C:535:GLU:O	1:C:539:GLU:HG3	1.95	0.66
1:C:45:ILE:HD11	1:C:78:TYR:CB	2.25	0.66
2:D:486:GLU:OE1	2:D:487:PRO:HD2	1.95	0.66
1:E:91:GLN:NE2	1:E:344:SER:H	1.92	0.66
1:A:584:ASN:ND2	1:A:694:HIS:H	1.93	0.66
1:C:192:TYR:HA	1:C:763:THR:HG21	1.78	0.66
1:C:315:GLU:CA	1:C:319:LEU:HB2	2.25	0.66
1:C:109:VAL:HG13	1:C:793:PHE:HE1	1.59	0.66
1:C:234:GLY:O	1:C:235:VAL:HG23	1.95	0.66
1:C:256:LYS:HA	1:C:256:LYS:CE	2.25	0.66
1:C:565:GLU:O	1:C:681:MET:HA	1.95	0.66
1:E:226:ALA:O	1:E:230:ALA:HB2	1.96	0.66
1:E:321:LYS:O	1:E:325:ARG:HG3	1.95	0.66
1:E:565:GLU:O	1:E:681:MET:HA	1.96	0.66
1:A:288:ILE:HG23	1:A:319:LEU:HD23	1.77	0.66
1:C:320:LEU:HD12	1:C:324:MET:HG3	1.77	0.66
1:E:142:VAL:O	1:E:145:GLN:HB2	1.96	0.66
1:A:392:GLY:HA2	1:A:513:LYS:HE2	1.76	0.66
2:B:417:TRP:NE1	2:B:568:PRO:HB2	2.10	0.66
1:E:584:ASN:ND2	1:E:694:HIS:H	1.93	0.66
1:C:288:ILE:HG23	1:C:319:LEU:HD23	1.77	0.65
1:A:644:ASN:HD22	1:A:684:VAL:HB	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:654:GLN:HG2	1:E:655:TYR:CD2	2.31	0.65
1:E:87:LYS:HE2	1:E:87:LYS:CA	2.26	0.65
2:F:465:ILE:HD12	2:F:535:LEU:HD12	1.77	0.65
1:A:581:ASN:ND2	1:A:699:DDE:O	2.28	0.65
1:C:162:ARG:HD2	1:C:166:GLU:OE2	1.97	0.65
1:C:703:GLY:HA2	2:D:493:ILE:HD13	1.78	0.65
1:E:536:LEU:HD11	1:E:540:ILE:HD11	1.77	0.65
1:E:279:ASP:O	1:E:283:ARG:HG2	1.97	0.65
1:E:45:ILE:HD11	1:E:78:TYR:HB3	1.78	0.65
1:A:258:THR:HG22	1:A:259:ASN:N	2.12	0.65
2:B:490:ARG:N	2:B:490:ARG:HD2	2.12	0.65
2:B:537:LEU:O	2:B:538:ARG:HD3	1.96	0.65
1:C:284:LEU:O	1:C:288:ILE:HB	1.97	0.65
1:E:292:LYS:HD3	1:E:295:GLU:OE2	1.96	0.64
1:A:220:PHE:HB3	1:A:328:LEU:HD13	1.78	0.64
1:C:243:ARG:NH1	1:C:257:TRP:CD1	2.65	0.64
1:A:373:ASP:OD2	1:A:376:ALA:HB2	1.98	0.64
1:E:211:PHE:HD2	1:E:220:PHE:CE1	2.15	0.64
1:C:685:ARG:HE	1:C:687:ASN:HD21	1.46	0.64
1:E:757:GLU:HG3	1:E:768:VAL:HG22	1.78	0.64
1:A:7:ASP:HA	1:A:10:ARG:HG2	1.79	0.64
1:A:103:ILE:HD11	1:A:453:ILE:HG12	1.80	0.64
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.78	0.64
1:C:588:LEU:C	1:C:588:LEU:HD12	2.18	0.64
1:E:391:LYS:HB3	1:E:393:ARG:HG2	1.80	0.64
1:C:166:GLU:HB3	1:C:167:LEU:CD1	2.28	0.64
1:C:509:LYS:HD2	1:C:509:LYS:N	2.11	0.64
1:C:545:LEU:O	1:C:550:ALA:CB	2.45	0.64
1:C:581:ASN:O	1:C:582:LYS:HB2	1.98	0.64
1:E:736:PRO:HB2	1:E:738:GLN:HG2	1.78	0.64
1:C:285:PHE:HE2	1:C:324:MET:SD	2.21	0.64
1:C:491:VAL:O	1:C:529:ILE:HA	1.97	0.64
1:C:492:ALA:HA	1:C:528:HIS:O	1.97	0.64
1:E:281:ILE:HG12	1:E:327:PHE:HE2	1.63	0.63
1:E:584:ASN:HD21	1:E:694:HIS:H	1.45	0.63
1:A:348:ALA:HA	1:A:351:TYR:CE2	2.33	0.63
1:C:157:ILE:HD12	1:C:181:THR:HG21	1.79	0.63
1:C:316:GLY:N	1:C:319:LEU:CB	2.61	0.63
1:C:757:GLU:HG3	1:C:768:VAL:HG22	1.79	0.63
1:C:192:TYR:HA	1:C:763:THR:CG2	2.29	0.63
1:A:580:PRO:O	1:A:582:LYS:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:LYS:HA	1:C:430:ALA:HA	1.81	0.63
1:A:454:ILE:HG13	1:A:455:GLY:N	2.11	0.63
1:C:239:LYS:O	1:C:243:ARG:HG3	1.99	0.63
1:A:222:ILE:HG22	1:A:241:MET:HB2	1.80	0.63
1:C:38:SER:HA	1:C:41:GLN:HG2	1.80	0.63
1:A:589:LYS:HE3	1:A:689:LEU:HD11	1.80	0.63
1:E:166:GLU:HB3	1:E:167:LEU:HD12	1.81	0.63
1:E:186:ASN:CG	1:E:201:GLN:HE21	2.03	0.62
1:A:719:LEU:HD21	1:A:835:TRP:CD2	2.35	0.62
1:C:220:PHE:HA	1:C:224:GLN:OE1	1.98	0.62
1:A:251:ASN:HB3	1:A:254:THR:OG1	1.99	0.62
2:B:524:ALA:O	2:B:528:GLU:HG3	1.99	0.62
1:E:75:ILE:HD13	1:E:439:GLY:HA3	1.81	0.62
1:E:495:VAL:CG1	1:E:554:LEU:HD23	2.28	0.62
1:A:568:GLU:HB3	1:A:721:ASP:OD2	1.99	0.62
1:C:256:LYS:HD3	1:C:257:TRP:N	2.11	0.62
1:E:704:GLN:O	1:E:707:PRO:HD2	1.99	0.62
1:C:157:ILE:HD11	1:C:181:THR:HG21	1.82	0.62
1:E:588:LEU:HD12	1:E:588:LEU:C	2.19	0.62
1:C:231:LYS:HE3	1:C:232:LYS:CG	2.23	0.62
1:C:277:ILE:O	1:C:280:PRO:HD2	1.99	0.62
1:E:307:LEU:HD13	1:E:312:LYS:HA	1.82	0.62
2:B:551:ARG:HH11	2:B:551:ARG:HG3	1.65	0.62
1:C:784:LEU:HD23	1:C:794:PRO:CG	2.26	0.62
1:E:635:CYS:SG	1:E:664:VAL:HG13	2.40	0.62
1:A:694:HIS:CD2	1:A:696:ASP:H	2.09	0.62
1:A:581:ASN:HD21	1:A:704:GLN:HG3	1.64	0.62
1:C:522:MET:HA	1:C:527:GLU:O	2.00	0.62
1:E:311:GLU:HB3	1:E:322:VAL:HG11	1.82	0.62
2:F:524:ALA:O	2:F:528:GLU:HG3	1.98	0.62
1:A:183:GLU:O	1:A:187:VAL:HG23	1.99	0.61
1:A:647:ILE:HG13	1:A:685:ARG:NE	2.13	0.61
2:B:440:HIS:HB2	2:B:471:ILE:HG22	1.82	0.61
1:A:2:VAL:HG22	1:A:3:ALA:N	2.14	0.61
1:A:32:LYS:HZ1	1:A:105:SER:HB2	1.63	0.61
2:B:495:ASN:ND2	2:B:495:ASN:H	1.97	0.61
1:E:285:PHE:CE2	1:E:320:LEU:HD11	2.35	0.61
1:A:321:LYS:NZ	1:A:325:ARG:HD3	2.15	0.61
1:A:591:GLU:HG2	1:A:685:ARG:HG2	1.81	0.61
1:C:354:GLU:OE2	1:C:361:ALA:HB1	2.00	0.61
1:C:4:PHE:HD1	1:C:8:GLN:OE1	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:496:LYS:HD3	1:E:555:LYS:CE	2.30	0.61
1:C:348:ALA:HA	1:C:351:TYR:CE2	2.35	0.61
1:E:472:SER:HB3	1:E:475:ALA:HB2	1.80	0.61
1:E:203:TYR:HD2	1:E:206:ARG:HD2	1.64	0.61
1:E:91:GLN:HE22	1:E:344:SER:N	1.94	0.61
1:A:391:LYS:HG3	1:A:392:GLY:H	1.65	0.61
1:C:316:GLY:H	1:C:319:LEU:HB2	1.64	0.61
1:E:132:ILE:N	1:E:132:ILE:HD12	2.15	0.61
1:E:89:ILE:C	1:E:91:GLN:H	2.03	0.61
1:C:288:ILE:HG23	1:C:319:LEU:CD2	2.31	0.61
1:C:72:SER:HA	1:C:439:GLY:O	2.00	0.61
1:E:759:GLN:HB2	1:E:766:PHE:CE2	2.35	0.61
1:A:186:ASN:HB3	1:A:201:GLN:HG2	1.81	0.61
1:A:30:HIS:HA	1:A:159:LYS:CE	2.31	0.61
1:E:591:GLU:O	1:E:685:ARG:HB3	2.01	0.61
1:A:594:ASP:HB2	1:A:597:VAL:HG23	1.83	0.61
2:D:417:TRP:NE1	2:D:568:PRO:HB2	2.15	0.61
1:E:78:TYR:HE1	1:E:97:SER:HB3	1.65	0.61
1:A:411:VAL:HG12	1:A:412:ARG:N	2.15	0.60
1:C:5:THR:OG1	1:C:8:GLN:HG3	2.00	0.60
1:E:552:VAL:HG22	1:E:553:PRO:HD2	1.82	0.60
2:B:457:ALA:HB2	2:B:558:TRP:CD2	2.36	0.60
1:E:412:ARG:HH12	1:E:428:ILE:HD11	1.66	0.60
1:C:707:PRO:O	1:C:711:ARG:HG3	2.00	0.60
1:E:211:PHE:CD2	1:E:220:PHE:CE1	2.89	0.60
1:E:536:LEU:O	1:E:539:GLU:N	2.34	0.60
1:A:823:ARG:NH1	1:A:829:LYS:O	2.34	0.60
1:A:501:LEU:HB3	1:A:502:PRO:HD3	1.84	0.60
1:A:485:VAL:O	1:A:487:PRO:HD3	2.01	0.60
1:C:221:THR:OG1	1:C:224:GLN:HG3	2.01	0.60
1:E:69:THR:O	1:E:389:SER:N	2.34	0.60
1:E:728:VAL:HB	1:E:800:HIS:CD2	2.36	0.60
1:E:381:TYR:O	1:E:398:GLY:HA3	2.01	0.60
1:A:186:ASN:HB3	1:A:201:GLN:HE21	1.67	0.60
1:C:591:GLU:CG	1:C:685:ARG:HG2	2.32	0.60
1:E:126:LEU:HD11	1:E:156:VAL:CG2	2.32	0.60
1:E:43:ALA:HB1	1:E:78:TYR:O	2.02	0.60
1:A:172:GLU:OE2	1:A:271:ARG:NH2	2.35	0.60
1:A:459:ILE:HD11	1:A:469:LEU:HD21	1.84	0.60
1:C:171:LYS:HG2	1:C:282:PHE:CE1	2.37	0.60
1:C:384:LYS:HB2	1:C:465:LYS:NZ	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ALA:HA	1:C:46:ILE:O	2.02	0.60
1:E:221:THR:OG1	1:E:224:GLN:HG3	2.02	0.60
1:C:500:ASP:OD2	1:C:552:VAL:HG21	2.02	0.59
2:D:477:LEU:HD13	2:D:551:ARG:NH1	2.17	0.59
2:D:551:ARG:HG3	2:D:551:ARG:HH11	1.67	0.59
1:A:690:ASP:OD1	1:A:691:VAL:N	2.30	0.59
1:A:544:ASP:O	1:A:549:HIS:HD2	1.85	0.59
1:C:581:ASN:ND2	1:C:699:DDE:O	2.35	0.59
1:C:581:ASN:HB3	1:C:583:HIS:HB2	1.84	0.59
1:E:730:LEU:HB2	1:E:799:ASP:HB2	1.84	0.59
1:A:258:THR:HG22	1:A:259:ASN:H	1.67	0.59
1:E:212:GLY:HA3	1:E:219:ALA:HA	1.84	0.59
1:E:303:LEU:O	1:E:304:GLU:HB2	2.03	0.59
1:A:321:LYS:HZ2	1:A:325:ARG:HD3	1.67	0.59
2:D:455:VAL:O	2:D:456:ARG:HG3	2.03	0.59
1:E:176:GLN:O	1:E:180:ARG:HG3	2.02	0.59
1:E:71:LYS:O	1:E:386:VAL:HG21	2.03	0.59
1:A:545:LEU:HD12	1:A:549:HIS:HB2	1.84	0.59
1:A:591:GLU:CG	1:A:685:ARG:HG2	2.32	0.59
1:C:316:GLY:H	1:C:319:LEU:CB	2.15	0.59
1:C:404:THR:HG22	1:C:449:PRO:CA	2.27	0.59
1:C:685:ARG:NE	1:C:687:ASN:HD21	1.99	0.59
1:C:784:LEU:CD2	1:C:794:PRO:HG3	2.26	0.59
1:E:690:ASP:OD1	1:E:691:VAL:N	2.35	0.59
1:C:644:ASN:ND2	1:C:684:VAL:H	2.00	0.59
1:E:10:ARG:NH1	1:E:449:PRO:HD3	2.16	0.59
1:E:581:ASN:O	1:E:582:LYS:HB2	2.01	0.59
1:A:258:THR:HG22	1:A:260:LYS:H	1.67	0.59
1:A:381:TYR:O	1:A:398:GLY:HA3	2.02	0.59
1:C:497:ASN:N	1:C:497:ASN:ND2	2.50	0.59
2:B:551:ARG:NH1	2:B:551:ARG:HG3	2.17	0.59
1:C:35:LEU:HD22	1:C:334:LEU:HD11	1.84	0.59
1:E:255:LYS:O	1:E:256:LYS:HG2	2.03	0.59
1:E:410:LYS:HA	1:E:430:ALA:HA	1.84	0.59
1:A:30:HIS:HA	1:A:159:LYS:HE3	1.84	0.58
1:C:454:ILE:HG13	1:C:455:GLY:N	2.18	0.58
1:E:183:GLU:OE1	1:E:186:ASN:ND2	2.36	0.58
2:B:420:GLU:N	2:B:420:GLU:OE1	2.35	0.58
1:C:10:ARG:NH2	1:C:449:PRO:HD3	2.18	0.58
1:E:219:ALA:HB3	1:E:330:ALA:HA	1.85	0.58
1:A:406:LYS:O	1:A:409:GLN:HB3	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:THR:HG22	1:E:259:ASN:H	1.68	0.58
1:C:226:ALA:O	1:C:230:ALA:HB2	2.04	0.58
1:C:614:ALA:O	1:C:618:ILE:HG12	2.03	0.58
1:C:258:THR:HG22	1:C:259:ASN:N	2.18	0.58
1:C:314:LEU:HD21	1:C:318:ALA:O	2.03	0.58
1:C:654:GLN:HG2	1:C:655:TYR:CD2	2.38	0.58
1:A:520:THR:HA	1:A:529:ILE:O	2.03	0.58
1:A:758:GLU:O	1:A:766:PHE:HD1	1.86	0.58
1:A:763:THR:HB	1:A:764:PRO:HD2	1.84	0.58
2:B:477:LEU:HD22	2:B:551:ARG:HB2	1.86	0.58
1:C:9:MET:O	1:C:13:MET:HG3	2.04	0.58
1:C:515:ASP:HB3	1:C:518:VAL:HG12	1.86	0.58
1:C:236:ASP:OD2	1:C:239:LYS:HE2	2.04	0.57
1:E:391:LYS:HG3	1:E:392:GLY:H	1.69	0.57
1:A:561:VAL:HG21	1:A:775:ASN:CA	2.34	0.57
1:C:529:ILE:N	1:C:529:ILE:HD12	2.19	0.57
2:F:520:ALA:HB1	2:F:522:GLU:OE2	2.05	0.57
1:E:685:ARG:HE	1:E:687:ASN:HD21	1.53	0.57
1:E:145:GLN:NE2	1:E:793:PHE:CZ	2.72	0.57
1:E:126:LEU:HD11	1:E:156:VAL:HG21	1.86	0.57
1:C:414:GLN:HB3	1:C:418:TYR:CD2	2.39	0.57
1:E:412:ARG:HG2	1:E:412:ARG:HH11	1.69	0.57
2:F:433:GLY:O	2:F:505:ARG:HB2	2.04	0.57
1:A:7:ASP:O	1:A:10:ARG:HG2	2.05	0.57
1:A:132:ILE:HD12	1:A:162:ARG:HD2	1.84	0.57
1:A:493:VAL:HG12	1:A:554:LEU:HD22	1.86	0.57
1:E:561:VAL:HG21	1:E:775:ASN:CB	2.34	0.57
2:D:445:GLU:OE1	2:D:494:ARG:NH2	2.38	0.57
1:A:784:LEU:HD23	1:A:794:PRO:HG3	1.86	0.57
1:C:644:ASN:HD22	1:C:684:VAL:H	1.53	0.57
1:E:284:LEU:HD13	1:E:324:MET:HE3	1.87	0.57
1:E:365:ASN:O	1:E:369:ILE:HG12	2.05	0.57
1:E:556:ILE:HD12	1:E:556:ILE:N	2.20	0.57
1:E:736:PRO:HB2	1:E:738:GLN:CG	2.35	0.57
1:C:251:ASN:OD1	1:C:269:LEU:HD11	2.05	0.57
1:C:509:LYS:O	1:C:513:LYS:HE3	2.05	0.57
1:E:591:GLU:CG	1:E:685:ARG:HG2	2.35	0.57
1:C:231:LYS:HG2	1:C:232:LYS:N	2.19	0.56
1:C:546:GLU:HG3	1:C:553:PRO:HA	1.87	0.56
1:C:627:VAL:HG21	1:C:631:ARG:NH2	2.20	0.56
1:E:258:THR:HG22	1:E:259:ASN:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:TYR:CE1	1:A:529:ILE:HD12	2.40	0.56
1:C:732:GLU:OE1	1:C:769:LYS:HE3	2.04	0.56
1:C:594:ASP:HB2	1:C:597:VAL:HG23	1.87	0.56
2:D:438:GLY:HA3	2:D:471:ILE:HD12	1.86	0.56
1:E:71:LYS:HB3	1:E:386:VAL:CG2	2.33	0.56
1:C:220:PHE:HB3	1:C:328:LEU:HD13	1.87	0.56
1:C:497:ASN:N	1:C:497:ASN:HD22	2.04	0.56
1:C:493:VAL:HG21	1:C:545:LEU:HD21	1.86	0.56
1:E:749:LYS:O	1:E:750:LYS:HD2	2.05	0.56
1:A:156:VAL:HG21	1:A:334:LEU:CD2	2.35	0.56
1:A:156:VAL:HG21	1:A:334:LEU:HD22	1.88	0.56
1:A:647:ILE:HB	1:A:687:ASN:HD22	1.70	0.56
2:B:484:ASP:OD2	2:B:494:ARG:HG2	2.05	0.56
1:C:155:VAL:HG12	1:C:156:VAL:N	2.19	0.56
1:C:251:ASN:H	1:C:251:ASN:HD22	1.54	0.56
1:C:494:GLU:OE1	1:C:494:GLU:HA	2.04	0.56
1:C:550:ALA:O	1:C:552:VAL:N	2.38	0.56
1:C:730:LEU:HB2	1:C:799:ASP:HB2	1.86	0.56
1:E:722:PRO:O	1:E:723:LYS:HD2	2.04	0.56
1:A:162:ARG:O	1:A:166:GLU:HB2	2.06	0.56
1:A:550:ALA:O	1:A:552:VAL:HG23	2.05	0.56
2:F:488:ASP:OD2	2:F:492:ARG:HD3	2.05	0.56
1:A:111:PHE:HB3	1:A:114:GLU:HG2	1.87	0.56
2:D:432:ARG:HA	2:D:432:ARG:CZ	2.35	0.56
1:E:37:ASP:O	1:E:41:GLN:HG3	2.05	0.56
1:A:734:GLN:HE21	1:A:734:GLN:N	2.04	0.56
1:E:225:PHE:CD2	1:E:277:ILE:HD12	2.41	0.56
1:E:158:ASN:HD22	1:E:159:LYS:HG3	1.70	0.56
2:F:473:GLY:HA3	2:F:597:LEU:HD11	1.88	0.56
1:C:240:MET:O	1:C:244:LEU:HG	2.05	0.56
1:C:484:SER:HB3	1:C:797:VAL:HG22	1.88	0.56
2:B:405:GLY:HA2	1:C:627:VAL:HG12	1.88	0.56
1:E:240:MET:O	1:E:244:LEU:HG	2.05	0.56
1:C:42:ARG:HG3	1:C:331:ALA:HB3	1.85	0.56
1:A:220:PHE:HA	1:A:224:GLN:OE1	2.04	0.55
1:C:538:LEU:O	1:C:542:LEU:HG	2.06	0.55
1:A:486:SER:O	1:A:488:VAL:HG13	2.05	0.55
1:E:114:GLU:O	1:E:117:ALA:HB3	2.06	0.55
1:E:432:GLN:HB2	1:E:457:VAL:O	2.06	0.55
1:E:707:PRO:O	1:E:711:ARG:HG3	2.06	0.55
1:A:172:GLU:HA	1:A:274:ASN:HD21	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:ASN:N	2:B:495:ASN:ND2	2.47	0.55
1:E:150:ARG:CZ	1:E:355:GLN:OE1	2.55	0.55
1:C:27:HIS:CD2	1:C:29:ASP:H	2.20	0.55
1:C:607:ASN:HB3	1:C:610:ASP:CG	2.26	0.55
1:E:26:ALA:O	1:E:32:LYS:HD2	2.06	0.55
1:A:140:GLU:HG3	1:A:188:ILE:HD11	1.85	0.55
2:B:495:ASN:HD22	2:B:495:ASN:H	1.53	0.55
1:C:155:VAL:HG21	1:C:185:VAL:HG11	1.88	0.55
1:C:675:PRO:HD3	1:C:714:TYR:CE1	2.41	0.55
1:A:229:TYR:HE2	1:A:276:PHE:HB3	1.68	0.55
1:A:3:ALA:HA	1:A:46:ILE:O	2.07	0.55
1:A:4:PHE:HA	1:A:8:GLN:OE1	2.07	0.55
1:A:820:LEU:CD1	1:A:830:GLU:HG2	2.34	0.55
2:B:518:LEU:H	2:B:518:LEU:HD22	1.72	0.55
1:C:563:TYR:O	1:C:564:ARG:HD2	2.07	0.55
1:C:585:ARG:HD2	1:C:692:THR:OG1	2.07	0.55
1:C:89:ILE:HG22	1:C:91:GLN:HG2	1.89	0.55
1:E:496:LYS:HD3	1:E:555:LYS:NZ	2.20	0.55
2:F:500:ARG:O	2:F:566:VAL:HG13	2.06	0.55
1:A:166:GLU:HB3	1:A:167:LEU:HD12	1.88	0.55
1:A:306:VAL:O	1:A:306:VAL:HG23	2.07	0.55
1:C:200:VAL:O	1:C:200:VAL:CG1	2.55	0.55
2:D:527:VAL:HG22	2:D:542:ILE:CD1	2.37	0.55
2:D:546:GLU:HG3	2:D:547:GLU:CG	2.33	0.55
1:E:9:MET:O	1:E:12:LEU:HB3	2.07	0.55
1:E:454:ILE:HG13	1:E:455:GLY:N	2.22	0.55
1:A:737:GLU:HG3	1:A:766:PHE:CD2	2.41	0.55
1:E:179:ALA:O	1:E:183:GLU:HB2	2.07	0.55
1:E:225:PHE:CG	1:E:277:ILE:HD12	2.42	0.55
1:E:429:LYS:HG3	1:E:462:PHE:CZ	2.41	0.55
2:F:420:GLU:H	2:F:420:GLU:CD	2.10	0.55
1:C:25:ILE:CD1	1:C:125:ALA:HB1	2.37	0.54
1:C:406:LYS:HB3	1:C:447:ASP:HB3	1.88	0.54
1:E:167:LEU:H	1:E:167:LEU:HD12	1.71	0.54
2:F:467:ARG:HG3	2:F:558:TRP:CD1	2.43	0.54
1:A:155:VAL:HG12	1:A:156:VAL:N	2.21	0.54
1:A:223:ARG:HG2	1:A:223:ARG:HH11	1.71	0.54
2:B:488:ASP:OD1	2:B:489:ALA:N	2.40	0.54
2:B:552:LEU:CD1	2:B:552:LEU:H	2.18	0.54
1:C:157:ILE:HD11	1:C:181:THR:CG2	2.37	0.54
1:C:288:ILE:HG23	1:C:319:LEU:HG	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:ASP:O	1:A:691:VAL:HG23	2.08	0.54
1:C:314:LEU:HG	1:C:319:LEU:HA	1.89	0.54
2:D:458:ARG:H	2:D:460:GLN:NE2	2.04	0.54
2:D:529:ARG:NH1	2:D:604:PRO:HG2	2.21	0.54
1:E:348:ALA:O	1:E:352:ARG:HB2	2.06	0.54
1:E:669:TRP:CZ2	2:F:492:ARG:HG2	2.42	0.54
1:E:80:GLU:HA	1:E:96:ASN:O	2.06	0.54
1:C:288:ILE:HG23	1:C:319:LEU:CG	2.37	0.54
1:C:77:LEU:HB2	1:C:100:ILE:HB	1.88	0.54
1:E:251:ASN:HB3	1:E:254:THR:OG1	2.07	0.54
1:A:737:GLU:CG	1:A:766:PHE:HE2	2.19	0.54
1:E:411:VAL:HG11	1:E:469:LEU:HB3	1.89	0.54
1:E:68:ILE:HG23	1:E:390:ASP:HB2	1.90	0.54
1:C:126:LEU:HD11	1:C:156:VAL:CG2	2.37	0.54
1:C:490:GLN:O	1:C:491:VAL:HG13	2.07	0.54
1:C:584:ASN:ND2	1:C:693:LEU:HA	2.20	0.54
1:A:388:THR:HG21	1:A:395:TYR:CD1	2.43	0.54
1:C:348:ALA:O	1:C:352:ARG:HB2	2.08	0.54
1:C:365:ASN:O	1:C:369:ILE:HG12	2.08	0.54
1:C:543:GLN:O	1:C:546:GLU:N	2.41	0.54
1:E:278:LEU:O	1:E:282:PHE:HB2	2.08	0.54
1:A:466:THR:HG22	1:A:467:GLY:N	2.23	0.54
2:B:477:LEU:HD11	2:B:546:GLU:OE1	2.08	0.54
1:C:316:GLY:O	1:C:319:LEU:HB3	2.07	0.54
1:E:109:VAL:CG2	1:E:138:GLN:HG3	2.38	0.54
2:F:505:ARG:NH1	2:F:505:ARG:HG3	2.23	0.54
1:A:285:PHE:CE2	1:A:320:LEU:HD11	2.43	0.54
1:A:501:LEU:C	1:A:501:LEU:HD23	2.29	0.54
1:C:10:ARG:CZ	1:C:449:PRO:HD3	2.38	0.54
2:D:447:ALA:HA	2:D:499:LEU:HD21	1.89	0.54
1:A:459:ILE:CD1	1:A:469:LEU:HD21	2.37	0.53
1:A:669:TRP:CZ2	2:B:492:ARG:HB3	2.43	0.53
1:A:710:ARG:HG3	1:A:710:ARG:HH11	1.72	0.53
1:C:200:VAL:O	1:C:200:VAL:HG13	2.08	0.53
1:C:750:LYS:O	1:C:751:ARG:HB2	2.08	0.53
1:E:150:ARG:NH1	1:E:355:GLN:HB2	2.23	0.53
2:B:505:ARG:NH1	2:B:505:ARG:HG3	2.22	0.53
1:C:311:GLU:OE2	1:C:322:VAL:HG11	2.09	0.53
1:C:45:ILE:HD11	1:C:78:TYR:N	2.24	0.53
1:C:836:GLN:N	1:C:836:GLN:HE21	1.98	0.53
1:E:739:ALA:HB2	1:E:791:GLN:OE1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:529:ARG:NH1	2:F:604:PRO:HG2	2.24	0.53
2:F:530:LEU:HA	2:F:604:PRO:HG3	1.89	0.53
1:E:75:ILE:HD13	1:E:439:GLY:HA2	1.89	0.53
1:A:117:ALA:HA	1:A:481:MET:SD	2.48	0.53
1:A:447:ASP:CG	1:A:448:CYS:N	2.61	0.53
1:A:89:ILE:HG22	1:A:91:GLN:HG2	1.91	0.53
2:B:445:GLU:OE1	2:B:494:ARG:NH2	2.37	0.53
1:C:109:VAL:HG13	1:C:793:PHE:CE1	2.42	0.53
1:A:189:VAL:CG1	1:A:200:VAL:HG12	2.39	0.53
1:A:235:VAL:CG2	1:A:240:MET:HB2	2.39	0.53
1:C:466:THR:HG22	1:C:467:GLY:N	2.24	0.53
1:C:569:SER:O	1:C:720:ALA:HB1	2.08	0.53
1:E:576:LEU:HD13	1:E:587:TYR:CE1	2.44	0.53
2:F:440:HIS:HB2	2:F:471:ILE:HG22	1.90	0.53
1:A:25:ILE:CD1	1:A:125:ALA:HB1	2.38	0.53
1:C:132:ILE:HG23	1:C:133:GLU:N	2.24	0.53
1:E:478:MET:O	1:E:479:LYS:C	2.47	0.53
1:A:472:SER:HB3	1:A:475:ALA:HB2	1.91	0.53
1:C:116:THR:HB	1:C:481:MET:HE3	1.90	0.53
1:C:509:LYS:O	1:C:513:LYS:HG3	2.09	0.53
1:C:782:GLY:O	1:C:785:ARG:HB3	2.09	0.53
2:D:551:ARG:HG3	2:D:551:ARG:NH1	2.23	0.53
2:D:457:ALA:HB2	2:D:558:TRP:CD2	2.44	0.53
1:A:348:ALA:HA	1:A:351:TYR:CZ	2.44	0.53
1:C:45:ILE:HG12	1:C:76:SER:O	2.09	0.53
1:E:70:ILE:HG22	1:E:388:THR:HG22	1.89	0.53
2:F:488:ASP:CG	2:F:492:ARG:HB2	2.28	0.53
2:F:522:GLU:CD	2:F:522:GLU:H	2.12	0.53
1:A:200:VAL:O	1:A:200:VAL:HG13	2.07	0.53
1:C:132:ILE:HG23	1:C:133:GLU:HG3	1.91	0.53
1:E:152:LYS:CD	1:E:200:VAL:HG23	2.38	0.53
1:E:307:LEU:HD12	1:E:312:LYS:HD3	1.91	0.53
1:C:129:VAL:HG13	1:C:134:GLY:O	2.09	0.52
1:C:429:LYS:HG3	1:C:462:PHE:CZ	2.43	0.52
1:E:644:ASN:HD22	1:E:684:VAL:HB	1.74	0.52
1:C:291:PHE:HE1	1:C:315:GLU:HB2	1.74	0.52
1:E:508:LEU:HD22	1:E:520:THR:HB	1.91	0.52
1:C:391:LYS:HD3	1:C:393:ARG:HG3	1.91	0.52
1:A:70:ILE:HG22	1:A:388:THR:HG22	1.90	0.52
1:A:71:LYS:HB3	1:A:386:VAL:CG2	2.38	0.52
1:C:647:ILE:HG13	1:C:685:ARG:HE	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:647:ILE:HB	1:C:687:ASN:HD22	1.74	0.52
1:A:797:VAL:HG22	1:A:798:PHE:N	2.24	0.52
1:C:544:ASP:O	1:C:549:HIS:HB2	2.10	0.52
1:E:17:THR:HB	1:E:92:LYS:O	2.09	0.52
2:D:508:LEU:N	2:D:509:PRO:CD	2.73	0.52
1:E:646:VAL:HG13	1:E:688:ILE:CD1	2.40	0.52
2:F:505:ARG:HH11	2:F:505:ARG:HG3	1.75	0.52
1:A:186:ASN:CB	1:A:201:GLN:HG2	2.40	0.52
1:A:72:SER:HA	1:A:439:GLY:O	2.10	0.52
1:C:155:VAL:CG1	1:C:156:VAL:N	2.72	0.52
1:C:26:ALA:HB2	1:C:128:VAL:HB	1.91	0.52
1:C:436:LEU:HD23	1:C:454:ILE:CD1	2.40	0.52
1:E:171:LYS:NZ	1:E:283:ARG:NH2	2.57	0.52
2:B:530:LEU:HD23	2:B:604:PRO:HD3	1.92	0.52
1:C:126:LEU:HD11	1:C:156:VAL:HG21	1.92	0.52
1:C:258:THR:HG22	1:C:259:ASN:H	1.74	0.52
1:C:742:GLY:O	1:C:745:SER:HB3	2.10	0.52
1:E:694:HIS:CE1	1:E:699:DDE:HD2	2.45	0.52
1:A:478:MET:O	1:A:479:LYS:C	2.48	0.52
2:B:429:LEU:HD21	2:B:565:VAL:HG11	1.91	0.52
1:C:384:LYS:HB2	1:C:465:LYS:HE3	1.92	0.52
1:C:743:ILE:HD13	1:C:784:LEU:HD11	1.91	0.52
1:E:103:ILE:HD12	1:E:103:ILE:N	2.23	0.52
1:E:493:VAL:HG12	1:E:494:GLU:N	2.25	0.52
1:A:172:GLU:CD	1:A:271:ARG:HH21	2.13	0.51
1:A:335:LEU:O	1:A:339:VAL:HG23	2.10	0.51
1:A:673:GLU:HG2	1:A:678:GLY:O	2.10	0.51
1:A:155:VAL:HG21	1:A:185:VAL:HG11	1.92	0.51
1:A:581:ASN:N	1:A:704:GLN:OE1	2.35	0.51
1:A:759:GLN:HB2	1:A:766:PHE:CE1	2.45	0.51
1:C:384:LYS:CB	1:C:465:LYS:HE3	2.40	0.51
1:E:13:MET:SD	1:E:436:LEU:HD21	2.50	0.51
1:E:9:MET:HE2	1:E:436:LEU:HD13	1.91	0.51
1:A:493:VAL:CG1	1:A:554:LEU:HD22	2.40	0.51
1:C:524:GLU:C	1:C:526:GLY:H	2.14	0.51
1:E:155:VAL:CG2	1:E:202:VAL:HG21	2.38	0.51
2:F:426:HIS:NE2	2:F:594:ILE:HB	2.25	0.51
1:A:273:PHE:CD1	1:A:277:ILE:HD12	2.45	0.51
1:A:707:PRO:O	1:A:711:ARG:HG3	2.10	0.51
1:A:809:LEU:O	1:A:811:PRO:HD3	2.11	0.51
2:B:575:PRO:HG2	2:B:576:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:529:ILE:HG22	1:C:530:VAL:N	2.25	0.51
1:C:571:SER:HB2	1:C:589:LYS:HG2	1.91	0.51
1:E:229:TYR:CE2	1:E:276:PHE:HB3	2.45	0.51
1:E:750:LYS:O	1:E:751:ARG:HB2	2.10	0.51
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.91	0.51
1:C:226:ALA:CB	1:C:241:MET:HB3	2.41	0.51
1:C:335:LEU:O	1:C:339:VAL:HG23	2.10	0.51
1:E:186:ASN:OD1	1:E:186:ASN:C	2.49	0.51
1:E:387:PRO:HG3	1:E:394:PHE:CE1	2.45	0.51
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.45	0.51
1:E:500:ASP:O	1:E:503:LYS:HB2	2.10	0.51
2:B:460:GLN:HB3	2:B:467:ARG:HD3	1.92	0.51
1:C:544:ASP:O	1:C:549:HIS:N	2.44	0.51
1:A:155:VAL:CG1	1:A:156:VAL:N	2.74	0.51
2:F:442:THR:OG1	2:F:443:PHE:N	2.42	0.51
1:A:9:MET:O	1:A:13:MET:HG3	2.11	0.51
1:A:7:ASP:CA	1:A:10:ARG:HG2	2.40	0.51
2:B:457:ALA:O	2:B:458:ARG:HG3	2.10	0.51
1:C:265:GLU:CG	1:C:266:GLY:H	2.14	0.51
1:C:91:GLN:O	1:C:93:THR:HG23	2.10	0.51
1:E:627:VAL:O	1:E:631:ARG:HG3	2.11	0.51
2:F:407:VAL:HG22	2:F:416:ASN:O	2.11	0.51
1:A:223:ARG:NH1	1:A:223:ARG:HG2	2.26	0.51
1:A:68:ILE:HG23	1:A:390:ASP:HB2	1.93	0.51
1:E:307:LEU:HB2	1:E:312:LYS:HE2	1.93	0.51
1:A:110:ASP:C	1:A:112:SER:H	2.14	0.51
1:A:644:ASN:ND2	1:A:684:VAL:H	2.09	0.51
2:D:548:GLU:O	2:D:548:GLU:HG3	2.11	0.51
1:A:231:LYS:C	1:A:233:PHE:H	2.15	0.50
1:C:262:THR:HA	1:C:269:LEU:HG	1.93	0.50
1:C:208:THR:HG22	1:C:341:HIS:CG	2.46	0.50
1:C:3:ALA:HA	1:C:46:ILE:HG22	1.93	0.50
1:C:578:LYS:HA	1:C:584:ASN:O	2.11	0.50
1:E:43:ALA:O	1:E:77:LEU:HA	2.11	0.50
1:E:10:ARG:HD3	1:E:445:ILE:HD11	1.92	0.50
1:A:423:LYS:HG2	1:A:423:LYS:O	2.11	0.50
1:E:454:ILE:HG13	1:E:455:GLY:H	1.75	0.50
2:F:426:HIS:CE1	2:F:594:ILE:HB	2.46	0.50
1:A:581:ASN:O	1:A:582:LYS:HG3	2.11	0.50
1:E:22:MET:HA	1:E:122:THR:HB	1.92	0.50
1:E:482:LYS:HB3	1:E:797:VAL:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:693:LEU:HB3	1:E:700:ARG:HD2	1.94	0.50
1:C:132:ILE:HG23	1:C:133:GLU:H	1.77	0.50
2:D:546:GLU:HG2	2:D:547:GLU:HG3	1.91	0.50
2:D:552:LEU:HD12	2:D:552:LEU:N	2.27	0.50
1:E:809:LEU:O	1:E:811:PRO:HD3	2.12	0.50
1:A:226:ALA:CB	1:A:241:MET:HB3	2.41	0.50
1:A:406:LYS:HG3	1:A:409:GLN:HB2	1.94	0.50
1:A:429:LYS:HG3	1:A:462:PHE:CZ	2.47	0.50
2:B:508:LEU:N	2:B:509:PRO:CD	2.74	0.50
1:E:39:LEU:CD1	1:E:334:LEU:HD12	2.42	0.50
1:E:524:GLU:HA	2:F:492:ARG:HH12	1.76	0.50
1:E:495:VAL:HA	1:E:554:LEU:HA	1.93	0.50
1:A:29:ASP:O	1:A:159:LYS:NZ	2.29	0.50
1:A:447:ASP:CG	1:A:448:CYS:H	2.15	0.50
1:A:485:VAL:HG22	1:A:485:VAL:O	2.12	0.50
1:A:7:ASP:HA	1:A:10:ARG:CG	2.42	0.50
1:C:129:VAL:HG12	1:C:130:ASP:N	2.27	0.50
2:D:484:ASP:OD2	2:D:494:ARG:HD3	2.12	0.50
2:D:524:ALA:O	2:D:528:GLU:HG3	2.11	0.50
1:E:597:VAL:O	1:E:601:ILE:HG13	2.11	0.50
1:A:3:ALA:HA	1:A:46:ILE:HG22	1.92	0.50
1:A:819:VAL:O	1:A:823:ARG:HG3	2.11	0.50
2:D:507:SER:C	2:D:509:PRO:HD2	2.32	0.50
1:E:729:PHE:CE2	1:E:774:VAL:HG22	2.47	0.50
2:F:426:HIS:O	2:F:429:LEU:HB2	2.11	0.50
2:F:513:ARG:CB	2:F:513:ARG:HH11	2.22	0.50
1:A:16:VAL:HG12	1:A:346:VAL:HG23	1.94	0.50
1:A:693:LEU:HB3	1:A:700:ARG:HD2	1.94	0.50
1:C:506:GLU:HG3	1:C:510:ARG:HE	1.75	0.50
1:C:578:LYS:HG2	1:C:585:ARG:HG2	1.94	0.50
1:E:784:LEU:HD23	1:E:794:PRO:CG	2.38	0.50
1:A:153:PRO:HD2	1:A:200:VAL:HG13	1.94	0.50
1:A:388:THR:HG21	1:A:395:TYR:CG	2.46	0.50
1:C:106:PRO:HG3	1:C:114:GLU:HG3	1.93	0.50
1:C:167:LEU:N	1:C:167:LEU:HD12	2.25	0.50
1:C:627:VAL:O	1:C:631:ARG:HG3	2.12	0.50
1:E:235:VAL:HG11	1:E:239:LYS:HD3	1.94	0.50
1:E:39:LEU:HB3	1:E:77:LEU:HD21	1.92	0.50
1:E:39:LEU:HD11	1:E:334:LEU:CD1	2.42	0.50
1:A:411:VAL:CG1	1:A:412:ARG:N	2.74	0.49
1:A:581:ASN:C	1:A:582:LYS:CG	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:LEU:CD2	1:A:730:LEU:C	2.81	0.49
1:C:39:LEU:HB3	1:C:77:LEU:HD21	1.93	0.49
1:C:384:LYS:HB2	1:C:465:LYS:CE	2.42	0.49
1:C:601:ILE:HG12	1:C:606:ILE:HB	1.94	0.49
1:C:669:TRP:HE1	1:C:710:ARG:HH21	1.59	0.49
1:C:823:ARG:NH1	1:C:828:MET:HB2	2.26	0.49
1:E:563:TYR:O	1:E:564:ARG:HD2	2.12	0.49
1:E:585:ARG:HD2	1:E:692:THR:OG1	2.12	0.49
1:A:584:ASN:ND2	1:A:693:LEU:HA	2.17	0.49
2:D:485:GLN:O	2:D:486:GLU:HG2	2.12	0.49
1:E:183:GLU:O	1:E:187:VAL:HG23	2.12	0.49
1:E:571:SER:HB2	1:E:589:LYS:HG2	1.93	0.49
1:A:132:ILE:HD12	1:A:162:ARG:NH1	2.22	0.49
1:A:129:VAL:HG13	1:A:134:GLY:C	2.32	0.49
1:A:26:ALA:HB2	1:A:128:VAL:HB	1.94	0.49
1:A:677:PHE:CZ	1:A:679:GLU:HG3	2.47	0.49
2:B:411:THR:OG1	2:B:495:ASN:ND2	2.43	0.49
2:B:410:SER:HB3	2:B:413:GLY:O	2.13	0.49
1:E:581:ASN:HB3	1:E:583:HIS:HD2	1.77	0.49
1:A:129:VAL:HG13	1:A:134:GLY:O	2.13	0.49
1:A:374:PRO:O	1:A:404:THR:HG23	2.12	0.49
1:C:478:MET:O	1:C:479:LYS:C	2.50	0.49
2:D:447:ALA:O	2:D:448:GLN:C	2.50	0.49
1:E:754:VAL:HA	1:E:770:ALA:HB2	1.94	0.49
1:E:823:ARG:NH1	1:E:828:MET:HB2	2.27	0.49
1:C:2:VAL:CG2	1:C:3:ALA:H	2.19	0.49
1:E:296:ILE:O	1:E:300:LEU:HB2	2.12	0.49
1:E:650:THR:CG2	1:E:688:ILE:HG22	2.42	0.49
2:F:504:PRO:HD3	2:F:563:ARG:O	2.11	0.49
1:C:703:GLY:HA2	2:D:493:ILE:CD1	2.42	0.49
1:E:167:LEU:HD12	1:E:167:LEU:N	2.28	0.49
1:E:284:LEU:HD11	1:E:303:LEU:CD1	2.41	0.49
2:F:552:LEU:H	2:F:552:LEU:HD12	1.75	0.49
1:A:27:HIS:HD2	1:A:29:ASP:N	2.01	0.49
1:A:594:ASP:O	1:A:597:VAL:HG23	2.12	0.49
2:D:488:ASP:CG	2:D:489:ALA:N	2.66	0.49
1:E:162:ARG:O	1:E:166:GLU:HB2	2.13	0.49
1:E:200:VAL:O	1:E:200:VAL:HG22	2.13	0.49
2:F:451:VAL:CG1	2:F:451:VAL:O	2.59	0.49
1:A:344:SER:C	1:A:346:VAL:H	2.15	0.49
1:C:729:PHE:CE2	1:C:774:VAL:HG22	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:THR:O	1:A:763:THR:HG22	2.13	0.49
2:B:453:GLY:O	2:B:456:ARG:HD3	2.12	0.49
1:C:729:PHE:O	1:C:771:TYR:HA	2.13	0.49
1:C:148:GLY:HA2	1:C:760:ARG:NH2	2.28	0.49
1:E:153:PRO:HD2	1:E:200:VAL:HG22	1.95	0.49
1:E:749:LYS:HG3	1:E:749:LYS:O	2.13	0.49
1:A:125:ALA:HB2	1:A:151:ILE:HG21	1.95	0.49
1:A:109:VAL:CG2	1:A:138:GLN:HG3	2.43	0.49
1:C:296:ILE:CD1	1:C:319:LEU:HD21	2.38	0.49
1:C:792:ALA:O	1:C:794:PRO:HD3	2.13	0.49
2:D:484:ASP:OD2	2:D:494:ARG:CD	2.60	0.49
1:E:710:ARG:NH1	1:E:710:ARG:HG3	2.28	0.49
1:A:106:PRO:HG3	1:A:114:GLU:HG3	1.95	0.48
1:A:230:ALA:O	1:A:235:VAL:HG22	2.12	0.48
2:B:436:PHE:HB2	2:B:502:TYR:CE2	2.48	0.48
2:B:479:TYR:CG	2:B:582:LEU:HB2	2.48	0.48
1:C:459:ILE:HG21	1:C:463:LEU:HD12	1.94	0.48
2:D:451:VAL:O	2:D:451:VAL:HG12	2.13	0.48
2:D:518:LEU:H	2:D:518:LEU:HD22	1.77	0.48
1:E:171:LYS:NZ	1:E:283:ARG:HH21	2.11	0.48
1:E:503:LYS:CB	1:E:551:GLY:HA3	2.38	0.48
1:A:175:TYR:HD2	1:A:176:GLN:HE21	1.61	0.48
1:A:615:ARG:HG2	1:A:619:MET:HE1	1.95	0.48
1:C:390:ASP:O	1:C:391:LYS:HB3	2.13	0.48
1:C:607:ASN:HB3	1:C:610:ASP:OD2	2.13	0.48
1:C:681:MET:CE	1:C:717:PHE:CD1	2.97	0.48
1:E:374:PRO:O	1:E:404:THR:HG23	2.13	0.48
2:F:556:LEU:HD22	2:F:560:LEU:HD13	1.95	0.48
1:A:126:LEU:HD11	1:A:156:VAL:CG2	2.43	0.48
1:A:45:ILE:HB	1:A:76:SER:HB2	1.94	0.48
2:B:551:ARG:CG	2:B:551:ARG:HH11	2.27	0.48
1:C:211:PHE:O	1:C:219:ALA:HA	2.13	0.48
1:C:2:VAL:CG2	1:C:3:ALA:N	2.71	0.48
1:E:606:ILE:HD12	1:E:619:MET:CG	2.43	0.48
2:F:427:ARG:HG2	2:F:428:GLN:N	2.28	0.48
1:A:77:LEU:HB2	1:A:100:ILE:HB	1.95	0.48
1:E:348:ALA:HA	1:E:351:TYR:CE2	2.49	0.48
1:E:646:VAL:HG13	1:E:688:ILE:HD12	1.95	0.48
1:A:100:ILE:HD13	1:A:338:ILE:HG21	1.94	0.48
1:A:307:LEU:HD13	1:A:312:LYS:HA	1.96	0.48
1:A:504:LEU:HD13	1:A:554:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:LEU:CD2	1:C:318:ALA:O	2.61	0.48
1:C:580:PRO:HD2	1:C:704:GLN:CD	2.34	0.48
1:C:712:ALA:O	1:C:715:ALA:HB3	2.13	0.48
1:E:186:ASN:HB2	1:E:201:GLN:HG2	1.96	0.48
1:A:2:VAL:CG2	1:A:3:ALA:N	2.77	0.48
1:E:536:LEU:CD1	1:E:540:ILE:HD11	2.42	0.48
1:E:644:ASN:ND2	1:E:684:VAL:H	2.11	0.48
1:A:387:PRO:HG3	1:A:394:PHE:CE1	2.47	0.48
2:B:438:GLY:HA3	2:B:471:ILE:CD1	2.43	0.48
1:C:344:SER:C	1:C:346:VAL:H	2.17	0.48
1:E:144:ARG:HG2	1:E:192:TYR:CD2	2.48	0.48
1:E:220:PHE:HA	1:E:224:GLN:OE1	2.12	0.48
1:E:237:LYS:HA	1:E:240:MET:CB	2.38	0.48
1:E:527:GLU:HB3	1:E:529:ILE:HD11	1.95	0.48
1:E:607:ASN:HB3	1:E:610:ASP:CG	2.34	0.48
1:E:569:SER:O	1:E:720:ALA:HB1	2.14	0.48
1:A:521:TYR:CZ	1:A:529:ILE:HD12	2.48	0.48
1:C:120:ARG:NH1	1:C:479:LYS:HG3	2.29	0.48
1:C:647:ILE:HG13	1:C:685:ARG:NE	2.28	0.48
2:D:465:ILE:HG13	2:D:466:TRP:CD1	2.49	0.48
1:E:647:ILE:HG13	1:E:685:ARG:HE	1.78	0.48
1:E:685:ARG:NE	1:E:687:ASN:HD21	2.11	0.48
2:F:508:LEU:N	2:F:509:PRO:CD	2.77	0.48
1:A:130:ASP:OD1	1:A:159:LYS:HD2	2.14	0.48
1:A:167:LEU:N	1:A:167:LEU:HD12	2.28	0.48
1:C:172:GLU:HA	1:C:274:ASN:HD21	1.79	0.48
2:D:476:ALA:HA	2:D:582:LEU:HD23	1.95	0.48
1:E:220:PHE:HB3	1:E:328:LEU:HD13	1.95	0.48
1:E:325:ARG:HH11	1:E:325:ARG:HG2	1.79	0.48
1:E:677:PHE:CZ	1:E:679:GLU:HG3	2.49	0.48
2:B:438:GLY:HA3	2:B:471:ILE:HD13	1.96	0.48
2:B:450:ILE:HG23	2:B:455:VAL:HG23	1.96	0.48
1:C:468:THR:C	1:C:469:LEU:HD12	2.34	0.48
1:C:571:SER:HB2	1:C:589:LYS:CG	2.43	0.48
1:E:412:ARG:HG2	1:E:412:ARG:NH1	2.29	0.48
1:E:528:HIS:O	1:E:529:ILE:HD13	2.14	0.48
1:A:91:GLN:HE22	1:A:343:PRO:HA	1.79	0.47
1:A:636:PHE:CE1	1:A:645:LEU:HD21	2.49	0.47
1:C:385:MET:SD	1:C:396:ALA:HA	2.54	0.47
1:C:42:ARG:HG3	1:C:331:ALA:HB1	1.93	0.47
1:C:647:ILE:HB	1:C:687:ASN:ND2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:SER:HB2	1:A:813:SER:HB2	1.97	0.47
1:C:189:VAL:HG13	1:C:200:VAL:HG12	1.96	0.47
1:E:181:THR:O	1:E:185:VAL:HG23	2.15	0.47
1:E:203:TYR:CD2	1:E:206:ARG:HD2	2.46	0.47
1:E:262:THR:CG2	1:E:266:GLY:HA2	2.44	0.47
1:E:606:ILE:HD12	1:E:619:MET:HG2	1.96	0.47
1:E:82:SER:O	1:E:86:VAL:HG23	2.14	0.47
1:A:225:PHE:CE2	1:A:277:ILE:HG23	2.49	0.47
1:A:647:ILE:CG1	1:A:685:ARG:HE	2.25	0.47
1:A:719:LEU:HD21	1:A:835:TRP:CE2	2.48	0.47
1:A:81:MET:O	1:A:96:ASN:HB3	2.14	0.47
1:C:386:VAL:HG11	1:C:437:MET:CE	2.45	0.47
1:C:488:VAL:HG23	1:C:489:VAL:HG22	1.95	0.47
1:E:129:VAL:HG12	1:E:130:ASP:N	2.28	0.47
2:F:470:TYR:CE2	2:F:555:ILE:HG12	2.50	0.47
1:A:569:SER:O	1:A:592:PRO:HD3	2.14	0.47
1:C:581:ASN:O	1:C:582:LYS:CB	2.62	0.47
2:D:488:ASP:OD1	2:D:489:ALA:N	2.47	0.47
1:E:436:LEU:HD23	1:E:454:ILE:CD1	2.44	0.47
1:E:10:ARG:NH1	1:E:449:PRO:HD2	2.20	0.47
2:B:560:LEU:O	2:B:560:LEU:HD22	2.14	0.47
2:D:570:ALA:HB3	2:D:591:GLU:OE1	2.15	0.47
1:E:172:GLU:HA	1:E:274:ASN:HD21	1.79	0.47
1:E:807:ASP:OD2	1:E:809:LEU:N	2.33	0.47
2:F:493:ILE:HG22	2:F:493:ILE:O	2.14	0.47
1:A:83:ASP:O	1:A:87:LYS:HG3	2.14	0.47
2:B:542:ILE:HD12	2:B:543:THR:H	1.80	0.47
1:C:43:ALA:HB1	1:C:78:TYR:O	2.13	0.47
1:C:116:THR:HB	1:C:481:MET:CE	2.45	0.47
2:F:422:LEU:HD13	2:F:594:ILE:HD11	1.97	0.47
2:B:490:ARG:N	2:B:490:ARG:CD	2.77	0.47
2:B:457:ALA:HB2	2:B:558:TRP:CE3	2.49	0.47
1:C:231:LYS:CG	1:C:232:LYS:N	2.77	0.47
1:C:411:VAL:HG12	1:C:412:ARG:N	2.29	0.47
1:E:155:VAL:HB	1:E:209:VAL:HG22	1.97	0.47
1:E:615:ARG:HG2	1:E:619:MET:HE2	1.97	0.47
1:E:734:GLN:N	1:E:734:GLN:NE2	2.58	0.47
1:C:186:ASN:HB3	1:C:201:GLN:HG2	1.97	0.47
1:C:256:LYS:CA	1:C:256:LYS:HE2	2.24	0.47
1:C:268:PRO:O	1:C:269:LEU:HD23	2.15	0.47
1:C:283:ARG:HB3	1:C:299:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:429:LEU:HD21	2:D:565:VAL:HG11	1.96	0.47
1:E:411:VAL:HG12	1:E:412:ARG:N	2.28	0.47
1:E:503:LYS:HB3	1:E:551:GLY:N	2.30	0.47
1:E:581:ASN:ND2	1:E:699:DDE:O	2.48	0.47
1:C:638:PRO:HB3	1:C:672:LYS:HG2	1.96	0.47
1:C:484:SER:HB3	1:C:797:VAL:HG23	1.97	0.47
1:E:147:LEU:HD12	1:E:192:TYR:HB2	1.92	0.47
1:E:739:ALA:HB1	1:E:788:THR:HB	1.97	0.47
2:F:556:LEU:HD22	2:F:560:LEU:CD1	2.45	0.47
1:C:384:LYS:HB2	1:C:465:LYS:HZ2	1.79	0.47
1:C:681:MET:HE1	1:C:717:PHE:CD1	2.50	0.47
1:C:729:PHE:CD2	1:C:774:VAL:HG22	2.50	0.47
2:D:465:ILE:HD12	2:D:535:LEU:HD12	1.97	0.47
1:E:773:PRO:HB2	1:E:776:GLU:HB2	1.97	0.47
1:A:348:ALA:O	1:A:352:ARG:HB2	2.15	0.47
2:B:546:GLU:HG3	2:B:553:GLU:OE1	2.15	0.47
2:B:552:LEU:CD1	2:B:552:LEU:N	2.70	0.47
1:C:223:ARG:HH11	1:C:223:ARG:HG2	1.80	0.47
1:C:809:LEU:O	1:C:811:PRO:HD3	2.14	0.47
1:E:284:LEU:HD13	1:E:324:MET:CE	2.45	0.47
1:E:285:PHE:CD2	1:E:320:LEU:HD11	2.50	0.47
2:F:427:ARG:CG	2:F:428:GLN:N	2.78	0.47
1:A:386:VAL:HA	1:A:387:PRO:HD3	1.78	0.46
1:A:112:SER:CB	1:A:794:PRO:O	2.63	0.46
1:C:45:ILE:HG12	1:C:76:SER:C	2.36	0.46
1:E:386:VAL:HG11	1:E:437:MET:CE	2.44	0.46
1:A:118:ALA:O	1:A:122:THR:HG23	2.14	0.46
2:B:556:LEU:HD22	2:B:560:LEU:CD1	2.45	0.46
1:C:275:MET:HE1	1:C:276:PHE:CZ	2.50	0.46
1:C:546:GLU:HB2	1:C:554:LEU:HD12	1.98	0.46
1:E:607:ASN:HA	1:E:608:PRO:HD3	1.87	0.46
1:A:16:VAL:HG21	1:A:450:ALA:O	2.14	0.46
1:A:495:VAL:HA	1:A:554:LEU:HD23	1.97	0.46
1:A:620:ALA:HA	1:A:625:TRP:O	2.15	0.46
1:C:140:GLU:HG3	1:C:188:ILE:HD11	1.93	0.46
1:E:307:LEU:HB2	1:E:312:LYS:CE	2.45	0.46
1:E:552:VAL:CG2	1:E:553:PRO:CD	2.80	0.46
1:E:829:LYS:HD2	1:E:829:LYS:N	2.30	0.46
1:A:103:ILE:HD12	1:A:122:THR:HG22	1.96	0.46
1:A:386:VAL:HG11	1:A:437:MET:CE	2.46	0.46
2:B:420:GLU:CD	2:B:420:GLU:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:THR:HG21	1:C:163:ALA:HB2	1.96	0.46
1:C:147:LEU:HD11	1:C:189:VAL:HA	1.96	0.46
1:C:385:MET:H	1:C:465:LYS:HD2	1.79	0.46
1:C:539:GLU:HA	1:C:542:LEU:HD12	1.98	0.46
1:C:706:ILE:HB	1:C:707:PRO:HD3	1.97	0.46
1:E:132:ILE:HD12	1:E:132:ILE:H	1.79	0.46
1:E:506:GLU:O	1:E:510:ARG:HG2	2.15	0.46
2:F:538:ARG:HD2	2:F:538:ARG:HA	1.49	0.46
1:A:7:ASP:HA	1:A:10:ARG:CD	2.44	0.46
1:E:39:LEU:HD11	1:E:334:LEU:CB	2.46	0.46
1:E:39:LEU:HD11	1:E:334:LEU:HD12	1.98	0.46
1:E:581:ASN:HB3	1:E:583:HIS:CD2	2.51	0.46
1:E:740:VAL:HG21	1:E:766:PHE:CD1	2.49	0.46
2:F:518:LEU:O	2:F:520:ALA:N	2.49	0.46
1:C:253:LYS:CE	1:C:253:LYS:HA	2.23	0.46
1:C:306:VAL:HG23	1:C:306:VAL:O	2.15	0.46
1:C:391:LYS:CG	1:C:392:GLY:N	2.61	0.46
1:C:589:LYS:HE3	1:C:689:LEU:HD11	1.97	0.46
1:C:669:TRP:C	1:C:669:TRP:CD1	2.88	0.46
1:E:595:GLU:OE2	1:E:682:ARG:NH2	2.41	0.46
1:E:710:ARG:HH11	1:E:710:ARG:HG3	1.81	0.46
1:E:784:LEU:CD2	1:E:794:PRO:HG3	2.38	0.46
1:E:807:ASP:C	1:E:807:ASP:OD2	2.53	0.46
1:E:829:LYS:HD2	1:E:829:LYS:H	1.81	0.46
1:A:365:ASN:O	1:A:369:ILE:HG12	2.16	0.46
1:C:235:VAL:CG1	1:C:236:ASP:N	2.79	0.46
1:C:374:PRO:O	1:C:404:THR:HG23	2.15	0.46
1:E:137:VAL:CG1	1:E:785:ARG:NH2	2.78	0.46
1:C:222:ILE:HG22	1:C:241:MET:HB2	1.98	0.46
1:C:552:VAL:CG2	1:C:553:PRO:CD	2.83	0.46
1:C:580:PRO:HD2	1:C:704:GLN:NE2	2.31	0.46
1:E:528:HIS:C	1:E:529:ILE:HD13	2.35	0.46
1:E:557:SER:O	1:E:558:PRO:O	2.33	0.46
1:E:647:ILE:HG13	1:E:685:ARG:NE	2.31	0.46
1:A:41:GLN:O	1:A:41:GLN:HG2	2.16	0.46
1:C:156:VAL:HG22	1:C:210:ALA:HB3	1.98	0.46
1:C:262:THR:OG1	1:C:263:ASP:N	2.49	0.46
1:E:345:PRO:HG2	1:E:451:GLY:O	2.16	0.46
1:E:493:VAL:CG1	1:E:494:GLU:N	2.79	0.46
1:A:228:ARG:C	1:A:230:ALA:H	2.17	0.46
1:A:436:LEU:HD23	1:A:454:ILE:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:GLU:HG3	1:A:768:VAL:HG22	1.97	0.46
1:C:228:ARG:C	1:C:230:ALA:H	2.20	0.46
1:C:331:ALA:O	1:C:335:LEU:HG	2.16	0.46
1:C:520:THR:HG22	1:C:530:VAL:HG22	1.97	0.46
1:C:89:ILE:CG2	1:C:91:GLN:HG2	2.45	0.46
1:E:545:LEU:HD12	1:E:549:HIS:CB	2.41	0.46
1:A:231:LYS:C	1:A:233:PHE:N	2.70	0.45
1:A:411:VAL:HG11	1:A:469:LEU:HB3	1.97	0.45
1:A:565:GLU:O	1:A:681:MET:HA	2.16	0.45
2:B:423:LEU:HD11	2:B:590:LYS:HD3	1.98	0.45
1:C:216:HIS:NE2	1:C:317:LYS:NZ	2.62	0.45
2:D:542:ILE:HG12	2:D:543:THR:N	2.31	0.45
1:E:654:GLN:HG2	1:E:655:TYR:CG	2.52	0.45
1:E:705:ILE:HD12	1:E:705:ILE:N	2.31	0.45
2:F:436:PHE:HB2	2:F:502:TYR:CE2	2.50	0.45
1:A:710:ARG:NH1	1:A:710:ARG:HG3	2.32	0.45
1:A:730:LEU:HB2	1:A:799:ASP:HB2	1.98	0.45
2:B:490:ARG:HD2	2:B:490:ARG:H	1.82	0.45
1:C:315:GLU:C	1:C:319:LEU:HB2	2.36	0.45
1:C:45:ILE:HD11	1:C:78:TYR:HB3	1.95	0.45
1:E:202:VAL:O	1:E:202:VAL:HG23	2.16	0.45
1:E:348:ALA:HA	1:E:351:TYR:CZ	2.51	0.45
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.98	0.45
1:E:732:GLU:N	1:E:795:GLN:O	2.46	0.45
1:C:515:ASP:HB3	1:C:518:VAL:CG1	2.47	0.45
1:C:493:VAL:HG21	1:C:545:LEU:CD2	2.45	0.45
1:C:558:PRO:HA	1:C:559:PRO:HD3	1.79	0.45
1:C:685:ARG:HE	1:C:687:ASN:ND2	2.13	0.45
1:C:816:GLY:O	1:C:820:LEU:HB3	2.16	0.45
1:E:150:ARG:HH12	1:E:355:GLN:HB2	1.81	0.45
1:E:10:ARG:NH1	1:E:449:PRO:CD	2.59	0.45
1:E:466:THR:HG22	1:E:467:GLY:N	2.32	0.45
1:E:117:ALA:HA	1:E:481:MET:SD	2.57	0.45
2:F:400:PHE:CD1	2:F:429:LEU:HD23	2.51	0.45
1:A:220:PHE:C	1:A:220:PHE:CD1	2.90	0.45
1:A:296:ILE:N	1:A:297:PRO:HD2	2.31	0.45
1:A:12:LEU:HG	1:A:99:LEU:HB2	1.96	0.45
2:B:417:TRP:CD1	2:B:568:PRO:HB2	2.51	0.45
1:C:277:ILE:HG22	1:C:278:LEU:N	2.31	0.45
1:C:311:GLU:OE2	1:C:322:VAL:CG1	2.64	0.45
1:E:143:LEU:O	1:E:147:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:735:CYS:HA	1:E:736:PRO:HD3	1.81	0.45
1:E:137:VAL:HG13	1:E:785:ARG:NH2	2.31	0.45
1:C:291:PHE:O	1:C:293:LYS:N	2.50	0.45
1:C:675:PRO:HD3	1:C:714:TYR:CD1	2.52	0.45
1:C:733:ILE:HG21	1:C:743:ILE:CD1	2.47	0.45
1:E:32:LYS:NZ	1:E:106:PRO:O	2.49	0.45
1:E:12:LEU:HG	1:E:99:LEU:HB2	1.98	0.45
1:E:485:VAL:HG22	1:E:485:VAL:O	2.17	0.45
1:A:126:LEU:HD11	1:A:156:VAL:HG23	1.99	0.45
1:A:454:ILE:CG1	1:A:455:GLY:H	2.27	0.45
1:A:647:ILE:HB	1:A:687:ASN:ND2	2.30	0.45
1:C:164:LEU:HD21	1:C:174:LEU:HD22	1.98	0.45
1:C:38:SER:CA	1:C:41:GLN:HG2	2.46	0.45
1:E:360:PRO:HB2	1:E:363:ASP:HB2	1.99	0.45
1:E:371:ASN:O	1:E:372:CYS:C	2.54	0.45
1:E:611:ASP:OD2	1:E:613:LYS:HB2	2.17	0.45
1:E:743:ILE:HD13	1:E:784:LEU:HD11	1.98	0.45
1:A:258:THR:HG21	1:A:260:LYS:HG2	1.97	0.45
1:A:338:ILE:O	1:A:342:LEU:HB2	2.17	0.45
1:A:561:VAL:HG21	1:A:775:ASN:CB	2.46	0.45
1:C:129:VAL:HG13	1:C:134:GLY:C	2.37	0.45
1:C:348:ALA:HA	1:C:351:TYR:CZ	2.52	0.45
1:C:581:ASN:ND2	1:C:704:GLN:HG3	2.32	0.45
1:E:507:GLY:CA	1:E:549:HIS:HB3	2.46	0.45
1:E:635:CYS:CB	1:E:664:VAL:HG13	2.46	0.45
1:E:823:ARG:NH2	1:E:833:PRO:HD3	2.31	0.45
2:B:420:GLU:CD	2:B:420:GLU:H	2.19	0.45
2:B:474:ASP:OD1	2:B:475:PRO:HD2	2.16	0.45
2:B:484:ASP:OD2	2:B:494:ARG:N	2.50	0.45
1:C:464:LEU:HD12	1:C:483:PHE:CZ	2.52	0.45
1:C:45:ILE:HB	1:C:76:SER:HB2	1.99	0.45
1:C:82:SER:O	1:C:86:VAL:HG23	2.17	0.45
1:E:508:LEU:HD22	1:E:520:THR:CG2	2.47	0.45
1:E:712:ALA:O	1:E:715:ALA:HB3	2.17	0.45
1:C:111:PHE:HB3	1:C:114:GLU:HG2	1.99	0.45
1:C:523:SER:O	1:C:526:GLY:N	2.50	0.45
1:C:729:PHE:HB2	1:C:772:LEU:O	2.17	0.45
2:D:535:LEU:HB3	2:D:536:PRO:HA	1.99	0.45
2:D:561:ALA:O	2:D:564:THR:HG23	2.17	0.45
1:E:149:GLU:O	1:E:150:ARG:HB2	2.16	0.45
2:F:451:VAL:HG12	2:F:451:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:450:ILE:O	2:F:454:GLY:N	2.50	0.45
1:A:7:ASP:O	1:A:10:ARG:CG	2.65	0.45
1:C:542:LEU:O	1:C:545:LEU:HB3	2.17	0.45
1:C:693:LEU:HB3	1:C:700:ARG:HD2	1.99	0.45
2:D:471:ILE:HG13	2:D:554:THR:HB	1.97	0.45
2:D:541:ALA:HB2	2:D:556:LEU:HD23	1.99	0.45
1:E:306:VAL:O	1:E:306:VAL:HG23	2.17	0.45
1:E:520:THR:HA	1:E:529:ILE:O	2.17	0.45
2:F:443:PHE:CE2	2:F:445:GLU:HB2	2.52	0.45
2:F:498:LEU:HD23	2:F:498:LEU:HA	1.72	0.45
1:A:200:VAL:O	1:A:200:VAL:CG1	2.65	0.44
1:A:43:ALA:HB1	1:A:78:TYR:O	2.17	0.44
1:A:690:ASP:O	1:A:691:VAL:CG2	2.65	0.44
1:C:552:VAL:CG2	1:C:553:PRO:HD3	2.39	0.44
1:C:567:VAL:HG23	1:C:592:PRO:HG3	1.99	0.44
2:D:558:TRP:O	2:D:559:PRO:C	2.55	0.44
1:E:72:SER:HA	1:E:439:GLY:O	2.18	0.44
1:A:249:PHE:CD2	1:A:249:PHE:N	2.85	0.44
1:A:7:ASP:HA	1:A:10:ARG:HD3	1.99	0.44
1:C:129:VAL:HB	1:C:157:ILE:HD13	1.98	0.44
1:C:211:PHE:CD2	1:C:211:PHE:N	2.85	0.44
1:C:251:ASN:HA	1:C:252:PRO:HD3	1.64	0.44
1:C:507:GLY:O	1:C:511:LEU:HB2	2.17	0.44
1:C:490:GLN:HB2	1:C:529:ILE:CG2	2.47	0.44
1:C:735:CYS:SG	1:C:739:ALA:HB3	2.58	0.44
1:E:109:VAL:O	1:E:109:VAL:HG12	2.16	0.44
1:E:386:VAL:HA	1:E:387:PRO:HD3	1.79	0.44
1:E:536:LEU:O	1:E:537:HIS:C	2.55	0.44
1:E:89:ILE:C	1:E:91:GLN:N	2.69	0.44
1:C:225:PHE:CE2	1:C:277:ILE:HG23	2.51	0.44
1:C:218:TRP:CA	1:C:330:ALA:HB2	2.47	0.44
1:C:371:ASN:O	1:C:372:CYS:C	2.55	0.44
1:C:381:TYR:O	1:C:398:GLY:HA3	2.18	0.44
1:E:158:ASN:HA	1:E:212:GLY:O	2.17	0.44
1:E:225:PHE:CZ	1:E:328:LEU:HD11	2.53	0.44
2:F:420:GLU:N	2:F:420:GLU:CD	2.71	0.44
2:F:570:ALA:HB3	2:F:591:GLU:OE1	2.18	0.44
1:A:582:LYS:HE3	1:A:582:LYS:HB3	1.49	0.44
1:C:301:GLU:HG3	1:C:301:GLU:O	2.18	0.44
1:C:413:ILE:HD13	1:C:459:ILE:HG23	1.98	0.44
1:C:644:ASN:HD22	1:C:684:VAL:HB	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:ILE:HG12	1:E:125:ALA:HB1	1.99	0.44
1:E:4:PHE:HA	1:E:8:GLN:OE1	2.18	0.44
1:A:32:LYS:HZ2	1:A:105:SER:HB2	1.79	0.44
1:A:30:HIS:HA	1:A:159:LYS:NZ	2.32	0.44
1:A:581:ASN:HB3	1:A:583:HIS:ND1	2.33	0.44
1:C:109:VAL:CG1	1:C:793:PHE:CE1	3.01	0.44
1:C:110:ASP:C	1:C:112:SER:H	2.20	0.44
1:C:223:ARG:HG2	1:C:223:ARG:NH1	2.33	0.44
1:C:42:ARG:HG3	1:C:331:ALA:HB2	1.90	0.44
1:C:501:LEU:CD2	1:C:501:LEU:C	2.86	0.44
1:E:500:ASP:HA	1:E:503:LYS:HD2	1.98	0.44
1:E:571:SER:HB2	1:E:589:LYS:CG	2.47	0.44
1:E:663:VAL:HG13	1:E:709:MET:SD	2.57	0.44
1:A:782:GLY:O	1:A:785:ARG:HB3	2.17	0.44
1:E:109:VAL:HG23	1:E:138:GLN:CD	2.38	0.44
1:E:349:GLN:O	1:E:370:LYS:HA	2.17	0.44
1:E:644:ASN:HD22	1:E:684:VAL:H	1.66	0.44
2:F:518:LEU:HD22	2:F:518:LEU:N	2.32	0.44
1:A:112:SER:HB3	1:A:794:PRO:O	2.18	0.44
2:B:490:ARG:CD	2:B:490:ARG:H	2.31	0.44
1:C:251:ASN:H	1:C:251:ASN:ND2	2.14	0.44
1:C:296:ILE:N	1:C:297:PRO:HD2	2.33	0.44
1:C:344:SER:C	1:C:346:VAL:N	2.70	0.44
1:C:500:ASP:HB3	1:C:552:VAL:HG11	2.00	0.44
1:E:503:LYS:HB3	1:E:551:GLY:H	1.83	0.44
1:A:357:TYR:CE2	1:A:359:GLY:HA3	2.53	0.44
1:A:589:LYS:HE3	1:A:689:LEU:CD1	2.45	0.44
2:B:447:ALA:HA	2:B:499:LEU:HD21	2.00	0.44
1:C:108:HIS:HD2	1:C:110:ASP:H	1.65	0.44
1:C:224:GLN:O	1:C:228:ARG:HG3	2.18	0.44
1:C:45:ILE:HD11	1:C:78:TYR:HB2	1.98	0.44
2:D:531:ILE:CD1	2:D:533:HIS:CE1	2.94	0.44
1:E:338:ILE:HA	1:E:342:LEU:HG	1.99	0.44
1:E:613:LYS:O	1:E:616:ALA:HB3	2.18	0.44
1:E:700:ARG:O	1:E:705:ILE:HD13	2.17	0.44
1:E:79:SER:O	1:E:98:PHE:N	2.50	0.44
1:A:258:THR:CG2	1:A:260:LYS:HG2	2.48	0.44
1:A:491:VAL:HG13	1:A:538:LEU:HD21	2.00	0.44
1:A:626:ASP:C	1:A:628:THR:N	2.71	0.44
1:E:118:ALA:O	1:E:122:THR:HG23	2.18	0.44
1:E:274:ASN:O	1:E:279:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:685:ARG:HE	1:E:687:ASN:ND2	2.15	0.44
1:E:735:CYS:SG	1:E:739:ALA:HB3	2.57	0.44
1:A:39:LEU:HB3	1:A:77:LEU:HD21	2.00	0.43
1:A:488:VAL:HG23	1:A:489:VAL:CG2	2.48	0.43
2:B:479:TYR:CD2	2:B:582:LEU:HB2	2.53	0.43
2:B:516:LEU:O	2:B:545:PRO:HD2	2.18	0.43
1:C:317:LYS:HD2	1:C:317:LYS:HA	1.28	0.43
1:C:411:VAL:HG12	1:C:412:ARG:O	2.17	0.43
1:E:250:PHE:HD2	1:E:275:MET:HE1	1.83	0.43
1:E:389:SER:O	1:E:391:LYS:N	2.51	0.43
1:E:40:VAL:C	1:E:42:ARG:H	2.21	0.43
1:E:694:HIS:NE2	1:E:699:DDE:HD2	2.33	0.43
2:F:479:TYR:CG	2:F:582:LEU:HB2	2.53	0.43
1:A:19:VAL:HA	1:A:99:LEU:O	2.18	0.43
1:C:494:GLU:OE1	1:C:494:GLU:CA	2.66	0.43
1:C:521:TYR:CD1	1:C:529:ILE:HD13	2.52	0.43
1:C:734:GLN:HE21	1:C:734:GLN:CA	2.29	0.43
1:E:381:TYR:OH	1:E:481:MET:HG3	2.18	0.43
1:E:68:ILE:HG21	1:E:395:TYR:OH	2.18	0.43
2:F:467:ARG:HG3	2:F:558:TRP:NE1	2.33	0.43
1:A:414:GLN:HB3	1:A:418:TYR:CD2	2.52	0.43
1:A:558:PRO:HA	1:A:559:PRO:HD3	1.92	0.43
1:A:690:ASP:C	1:A:691:VAL:HG23	2.38	0.43
1:A:19:VAL:HG22	1:A:99:LEU:HB3	2.00	0.43
1:C:16:VAL:HG12	1:C:346:VAL:HG23	2.00	0.43
1:C:606:ILE:HD12	1:C:619:MET:CG	2.48	0.43
1:E:296:ILE:N	1:E:297:PRO:HD2	2.34	0.43
2:F:476:ALA:HA	2:F:582:LEU:HD23	2.01	0.43
1:A:654:GLN:HG2	1:A:655:TYR:CG	2.54	0.43
1:C:156:VAL:HG21	1:C:334:LEU:HD22	2.00	0.43
2:D:436:PHE:CE1	2:D:438:GLY:O	2.71	0.43
1:E:153:PRO:HD2	1:E:200:VAL:CG2	2.48	0.43
1:E:4:PHE:CE2	1:E:45:ILE:HD12	2.53	0.43
1:E:461:GLN:NE2	1:E:462:PHE:CE2	2.87	0.43
1:E:749:LYS:HG3	1:E:750:LYS:HD2	1.98	0.43
1:C:411:VAL:HG13	1:C:470:THR:O	2.19	0.43
2:D:437:VAL:HG11	2:D:511:PHE:CE2	2.54	0.43
2:F:443:PHE:CD2	2:F:445:GLU:HB2	2.53	0.43
1:A:549:HIS:H	1:A:549:HIS:CD2	2.35	0.43
1:A:733:ILE:O	1:A:767:THR:HA	2.19	0.43
2:B:489:ALA:HB3	2:B:490:ARG:HH11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:THR:CA	1:C:269:LEU:HG	2.48	0.43
1:C:288:ILE:CG2	1:C:319:LEU:HG	2.47	0.43
1:C:387:PRO:HG3	1:C:394:PHE:CE1	2.54	0.43
1:C:411:VAL:CG1	1:C:412:ARG:N	2.81	0.43
1:C:659:ILE:HD13	1:C:693:LEU:HD21	2.00	0.43
2:D:470:TYR:CE2	2:D:555:ILE:HD11	2.54	0.43
1:A:569:SER:O	1:A:720:ALA:HB1	2.18	0.43
1:A:580:PRO:HB2	1:A:704:GLN:HE22	1.83	0.43
2:D:541:ALA:CB	2:D:556:LEU:HD23	2.49	0.43
1:E:229:TYR:CD1	1:E:232:LYS:HD2	2.54	0.43
1:E:350:ALA:O	1:E:370:LYS:HG2	2.18	0.43
1:E:490:GLN:HA	1:E:531:ALA:HA	2.01	0.43
1:E:782:GLY:O	1:E:786:GLN:NE2	2.52	0.43
1:A:522:MET:CE	1:A:526:GLY:O	2.66	0.43
1:A:504:LEU:HD22	1:A:554:LEU:CD2	2.49	0.43
1:A:824:LYS:HE3	1:A:830:GLU:OE2	2.19	0.43
1:A:240:MET:O	1:A:244:LEU:HG	2.18	0.43
1:A:704:GLN:O	1:A:707:PRO:HD2	2.19	0.43
1:C:186:ASN:CB	1:C:201:GLN:HG2	2.49	0.43
1:C:216:HIS:CE1	1:C:317:LYS:HZ1	2.36	0.43
1:C:459:ILE:O	1:C:462:PHE:N	2.48	0.43
1:C:497:ASN:H	1:C:497:ASN:HD22	1.67	0.43
1:E:209:VAL:HG12	1:E:211:PHE:CE1	2.53	0.43
1:E:171:LYS:HZ3	1:E:283:ARG:HH21	1.67	0.43
1:A:408:GLY:O	1:A:409:GLN:C	2.57	0.43
1:A:411:VAL:HG13	1:A:470:THR:O	2.19	0.43
1:A:591:GLU:OE2	1:A:685:ARG:NH1	2.52	0.43
2:B:499:LEU:HB3	2:B:566:VAL:CG1	2.49	0.43
2:B:583:ASP:HA	2:B:584:PRO:HD2	1.86	0.43
1:C:253:LYS:HG3	1:C:253:LYS:O	2.19	0.43
1:C:587:TYR:CD2	1:C:690:ASP:HB3	2.53	0.43
1:C:655:TYR:O	1:C:656:LEU:C	2.57	0.43
1:C:646:VAL:HG13	1:C:688:ILE:HD13	2.01	0.43
1:C:749:LYS:O	1:C:750:LYS:HD2	2.19	0.43
1:E:4:PHE:CD2	1:E:45:ILE:HD12	2.54	0.43
2:F:427:ARG:O	2:F:428:GLN:C	2.55	0.43
2:B:503:VAL:HB	2:B:504:PRO:CD	2.49	0.42
2:B:520:ALA:HB1	2:B:521:PRO:CD	2.48	0.42
1:C:694:HIS:HD2	1:C:696:ASP:N	2.00	0.42
1:C:760:ARG:O	1:C:761:PRO:C	2.58	0.42
1:E:737:GLU:HG3	1:E:766:PHE:CZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:HG12	1:A:345:PRO:HG2	1.94	0.42
1:A:588:LEU:CD1	1:A:588:LEU:C	2.86	0.42
1:A:597:VAL:O	1:A:601:ILE:HG13	2.20	0.42
2:B:518:LEU:H	2:B:518:LEU:CD2	2.33	0.42
1:A:711:ARG:HH11	2:B:577:ASN:HD21	1.67	0.42
1:C:285:PHE:CE2	1:C:324:MET:SD	3.09	0.42
1:C:515:ASP:HA	1:C:516:PRO:HD3	1.85	0.42
1:E:21:ASN:ND2	1:E:345:PRO:HG3	2.34	0.42
1:A:576:LEU:HD13	1:A:587:TYR:CE1	2.54	0.42
1:A:729:PHE:CD2	1:A:774:VAL:HG22	2.54	0.42
2:B:458:ARG:O	2:B:459:SER:HB2	2.18	0.42
1:C:158:ASN:HD22	1:C:159:LYS:HG2	1.78	0.42
1:C:236:ASP:OD1	1:C:238:ALA:HB3	2.19	0.42
1:E:800:HIS:CD2	1:E:800:HIS:N	2.87	0.42
1:E:814:LYS:O	1:E:817:GLU:HB3	2.20	0.42
1:A:488:VAL:HG23	1:A:489:VAL:HG23	2.01	0.42
1:A:591:GLU:HG2	1:A:685:ARG:CG	2.46	0.42
1:C:494:GLU:HG2	1:C:528:HIS:HE1	1.85	0.42
1:C:565:GLU:CD	1:C:676:ILE:HB	2.40	0.42
2:F:401:LEU:O	2:F:421:ARG:NE	2.48	0.42
1:A:626:ASP:O	1:A:628:THR:N	2.53	0.42
1:C:410:LYS:HE2	1:C:430:ALA:HB2	2.02	0.42
1:C:522:MET:SD	1:C:528:HIS:HA	2.59	0.42
1:C:650:THR:CG2	1:C:688:ILE:HG22	2.50	0.42
1:C:690:ASP:OD1	1:C:691:VAL:N	2.47	0.42
1:E:564:ARG:HD3	1:E:801:TRP:CH2	2.55	0.42
1:E:698:ILE:HD13	1:E:698:ILE:N	2.35	0.42
1:A:580:PRO:HD2	1:A:704:GLN:CD	2.40	0.42
1:A:644:ASN:HD22	1:A:684:VAL:H	1.68	0.42
2:B:410:SER:OG	2:B:412:ARG:HB3	2.19	0.42
1:C:4:PHE:HD2	1:C:45:ILE:HG23	1.84	0.42
1:C:525:SER:OG	1:C:527:GLU:HG3	2.20	0.42
2:D:498:LEU:HA	2:D:498:LEU:HD23	1.69	0.42
1:E:108:HIS:O	1:E:111:PHE:HD2	2.01	0.42
1:E:202:VAL:HB	1:E:209:VAL:CG2	2.49	0.42
1:E:89:ILE:HG22	1:E:91:GLN:HB3	2.01	0.42
1:A:556:ILE:HG22	1:A:557:SER:O	2.19	0.42
1:A:760:ARG:O	1:A:761:PRO:C	2.58	0.42
2:D:582:LEU:HD12	2:D:583:ASP:N	2.35	0.42
1:E:132:ILE:CD1	1:E:132:ILE:N	2.82	0.42
1:E:25:ILE:HD12	1:E:142:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:ILE:HD12	1:E:142:VAL:CG1	2.50	0.42
1:E:636:PHE:CE1	1:E:645:LEU:HD21	2.54	0.42
2:F:531:ILE:HG22	2:F:533:HIS:H	1.85	0.42
1:A:144:ARG:NH2	1:A:791:GLN:O	2.53	0.42
1:A:46:ILE:HD12	1:A:46:ILE:HA	1.91	0.42
1:A:607:ASN:HA	1:A:608:PRO:HD3	1.82	0.42
2:B:484:ASP:OD2	2:B:494:ARG:CG	2.68	0.42
1:C:501:LEU:O	1:C:501:LEU:HD23	2.17	0.42
1:C:569:SER:O	1:C:592:PRO:HD3	2.20	0.42
2:D:523:ALA:O	2:D:524:ALA:C	2.57	0.42
1:E:121:VAL:HG11	1:E:383:SER:HB3	2.01	0.42
1:E:418:TYR:HD1	1:E:424:ASP:O	2.02	0.42
1:E:525:SER:O	2:F:412:ARG:CZ	2.67	0.42
1:A:590:ALA:HA	1:A:685:ARG:O	2.20	0.42
2:B:443:PHE:CD2	2:B:445:GLU:HB2	2.55	0.42
1:C:487:PRO:HB3	1:C:531:ALA:HB1	2.02	0.42
1:C:828:MET:CE	2:D:576:ARG:HE	2.32	0.42
1:E:694:HIS:CE1	1:E:699:DDE:CD2	3.03	0.42
1:E:740:VAL:HG21	1:E:766:PHE:HD1	1.85	0.42
1:E:89:ILE:O	1:E:91:GLN:N	2.53	0.42
1:E:78:TYR:CE1	1:E:97:SER:HB3	2.48	0.42
2:F:470:TYR:CD2	2:F:555:ILE:HG12	2.55	0.42
1:A:154:VAL:CG1	1:A:337:MET:HE3	2.50	0.42
1:A:607:ASN:HB3	1:A:610:ASP:CG	2.40	0.42
2:B:558:TRP:O	2:B:559:PRO:C	2.55	0.42
1:C:237:LYS:O	1:C:241:MET:HG2	2.20	0.42
1:C:46:ILE:HD12	1:C:46:ILE:HA	1.92	0.42
2:D:518:LEU:CD2	2:D:518:LEU:H	2.33	0.42
1:E:536:LEU:O	1:E:539:GLU:HB3	2.20	0.42
1:A:10:ARG:HG3	1:A:11:SER:N	2.35	0.41
1:A:380:LEU:HD23	1:A:381:TYR:N	2.35	0.41
1:A:600:ALA:HB1	1:A:606:ILE:HG12	2.00	0.41
1:C:426:LEU:O	1:C:427:PHE:CD1	2.73	0.41
1:C:511:LEU:HD22	1:C:545:LEU:HD13	2.02	0.41
1:C:543:GLN:O	1:C:547:HIS:N	2.46	0.41
1:C:739:ALA:HB2	1:C:791:GLN:OE1	2.20	0.41
2:D:518:LEU:HD11	2:D:542:ILE:HD13	2.02	0.41
2:D:570:ALA:O	2:D:572:PRO:HD3	2.20	0.41
1:E:237:LYS:O	1:E:241:MET:HE2	2.19	0.41
1:E:515:ASP:HA	1:E:516:PRO:HD3	1.80	0.41
1:E:600:ALA:HB1	1:E:606:ILE:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:457:ALA:HB2	2:F:558:TRP:CD2	2.55	0.41
1:A:258:THR:CG2	1:A:259:ASN:N	2.79	0.41
1:A:515:ASP:HA	1:A:516:PRO:HD3	1.89	0.41
1:C:19:VAL:HG12	1:C:20:ARG:N	2.35	0.41
1:C:646:VAL:HG13	1:C:688:ILE:CD1	2.50	0.41
1:C:73:THR:HG22	1:C:73:THR:O	2.21	0.41
1:E:305:ILE:HG21	1:E:323:VAL:HG13	2.02	0.41
1:E:123:ASP:HB3	1:E:343:PRO:HG2	2.00	0.41
1:E:406:LYS:O	1:E:409:GLN:HB3	2.19	0.41
1:E:524:GLU:C	1:E:526:GLY:H	2.24	0.41
1:E:584:ASN:HD22	1:E:693:LEU:HA	1.84	0.41
1:E:804:LEU:N	1:E:804:LEU:HD23	2.35	0.41
1:A:395:TYR:CE1	1:A:457:VAL:HG13	2.55	0.41
1:A:556:ILE:N	1:A:556:ILE:HD12	2.35	0.41
2:B:535:LEU:HB3	2:B:536:PRO:HA	2.02	0.41
1:C:192:TYR:HA	1:C:763:THR:HG22	2.02	0.41
1:C:38:SER:HA	1:C:41:GLN:CG	2.49	0.41
1:C:530:VAL:O	1:C:538:LEU:HD11	2.21	0.41
1:C:609:ARG:NH1	1:C:609:ARG:HG3	2.35	0.41
1:E:164:LEU:HD12	1:E:285:PHE:CE1	2.56	0.41
1:E:144:ARG:HG2	1:E:192:TYR:CG	2.55	0.41
1:E:314:LEU:O	1:E:319:LEU:HB2	2.20	0.41
1:E:314:LEU:C	1:E:319:LEU:HB2	2.40	0.41
1:E:760:ARG:O	1:E:761:PRO:C	2.59	0.41
1:A:221:THR:OG1	1:A:224:GLN:HG3	2.20	0.41
1:A:503:LYS:HB2	1:A:552:VAL:HG21	2.01	0.41
2:B:518:LEU:N	2:B:518:LEU:HD22	2.34	0.41
1:C:274:ASN:HA	1:C:278:LEU:HB2	2.02	0.41
1:C:485:VAL:O	1:C:485:VAL:HG22	2.19	0.41
1:C:740:VAL:HG21	1:C:766:PHE:HB2	2.01	0.41
1:C:192:TYR:HE1	1:C:765:LEU:HB2	1.86	0.41
1:E:239:LYS:NZ	1:E:243:ARG:NH2	2.69	0.41
1:E:46:ILE:HG22	1:E:47:SER:N	2.27	0.41
1:A:103:ILE:HD13	1:A:121:VAL:HG23	2.01	0.41
1:A:406:LYS:HB3	1:A:447:ASP:HB2	2.03	0.41
2:B:484:ASP:OD2	2:B:494:ARG:CD	2.69	0.41
1:C:418:TYR:HB3	1:C:477:ASN:HD21	1.85	0.41
1:C:501:LEU:N	1:C:502:PRO:CD	2.83	0.41
1:C:600:ALA:HB1	1:C:606:ILE:HG12	2.00	0.41
1:C:758:GLU:O	1:C:759:GLN:HB3	2.19	0.41
2:D:530:LEU:HD23	2:D:604:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:734:GLN:H	1:E:734:GLN:HE21	1.65	0.41
1:A:634:TRP:O	1:A:635:CYS:HB3	2.20	0.41
2:B:446:ALA:O	2:B:447:ALA:C	2.59	0.41
1:C:124:GLY:HA3	1:C:342:LEU:HD22	2.01	0.41
1:C:523:SER:HG	1:C:527:GLU:HB2	1.85	0.41
2:D:451:VAL:O	2:D:451:VAL:CG1	2.68	0.41
2:D:518:LEU:N	2:D:518:LEU:HD22	2.35	0.41
1:E:807:ASP:HA	1:E:808:PRO:HD2	1.95	0.41
2:F:423:LEU:HD11	2:F:590:LYS:HD3	2.03	0.41
2:F:571:ILE:HD11	2:F:587:ILE:HD12	2.02	0.41
1:A:239:LYS:HG2	1:A:239:LYS:O	2.20	0.41
1:A:606:ILE:HD12	1:A:619:MET:HG3	2.01	0.41
1:A:654:GLN:HG2	1:A:655:TYR:CE2	2.54	0.41
1:C:167:LEU:N	1:C:167:LEU:CD1	2.84	0.41
1:C:218:TRP:C	1:C:330:ALA:HB2	2.41	0.41
1:C:397:PHE:HD1	1:C:437:MET:HG3	1.86	0.41
1:C:804:LEU:N	1:C:804:LEU:HD23	2.35	0.41
1:E:126:LEU:HD11	1:E:156:VAL:HG23	2.00	0.41
1:A:124:GLY:HA3	1:A:342:LEU:HD22	2.02	0.41
1:A:27:HIS:CD2	1:A:29:ASP:HB2	2.56	0.41
1:A:512:SER:HA	1:A:518:VAL:CG1	2.51	0.41
2:B:450:ILE:HG23	2:B:455:VAL:CG2	2.51	0.41
1:E:10:ARG:HA	1:E:10:ARG:HD2	1.91	0.41
1:A:71:LYS:O	1:A:386:VAL:HG21	2.21	0.41
1:C:152:LYS:HD2	1:C:200:VAL:HG22	2.03	0.41
1:C:597:VAL:O	1:C:601:ILE:HG13	2.20	0.41
1:E:594:ASP:HB2	1:E:597:VAL:HG23	2.03	0.41
1:E:806:SER:HB2	1:E:813:SER:HB2	2.02	0.41
1:A:254:THR:O	1:A:255:LYS:HB2	2.21	0.41
1:A:363:ASP:O	1:A:367:ILE:HG13	2.21	0.41
2:B:467:ARG:HG3	2:B:558:TRP:HD1	1.84	0.41
1:C:169:VAL:HG13	1:C:169:VAL:O	2.21	0.41
1:C:338:ILE:O	1:C:342:LEU:HB2	2.21	0.41
2:D:445:GLU:CD	2:D:494:ARG:HH22	2.23	0.41
2:D:495:ASN:OD1	2:D:495:ASN:N	2.53	0.41
1:E:186:ASN:HA	1:E:189:VAL:HB	2.03	0.41
1:E:221:THR:HG21	1:E:336:GLU:OE1	2.21	0.41
1:E:303:LEU:O	1:E:304:GLU:CB	2.69	0.41
1:E:397:PHE:HD1	1:E:437:MET:HG3	1.85	0.41
1:A:729:PHE:CE2	1:A:774:VAL:HG22	2.56	0.41
1:A:784:LEU:CD2	1:A:794:PRO:HG3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:PHE:CE1	1:C:315:GLU:HB2	2.52	0.41
1:C:316:GLY:O	1:C:319:LEU:N	2.54	0.41
1:C:521:TYR:O	1:C:529:ILE:HD12	2.21	0.41
2:D:448:GLN:HB2	2:D:448:GLN:HE21	1.71	0.41
1:E:262:THR:HG21	1:E:266:GLY:HA2	2.02	0.41
1:E:39:LEU:HD11	1:E:334:LEU:HB2	2.03	0.41
1:E:5:THR:OG1	1:E:8:GLN:HG3	2.21	0.41
1:E:70:ILE:HA	1:E:388:THR:HA	2.03	0.41
2:F:464:ALA:O	2:F:467:ARG:HB3	2.21	0.41
1:C:379:MET:SD	1:C:470:THR:HG22	2.61	0.40
1:C:495:VAL:CG1	1:C:554:LEU:HD23	2.50	0.40
1:C:588:LEU:CD1	1:C:588:LEU:C	2.87	0.40
1:C:611:ASP:O	1:C:612:PHE:C	2.59	0.40
1:C:799:ASP:OD1	1:C:800:HIS:HD2	2.04	0.40
1:E:731:VAL:HG13	1:E:731:VAL:O	2.20	0.40
1:E:797:VAL:HG22	1:E:798:PHE:N	2.35	0.40
2:F:400:PHE:O	2:F:425:ALA:HB1	2.20	0.40
2:F:558:TRP:O	2:F:559:PRO:C	2.57	0.40
1:A:576:LEU:HD13	1:A:587:TYR:CD1	2.56	0.40
1:A:700:ARG:HB2	1:A:700:ARG:HE	1.49	0.40
1:A:91:GLN:O	1:A:93:THR:HG23	2.21	0.40
1:C:550:ALA:C	1:C:552:VAL:H	2.24	0.40
1:E:189:VAL:O	1:E:193:ALA:CB	2.69	0.40
1:E:205:ALA:HB2	1:E:245:TRP:HB3	2.02	0.40
1:E:267:LYS:HA	1:E:268:PRO:HD3	1.86	0.40
1:E:391:LYS:CG	1:E:392:GLY:H	2.34	0.40
1:E:500:ASP:O	1:E:503:LYS:N	2.50	0.40
1:E:823:ARG:HG2	1:E:823:ARG:NH1	2.36	0.40
2:F:429:LEU:O	2:F:434:TYR:HB2	2.22	0.40
1:A:26:ALA:CB	1:A:128:VAL:HB	2.51	0.40
1:A:404:THR:HB	1:A:447:ASP:OD2	2.21	0.40
1:A:694:HIS:HD2	1:A:696:ASP:N	1.99	0.40
1:C:237:LYS:HA	1:C:240:MET:HB3	2.04	0.40
1:E:108:HIS:HB2	1:E:111:PHE:CE2	2.57	0.40
1:E:167:LEU:CD1	1:E:167:LEU:H	2.34	0.40
1:E:388:THR:HG21	1:E:395:TYR:CD1	2.56	0.40
1:E:74:ALA:O	1:E:439:GLY:CA	2.67	0.40
1:C:360:PRO:C	1:C:362:ASP:H	2.24	0.40
1:C:411:VAL:HG11	1:C:469:LEU:HB3	2.04	0.40
1:C:454:ILE:CG1	1:C:455:GLY:N	2.85	0.40
1:C:116:THR:CB	1:C:481:MET:HE3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:GLU:OE2	1:C:685:ARG:NH1	2.55	0.40
1:E:169:VAL:CG2	1:E:173:ASP:HB2	2.51	0.40
1:E:68:ILE:HG23	1:E:390:ASP:CB	2.50	0.40
1:A:512:SER:HA	1:A:518:VAL:HG13	2.04	0.40
1:A:644:ASN:ND2	1:A:684:VAL:HB	2.31	0.40
1:C:146:ALA:O	1:C:151:ILE:HG12	2.22	0.40
1:C:319:LEU:O	1:C:323:VAL:HG23	2.20	0.40
1:C:591:GLU:HA	1:C:592:PRO:HD3	1.84	0.40
1:C:736:PRO:O	1:C:739:ALA:N	2.52	0.40
2:D:436:PHE:HB2	2:D:502:TYR:CE2	2.56	0.40
2:D:479:TYR:CD2	2:D:582:LEU:HB2	2.56	0.40
1:E:111:PHE:O	1:E:112:SER:C	2.59	0.40
2:F:535:LEU:HB3	2:F:536:PRO:HA	2.04	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	818/842 (97%)	729 (89%)	75 (9%)	14 (2%)	9	34
1	C	818/842 (97%)	716 (88%)	80 (10%)	22 (3%)	5	23
1	E	818/842 (97%)	712 (87%)	90 (11%)	16 (2%)	7	29
2	B	205/207 (99%)	181 (88%)	22 (11%)	2 (1%)	15	47
2	D	205/207 (99%)	182 (89%)	17 (8%)	6 (3%)	4	22
2	F	205/207 (99%)	179 (87%)	21 (10%)	5 (2%)	6	25
All	All	3069/3147 (98%)	2699 (88%)	305 (10%)	65 (2%)	7	28

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	SER
1	A	761	PRO
2	B	518	LEU
2	B	519	ALA
1	C	235	VAL
1	C	264	ALA
1	C	761	PRO
2	D	518	LEU
2	D	519	ALA
1	E	112	SER
1	E	558	PRO
1	E	761	PRO
2	F	519	ALA
1	A	309	GLY
1	A	390	ASP
1	A	498	ALA
1	C	112	SER
1	C	309	GLY
1	C	460	ASP
1	C	549	HIS
1	C	551	GLY
1	C	737	GLU
2	D	491	GLY
1	E	304	GLU
1	E	390	ASP
1	E	479	LYS
2	F	454	GLY
1	A	111	PHE
1	A	237	LYS
1	A	479	LYS
1	C	266	GLY
1	C	479	LYS
1	E	90	LYS
1	E	233	PHE
2	F	577	ASN
1	A	460	ASP
1	A	677	PHE
1	C	265	GLU
1	C	314	LEU
1	C	558	PRO
1	C	743	ILE
1	C	785	ARG
1	E	372	CYS

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Mol	Chain	Res	Type
1	E	621	ASP
1	A	446	ASP
1	C	120	ARG
1	C	329	PRO
1	C	446	ASP
1	C	525	SER
2	D	604	PRO
1	E	446	ASP
1	E	737	GLU
1	E	743	ILE
2	F	404	GLY
1	A	621	ASP
1	E	428	ILE
2	D	404	GLY
2	D	405	GLY
1	E	338	ILE
2	F	450	ILE
1	C	491	VAL
1	A	604	GLY
1	A	329	PRO
1	E	556	ILE
1	C	604	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	699/714 (98%)	662 (95%)	37 (5%)	22	53
1	C	699/714 (98%)	649 (93%)	50 (7%)	14	42
1	E	699/714 (98%)	659 (94%)	40 (6%)	20	50
2	B	161/162 (99%)	142 (88%)	19 (12%)	5	20
2	D	161/162 (99%)	146 (91%)	15 (9%)	9	31
2	F	161/162 (99%)	144 (89%)	17 (11%)	6	24
All	All	2580/2628 (98%)	2402 (93%)	178 (7%)	15	44



All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	15	LYS
1	A	36	THR
1	A	68	ILE
1	A	81	MET
1	A	83	ASP
1	A	91	GLN
1	A	113	SER
1	A	152	LYS
1	A	162	ARG
1	A	200	VAL
1	A	236	ASP
1	A	261	ASP
1	A	262	THR
1	A	275	MET
1	A	347	THR
1	A	352	ARG
1	A	362	ASP
1	A	460	ASP
1	A	489	VAL
1	A	536	LEU
1	A	544	ASP
1	A	582	LYS
1	A	597	VAL
1	A	599	LEU
1	A	609	ARG
1	A	677	PHE
1	A	710	ARG
1	A	718	LEU
1	A	724	ILE
1	A	730	LEU
1	A	734	GLN
1	A	738	GLN
1	A	767	THR
1	A	775	ASN
1	A	785	ARG
1	A	836	GLN
2	B	412	ARG
2	B	420	GLU
2	B	422	LEU
2	B	456	ARG
2	B	467	ARG

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Mol	Chain	Res	Type
2	B	488	ASP
2	B	492	ARG
2	B	494	ARG
2	B	495	ASN
2	B	499	LEU
2	B	506	SER
2	B	540	ASP
2	B	547	GLU
2	B	551	ARG
2	B	552	LEU
2	B	559	PRO
2	B	560	LEU
2	B	577	ASN
2	B	602	SER
1	C	14	ASP
1	C	36	THR
1	C	68	ILE
1	C	81	MET
1	C	83	ASP
1	C	94	ASP
1	C	113	SER
1	C	164	LEU
1	C	167	LEU
1	C	183	GLU
1	C	195	GLU
1	C	231	LYS
1	C	242	ASP
1	C	253	LYS
1	C	256	LYS
1	C	282	PHE
1	C	299	LEU
1	C	301	GLU
1	C	317	LYS
1	C	320	LEU
1	C	347	THR
1	C	362	ASP
1	C	432	GLN
1	C	460	ASP
1	C	461	GLN
1	C	489	VAL
1	C	494	GLU
1	C	495	VAL

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Mol	Chain	Res	Type
1	C	497	ASN
1	C	500	ASP
1	C	506	GLU
1	C	524	GLU
1	C	528	HIS
1	C	544	ASP
1	C	552	VAL
1	C	556	ILE
1	C	599	LEU
1	C	609	ARG
1	C	625	TRP
1	C	677	PHE
1	C	718	LEU
1	C	730	LEU
1	C	734	GLN
1	C	738	GLN
1	C	761	PRO
1	C	767	THR
1	C	775	ASN
1	C	820	LEU
1	C	836	GLN
1	C	837	GLU
2	D	403	ASP
2	D	410	SER
2	D	411	THR
2	D	422	LEU
2	D	483	GLN
2	D	488	ASP
2	D	494	ARG
2	D	499	LEU
2	D	538	ARG
2	D	540	ASP
2	D	547	GLU
2	D	551	ARG
2	D	560	LEU
2	D	577	ASN
2	D	602	SER
1	E	23	SER
1	E	46	ILE
1	E	87	LYS
1	E	94	ASP
1	E	161	ASP

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Mol	Chain	Res	Type
1	E	183	GLU
1	E	186	ASN
1	E	194	ASP
1	E	211	PHE
1	E	216	HIS
1	E	263	ASP
1	E	275	MET
1	E	282	PHE
1	E	313	ASP
1	E	347	THR
1	E	362	ASP
1	E	440	ARG
1	E	460	ASP
1	E	489	VAL
1	E	544	ASP
1	E	552	VAL
1	E	558	PRO
1	E	599	LEU
1	E	625	TRP
1	E	677	PHE
1	E	698	ILE
1	E	710	ARG
1	E	718	LEU
1	E	724	ILE
1	E	730	LEU
1	E	734	GLN
1	E	738	GLN
1	E	749	LYS
1	E	761	PRO
1	E	767	THR
1	E	775	ASN
1	E	786	GLN
1	E	800	HIS
1	E	836	GLN
1	E	837	GLU
2	F	403	ASP
2	F	411	THR
2	F	422	LEU
2	F	467	ARG
2	F	494	ARG
2	F	498	LEU
2	F	499	LEU

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Mol	Chain	Res	Type
2	F	513	ARG
2	F	522	GLU
2	F	538	ARG
2	F	540	ASP
2	F	547	GLU
2	F	552	LEU
2	F	560	LEU
2	F	577	ASN
2	F	599	ASP
2	F	604	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	30	HIS
1	A	91	GLN
1	A	101	ASN
1	A	108	HIS
1	A	138	GLN
1	A	176	GLN
1	A	201	GLN
1	A	274	ASN
1	A	371	ASN
1	A	537	HIS
1	A	547	HIS
1	A	549	HIS
1	A	581	ASN
1	A	584	ASN
1	A	644	ASN
1	A	654	GLN
1	A	687	ASN
1	A	694	HIS
1	A	734	GLN
1	A	738	GLN
1	A	753	GLN
1	A	800	HIS
1	A	836	GLN
2	B	428	GLN
2	B	448	GLN
2	B	495	ASN
2	B	577	ASN

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Mol	Chain	Res	Type
1	C	21	ASN
1	C	27	HIS
1	C	91	GLN
1	C	108	HIS
1	C	138	GLN
1	C	201	GLN
1	C	251	ASN
1	C	371	ASN
1	C	414	GLN
1	C	452	ASN
1	C	497	ASN
1	C	528	HIS
1	C	537	HIS
1	C	547	HIS
1	C	549	HIS
1	C	581	ASN
1	C	583	HIS
1	C	584	ASN
1	C	644	ASN
1	C	687	ASN
1	C	694	HIS
1	C	734	GLN
1	C	738	GLN
1	C	753	GLN
1	C	800	HIS
1	C	836	GLN
2	D	448	GLN
2	D	460	GLN
2	D	577	ASN
1	E	27	HIS
1	E	91	GLN
1	E	138	GLN
1	E	201	GLN
1	E	371	ASN
1	E	528	HIS
1	E	537	HIS
1	E	547	HIS
1	E	581	ASN
1	E	583	HIS
1	E	584	ASN
1	E	644	ASN
1	E	654	GLN

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Mol	Chain	Res	Type
1	E	687	ASN
1	E	694	HIS
1	E	734	GLN
1	E	753	GLN
1	E	800	HIS
1	E	836	GLN
2	F	428	GLN
2	F	448	GLN
2	F	460	GLN
2	F	577	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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
1	DDE	A	699	1	5,10,21	0.63	0	3,12,30	1.51	1 (33%)
1	DDE	C	699	1	5,10,21	0.52	0	3,12,30	1.53	1 (33%)
1	DDE	E	699	1	5,10,21	0.58	0	3,12,30	1.37	1 (33%)

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
1	DDE	A	699	1	-	0/5/6/23	0/1/1/1
1	DDE	C	699	1	-	0/5/6/23	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DDE	E	699	1	-	0/5/6/23	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	699	DDE	CD2-NE2-CE1	2.13	109.11	105.78
1	A	699	DDE	CD2-NE2-CE1	2.10	109.05	105.78
1	E	699	DDE	CD2-NE2-CE1	2.06	109.00	105.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	699	DDE	1	0
1	C	699	DDE	1	0
1	E	699	DDE	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	822/842 (97%)	-0.22	14 (1%) 70 48	8, 57, 85, 104	0
1	C	822/842 (97%)	0.10	39 (4%) 31 14	10, 69, 123, 135	0
1	E	822/842 (97%)	0.78	154 (18%) 1 0	6, 105, 128, 146	0
2	B	207/207 (100%)	-0.59	2 (0%) 82 66	5, 24, 57, 74	0
2	D	207/207 (100%)	-0.60	0 100 100	5, 23, 61, 76	0
2	F	207/207 (100%)	-0.54	0 100 100	10, 31, 63, 82	0
All	All	3087/3147 (98%)	0.06	209 (6%) 17 7	5, 60, 123, 146	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	107	GLY	8.6
1	E	189	VAL	7.2
1	C	551	GLY	6.5
1	C	251	ASN	6.2
1	E	759	GLN	6.0
1	E	194	ASP	5.8
1	E	193	ALA	5.8
1	E	554	LEU	5.6
1	E	546	GLU	5.5
1	E	343	PRO	5.4
1	C	499	ASN	5.3
1	E	257	TRP	5.2
1	E	47	SER	5.1
1	E	97	SER	5.1
1	E	737	GLU	5.1
1	E	108	HIS	5.0
1	E	280	PRO	5.0
1	C	296	ILE	4.8
1	C	291	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	276	PHE	4.8
1	E	33	SER	4.6
1	E	143	LEU	4.6
1	E	231	LYS	4.5
1	C	168	GLN	4.4
1	E	179	ALA	4.2
1	C	493	VAL	4.2
1	E	175	TYR	4.1
1	E	67	GLY	4.1
1	E	240	MET	4.0
1	E	110	ASP	4.0
1	E	146	ALA	4.0
1	E	313	ASP	3.9
1	E	256	LYS	3.9
1	E	314	LEU	3.9
1	E	525	SER	3.9
1	E	339	VAL	3.8
1	E	245	TRP	3.7
1	C	552	VAL	3.7
1	C	108	HIS	3.7
1	E	5	THR	3.7
1	E	89	ILE	3.7
1	E	155	VAL	3.7
1	C	307	LEU	3.6
1	E	80	GLU	3.6
1	E	167	LEU	3.6
1	E	335	LEU	3.6
1	E	310	ASP	3.5
1	E	551	GLY	3.5
1	E	99	LEU	3.5
1	E	348	ALA	3.4
1	E	279	ASP	3.4
1	E	398	GLY	3.4
1	E	317	LYS	3.4
1	C	306	VAL	3.3
1	E	269	LEU	3.3
1	C	544	ASP	3.3
1	A	47	SER	3.3
1	E	392	GLY	3.3
1	E	501	LEU	3.3
1	E	777	SER	3.3
2	B	519	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	547	HIS	3.3
1	C	264	ALA	3.2
1	C	549	HIS	3.2
1	E	349	GLN	3.2
1	E	334	LEU	3.2
1	E	499	ASN	3.2
1	E	201	GLN	3.2
1	E	444	PRO	3.2
1	E	510	ARG	3.1
1	C	300	LEU	3.1
1	E	290	ASN	3.1
1	E	311	GLU	3.1
1	E	273	PHE	3.0
1	A	398	GLY	3.0
1	E	132	ILE	3.0
1	E	134	GLY	3.0
1	C	555	LYS	3.0
1	E	96	ASN	3.0
1	E	243	ARG	3.0
1	E	78	TYR	3.0
1	E	553	PRO	3.0
1	E	166	GLU	3.0
1	E	498	ALA	2.9
1	E	209	VAL	2.9
1	C	29	ASP	2.9
1	A	420	PRO	2.9
1	E	494	GLU	2.9
1	C	323	VAL	2.9
1	E	242	ASP	2.9
1	E	200	VAL	2.9
1	E	784	LEU	2.9
1	E	315	GLU	2.9
1	E	442	VAL	2.8
1	E	302	LYS	2.8
1	E	362	ASP	2.8
1	E	188	ILE	2.8
1	E	275	MET	2.8
1	A	33	SER	2.8
1	E	421	GLY	2.8
1	E	216	HIS	2.8
1	C	554	LEU	2.8
1	E	258	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	266	GLY	2.8
1	E	758	GLU	2.8
1	E	541	CYS	2.8
1	E	745	SER	2.8
1	E	766	PHE	2.8
1	E	390	ASP	2.7
1	E	336	GLU	2.7
1	A	7	ASP	2.7
1	E	196	VAL	2.7
1	C	7	ASP	2.7
1	E	356	LEU	2.7
1	E	230	ALA	2.7
1	E	244	LEU	2.7
1	E	32	LYS	2.7
1	E	790	GLY	2.7
1	E	48	ALA	2.7
1	E	308	LYS	2.7
1	A	495	VAL	2.7
1	E	93	THR	2.6
1	E	111	PHE	2.6
1	E	7	ASP	2.6
1	E	255	LYS	2.6
1	A	46	ILE	2.6
1	C	263	ASP	2.6
1	E	239	LYS	2.6
1	E	360	PRO	2.6
1	C	504	LEU	2.6
1	E	68	ILE	2.6
1	E	301	GLU	2.6
1	E	420	PRO	2.5
1	E	757	GLU	2.5
1	E	419	VAL	2.5
1	E	126	LEU	2.5
1	E	474	THR	2.5
1	E	472	SER	2.5
1	E	187	VAL	2.5
1	E	316	GLY	2.5
1	E	277	ILE	2.5
1	A	5	THR	2.4
1	C	299	LEU	2.4
1	E	522	MET	2.4
1	E	391	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	477	ASN	2.4
1	E	367	ILE	2.4
1	E	761	PRO	2.4
1	E	781	THR	2.4
1	E	197	LEU	2.4
1	A	392	GLY	2.4
1	A	107	GLY	2.3
1	E	221	THR	2.3
1	E	418	TYR	2.3
1	E	158	ASN	2.3
1	E	452	ASN	2.3
1	C	548	ASP	2.3
1	E	82	SER	2.3
1	E	770	ALA	2.3
1	C	107	GLY	2.3
1	E	20	ARG	2.3
1	C	216	HIS	2.3
1	E	338	ILE	2.3
1	E	476	HIS	2.3
1	E	228	ARG	2.3
1	E	260	LYS	2.3
1	E	46	ILE	2.3
1	E	131	THR	2.3
1	E	764	PRO	2.2
1	C	233	PHE	2.2
1	C	252	PRO	2.2
1	E	195	GLU	2.2
1	C	292	LYS	2.2
1	E	94	ASP	2.2
1	E	443	GLU	2.2
1	C	553	PRO	2.2
1	E	192	TYR	2.2
1	E	358	GLU	2.2
1	E	294	ASP	2.2
1	E	306	VAL	2.2
1	E	366	CYS	2.2
1	E	254	THR	2.2
1	E	31	GLY	2.2
1	E	738	GLN	2.2
1	E	232	LYS	2.2
1	A	763	THR	2.2
1	E	163	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	236	ASP	2.1
1	C	362	ASP	2.1
1	E	137	VAL	2.1
1	C	270	GLU	2.1
1	E	309	GLY	2.1
1	A	361	ALA	2.1
1	C	293	LYS	2.1
1	C	513	LYS	2.1
1	E	151	ILE	2.1
1	E	455	GLY	2.1
1	A	233	PHE	2.1
1	E	186	ASN	2.1
1	E	127	VAL	2.1
1	C	294	ASP	2.1
1	E	298	VAL	2.0
1	A	417	ASN	2.0
1	C	556	ILE	2.0
2	B	521	PRO	2.0
1	E	21	ASN	2.0
1	E	263	ASP	2.0
1	E	363	ASP	2.0
1	E	154	VAL	2.0

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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	DDE	E	699	10/21	0.93	0.16	44,48,49,50	0
1	DDE	C	699	10/21	0.95	0.14	43,47,48,50	0
1	DDE	A	699	10/21	0.96	0.12	40,42,44,45	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.