



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2022 – 10:04 AM EDT

PDB ID : 7UJB  
Title : N-terminal domain deletion variant of Eta  
Authors : Qayyum, M.Z.; Murakami, K.S.  
Deposited on : 2022-03-30  
Resolution : 4.12 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.

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

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

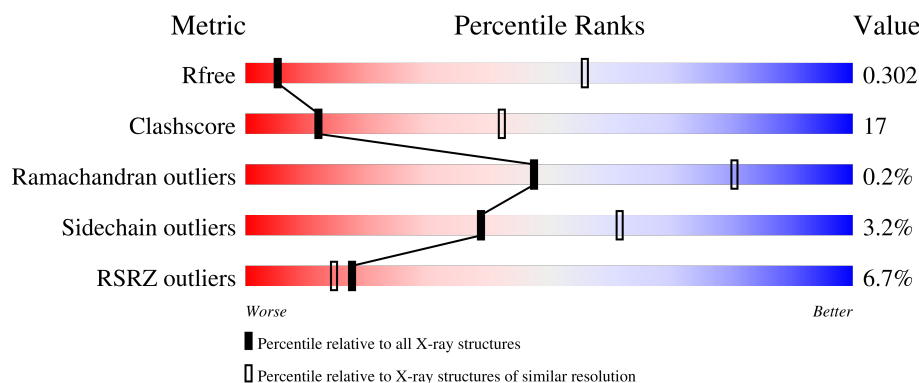
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.12 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	1024 (4.50-3.74)
Clashscore	141614	1011 (4.48-3.76)
Ramachandran outliers	138981	1043 (4.50-3.74)
Sidechain outliers	138945	1030 (4.50-3.74)
RSRZ outliers	127900	1041 (4.54-3.70)

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  $\geq 3$ , 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	639	<div> <div>6%</div> <div>64%</div> <div>34%</div> <div>..</div> </div>
1	B	639	<div> <div>7%</div> <div>64%</div> <div>34%</div> <div>..</div> </div>
1	C	639	<div> <div>8%</div> <div>59%</div> <div>39%</div> <div>.</div> </div>
1	D	639	<div> <div>6%</div> <div>60%</div> <div>37%</div> <div>.</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20234 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.

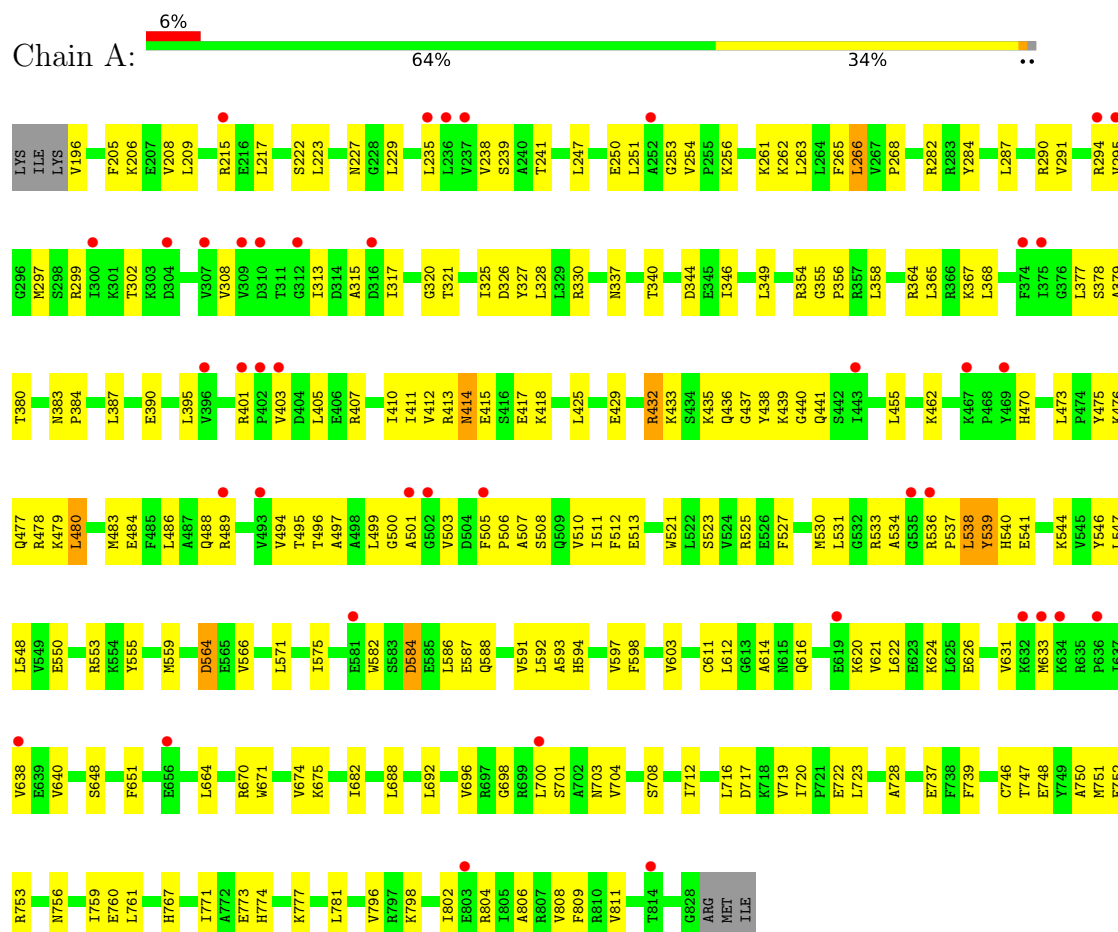
- Molecule 1 is a protein called DEAD/DEAH box RNA helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	633	Total	C	N	O	S	0	0	0
			5034	3219	877	921	17			
1	B	633	Total	C	N	O	S	0	0	0
			5034	3219	877	921	17			
1	C	639	Total	C	N	O	S	0	0	0
			5087	3254	888	927	18			
1	D	638	Total	C	N	O	S	0	0	0
			5079	3248	887	926	18			

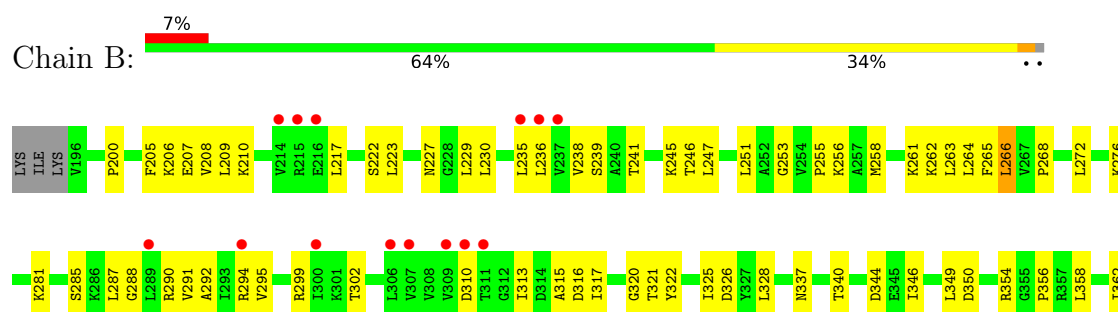
### 3 Residue-property plots

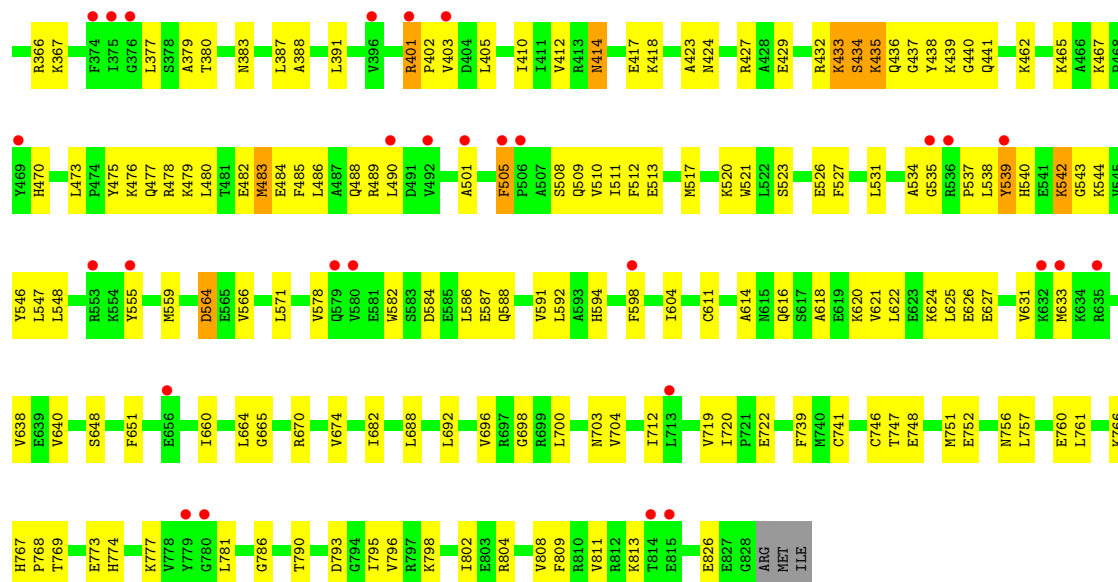
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DEAD/DEAH box RNA helicase

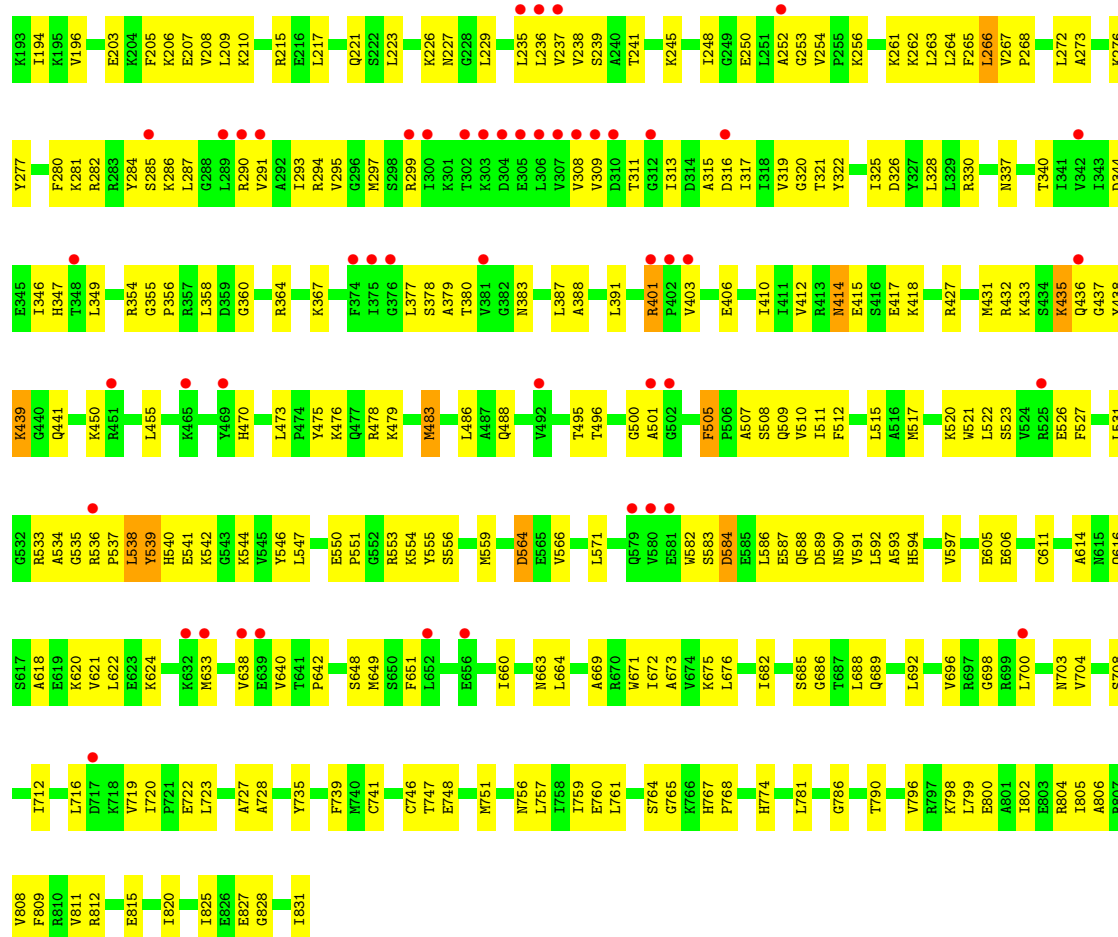


#### • Molecule 1: DEAD/DEAH box RNA helicase

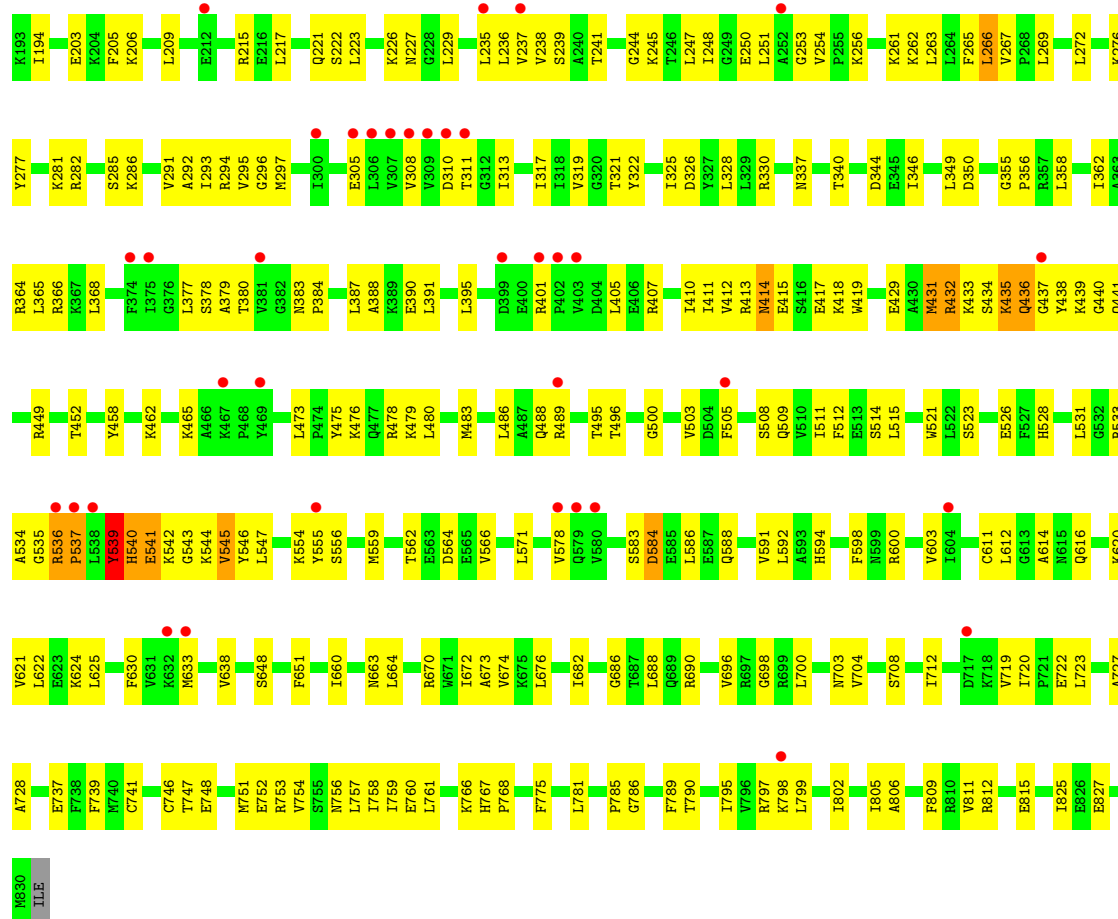




• Molecule 1: DEAD/DEAH box RNA helicase



• Molecule 1: DEAD/DEAH box RNA helicase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.24Å 135.24Å 262.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.48 – 4.12 48.66 – 4.12	Depositor EDS
% Data completeness (in resolution range)	90.0 (43.48-4.12) 90.1 (48.66-4.12)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.250 , 0.303 0.252 , 0.302	Depositor DCC
$R_{free}$ test set	1997 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	177.0	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 302.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.378 for -h,-k,l 0.389 for h,-h-k,-l 0.388 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	20234	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	242.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.36	0/5123	0.61	0/6907
1	B	0.36	0/5123	0.62	1/6907 (0.0%)
1	C	0.36	0/5176	0.61	0/6975
1	D	0.36	0/5168	0.62	1/6964 (0.0%)
All	All	0.36	0/20590	0.61	2/27753 (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	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	766	LYS	C-N-CA	6.18	137.14	121.70
1	D	766	LYS	C-N-CA	5.36	135.10	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	538	LEU	Peptide
1	D	539	TYR	Peptide



## 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	5034	0	5187	170	0
1	B	5034	0	5187	167	0
1	C	5087	0	5257	198	0
1	D	5079	0	5246	193	0
All	All	20234	0	20877	706	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 17.

All (706) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:PRO:HA	1:A:537:PRO:HB3	1.47	0.95
1:D:412:VAL:HG21	1:D:418:LYS:HB2	1.57	0.87
1:D:535:GLY:HA2	1:D:540:HIS:HE1	1.41	0.86
1:B:435:LYS:HD2	1:B:436:GLN:H	1.39	0.86
1:A:412:VAL:HG21	1:A:418:LYS:HB2	1.59	0.85
1:A:356:PRO:HG2	1:A:586:LEU:HD13	1.65	0.79
1:C:412:VAL:HG21	1:C:418:LYS:HB2	1.63	0.79
1:A:326:ASP:HB3	1:A:651:PHE:HZ	1.48	0.78
1:B:326:ASP:HB3	1:B:651:PHE:HZ	1.47	0.78
1:D:238:VAL:HG12	1:D:380:THR:HA	1.66	0.78
1:C:439:LYS:NZ	1:C:488:GLN:O	2.16	0.78
1:D:412:VAL:HG11	1:D:418:LYS:HA	1.66	0.78
1:B:412:VAL:HG21	1:B:418:LYS:HB2	1.65	0.78
1:D:664:LEU:HD13	1:D:811:VAL:HG21	1.66	0.78
1:C:263:LEU:HD13	1:C:340:THR:HB	1.65	0.77
1:D:533:ARG:HA	1:D:536:ARG:HD2	1.68	0.76
1:B:433:LYS:HD3	1:B:434:SER:H	1.49	0.76
1:C:412:VAL:HG11	1:C:418:LYS:HA	1.67	0.75
1:C:207:GLU:HA	1:D:215:ARG:HH22	1.52	0.75
1:D:418:LYS:NZ	1:D:555:TYR:OH	2.19	0.75
1:D:433:LYS:HD2	1:D:438:TYR:HB2	1.68	0.75
1:A:418:LYS:NZ	1:A:555:TYR:OH	2.19	0.74
1:A:412:VAL:HG11	1:A:418:LYS:HA	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:LYS:NZ	1:B:555:TYR:OH	2.19	0.74
1:D:294:ARG:HG2	1:D:328:LEU:HD11	1.70	0.74
1:B:263:LEU:HD13	1:B:340:THR:HB	1.69	0.73
1:A:413:ARG:NH2	1:D:405:LEU:O	2.20	0.73
1:A:435:LYS:HD2	1:B:288:GLY:HA2	1.71	0.73
1:A:664:LEU:HD13	1:A:811:VAL:HG21	1.71	0.73
1:C:266:LEU:HD21	1:C:325:ILE:HG13	1.71	0.73
1:C:501:ALA:HA	1:C:533:ARG:HH22	1.54	0.73
1:A:263:LEU:HD13	1:A:340:THR:HB	1.68	0.72
1:D:483:MET:HA	1:D:486:LEU:HD12	1.72	0.72
1:A:241:THR:HG23	1:A:379:ALA:HB2	1.72	0.72
1:C:194:ILE:HB	1:C:217:LEU:HD12	1.70	0.71
1:C:664:LEU:HD13	1:C:811:VAL:HG21	1.72	0.71
1:D:433:LYS:HB3	1:D:438:TYR:HB3	1.73	0.70
1:B:356:PRO:HG2	1:B:586:LEU:HD13	1.73	0.70
1:A:217:LEU:HD13	1:A:222:SER:HA	1.72	0.70
1:A:439:LYS:NZ	1:A:488:GLN:O	2.25	0.70
1:A:294:ARG:HG2	1:A:328:LEU:HD11	1.74	0.70
1:D:263:LEU:HD13	1:D:340:THR:HB	1.74	0.69
1:D:616:GLN:HB3	1:D:620:LYS:HD2	1.73	0.69
1:C:435:LYS:HD3	1:C:435:LYS:H	1.57	0.69
1:B:621:VAL:HA	1:B:624:LYS:HD2	1.73	0.69
1:A:483:MET:HA	1:A:486:LEU:HD12	1.73	0.69
1:B:664:LEU:HD13	1:B:811:VAL:HG21	1.74	0.69
1:C:272:LEU:HD22	1:C:501:ALA:HB3	1.75	0.69
1:D:296:GLY:O	1:D:797:ARG:NH2	2.26	0.68
1:B:356:PRO:HB2	1:B:586:LEU:HD22	1.74	0.68
1:D:266:LEU:HD21	1:D:325:ILE:HG13	1.75	0.68
1:B:266:LEU:HD21	1:B:325:ILE:HG13	1.74	0.68
1:C:508:SER:HB3	1:C:538:LEU:HB2	1.75	0.68
1:D:407:ARG:HA	1:D:545:VAL:HG23	1.73	0.68
1:B:429:GLU:O	1:B:440:GLY:HA3	1.93	0.68
1:C:418:LYS:NZ	1:C:555:TYR:OH	2.27	0.68
1:D:737:GLU:OE2	1:D:753:ARG:NH2	2.27	0.67
1:C:356:PRO:HB2	1:C:586:LEU:HD22	1.76	0.67
1:C:294:ARG:HG2	1:C:328:LEU:HD11	1.76	0.67
1:D:756:ASN:HA	1:D:759:ILE:HD12	1.77	0.67
1:C:432:ARG:O	1:C:439:LYS:HA	1.94	0.67
1:A:356:PRO:HB2	1:A:586:LEU:HD22	1.76	0.67
1:B:294:ARG:HG2	1:B:328:LEU:HD11	1.75	0.66
1:C:194:ILE:HD11	1:C:226:LYS:HE3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:LYS:HA	1:D:291:VAL:HG21	1.78	0.66
1:C:756:ASN:HA	1:C:759:ILE:HD12	1.77	0.66
1:A:621:VAL:HA	1:A:624:LYS:HD2	1.76	0.66
1:B:674:VAL:HG11	1:B:752:GLU:HG3	1.78	0.66
1:B:349:LEU:HG	1:B:358:LEU:HD23	1.77	0.66
1:C:206:LYS:HA	1:C:209:LEU:HD12	1.78	0.65
1:C:238:VAL:HG12	1:C:380:THR:HA	1.78	0.65
1:A:326:ASP:HB3	1:A:651:PHE:CZ	2.31	0.65
1:A:436:GLN:HA	1:B:290:ARG:HG2	1.78	0.65
1:A:588:GLN:HA	1:A:621:VAL:HG11	1.77	0.65
1:B:291:VAL:HG22	1:B:317:ILE:HD12	1.79	0.65
1:B:622:LEU:HD22	1:B:638:VAL:HG11	1.79	0.65
1:B:326:ASP:HB3	1:B:651:PHE:CZ	2.32	0.64
1:A:507:ALA:H	1:A:537:PRO:CB	2.09	0.64
1:D:512:PHE:HB2	1:D:547:LEU:HG	1.78	0.64
1:A:262:LYS:N	1:A:337:ASN:O	2.31	0.64
1:A:507:ALA:H	1:A:537:PRO:HB3	1.63	0.64
1:B:712:ILE:HG23	1:B:719:VAL:HG11	1.81	0.63
1:D:206:LYS:HA	1:D:209:LEU:HD12	1.80	0.63
1:C:748:GLU:HA	1:C:751:MET:SD	2.38	0.63
1:A:712:ILE:HG23	1:A:719:VAL:HG11	1.78	0.63
1:B:439:LYS:NZ	1:B:490:LEU:O	2.30	0.63
1:D:621:VAL:HA	1:D:624:LYS:HD2	1.80	0.63
1:D:748:GLU:HA	1:D:751:MET:SD	2.38	0.63
1:A:700:LEU:HD12	1:A:708:SER:HB2	1.81	0.63
1:D:584:ASP:OD1	1:D:584:ASP:N	2.30	0.63
1:A:538:LEU:HD22	1:A:541:GLU:H	1.62	0.62
1:D:356:PRO:HB2	1:D:586:LEU:HD22	1.80	0.62
1:C:229:LEU:HD11	1:C:252:ALA:HB2	1.82	0.62
1:C:476:LYS:HE2	1:D:476:LYS:HE2	1.81	0.62
1:A:674:VAL:HG11	1:A:752:GLU:HG3	1.80	0.62
1:C:207:GLU:O	1:D:215:ARG:NH2	2.32	0.62
1:B:241:THR:HG23	1:B:379:ALA:HB2	1.81	0.62
1:B:262:LYS:N	1:B:337:ASN:O	2.33	0.62
1:B:786:GLY:O	1:B:790:THR:OG1	2.17	0.62
1:C:432:ARG:NH1	1:C:539:TYR:OH	2.32	0.62
1:D:622:LEU:HD22	1:D:638:VAL:HG11	1.82	0.62
1:A:223:LEU:O	1:A:227:ASN:ND2	2.33	0.62
1:A:390:GLU:HB3	1:A:612:LEU:HD21	1.80	0.62
1:B:434:SER:OG	1:B:435:LYS:N	2.33	0.62
1:B:510:VAL:HG23	1:B:534:ALA:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:GLN:HA	1:B:621:VAL:HG11	1.82	0.61
1:D:295:VAL:HG23	1:D:297:MET:HA	1.82	0.61
1:C:223:LEU:O	1:C:227:ASN:ND2	2.33	0.61
1:C:512:PHE:HB2	1:C:547:LEU:HG	1.83	0.61
1:A:622:LEU:HD22	1:A:638:VAL:HG11	1.83	0.60
1:B:692:LEU:HB2	1:B:700:LEU:HD22	1.84	0.60
1:C:309:VAL:HG21	1:D:439:LYS:HZ1	1.65	0.60
1:B:537:PRO:HG2	1:B:540:HIS:HB2	1.83	0.60
1:B:611:CYS:HB2	1:B:614:ALA:HB2	1.84	0.60
1:C:299:ARG:HD3	1:C:796:VAL:HG12	1.83	0.60
1:C:403:VAL:HG11	1:C:537:PRO:HG3	1.83	0.60
1:D:344:ASP:HA	1:D:377:LEU:HB2	1.84	0.60
1:B:344:ASP:HA	1:B:377:LEU:HB2	1.82	0.60
1:A:205:PHE:O	1:A:209:LEU:HG	2.02	0.60
1:A:696:VAL:HG23	1:A:698:GLY:H	1.67	0.59
1:A:756:ASN:HA	1:A:759:ILE:HD12	1.84	0.59
1:A:297:MET:HG2	1:A:308:VAL:HG11	1.84	0.59
1:C:262:LYS:HG2	1:C:316:ASP:HA	1.84	0.59
1:D:503:VAL:O	1:D:533:ARG:NH1	2.32	0.59
1:D:433:LYS:HB3	1:D:438:TYR:CB	2.31	0.59
1:A:475:TYR:CZ	1:A:479:LYS:HG3	2.37	0.59
1:A:703:ASN:OD1	1:A:704:VAL:N	2.36	0.59
1:C:281:LYS:HA	1:C:291:VAL:HG21	1.84	0.59
1:C:349:LEU:HA	1:C:355:GLY:HA2	1.83	0.59
1:A:253:GLY:HA3	1:A:263:LEU:HD22	1.84	0.59
1:C:356:PRO:HG2	1:C:586:LEU:HD13	1.83	0.59
1:C:476:LYS:HG3	1:D:480:LEU:HD11	1.84	0.59
1:C:507:ALA:O	1:C:537:PRO:HA	2.03	0.59
1:C:703:ASN:OD1	1:C:704:VAL:N	2.35	0.59
1:D:194:ILE:HB	1:D:217:LEU:HD12	1.84	0.59
1:D:528:HIS:O	1:D:531:LEU:HG	2.04	0.58
1:B:616:GLN:HB3	1:B:620:LYS:HD2	1.85	0.58
1:C:326:ASP:HB3	1:C:651:PHE:HZ	1.68	0.58
1:D:237:VAL:HG11	1:D:248:ILE:HD13	1.85	0.58
1:A:473:LEU:HB2	1:A:478:ARG:HG3	1.85	0.58
1:D:236:LEU:HD23	1:D:388:ALA:HB2	1.86	0.58
1:D:521:TRP:CD2	1:D:566:VAL:HG21	2.38	0.58
1:B:223:LEU:O	1:B:227:ASN:ND2	2.36	0.58
1:C:205:PHE:O	1:C:209:LEU:HG	2.02	0.58
1:D:205:PHE:O	1:D:209:LEU:HG	2.03	0.58
1:B:756:ASN:O	1:B:760:GLU:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:VAL:HG11	1:C:621:VAL:HB	1.86	0.58
1:A:432:ARG:HG2	1:A:433:LYS:N	2.17	0.58
1:C:293:ILE:O	1:C:311:THR:HG22	2.04	0.58
1:D:588:GLN:HA	1:D:621:VAL:HG11	1.85	0.58
1:B:703:ASN:OD1	1:B:704:VAL:N	2.36	0.58
1:C:588:GLN:HA	1:C:621:VAL:HG11	1.85	0.58
1:D:356:PRO:HG2	1:D:586:LEU:HD13	1.86	0.58
1:A:299:ARG:HD3	1:A:796:VAL:HG12	1.85	0.58
1:A:349:LEU:HG	1:A:358:LEU:HD23	1.85	0.57
1:A:291:VAL:HG22	1:A:317:ILE:HD12	1.84	0.57
1:C:756:ASN:O	1:C:760:GLU:HG2	2.04	0.57
1:A:527:PHE:O	1:A:531:LEU:HG	2.04	0.57
1:B:205:PHE:O	1:B:209:LEU:HG	2.04	0.57
1:D:786:GLY:O	1:D:790:THR:OG1	2.20	0.57
1:A:584:ASP:OD1	1:A:584:ASP:N	2.32	0.57
1:A:723:LEU:HB2	1:A:728:ALA:HB2	1.86	0.57
1:B:208:VAL:HG21	1:B:287:LEU:HG	1.85	0.57
1:B:622:LEU:HD13	1:B:638:VAL:HG21	1.86	0.57
1:C:281:LYS:HE3	1:D:437:GLY:HA2	1.86	0.57
1:C:295:VAL:HG12	1:C:321:THR:HG23	1.86	0.57
1:D:223:LEU:O	1:D:227:ASN:ND2	2.38	0.57
1:D:720:ILE:O	1:D:722:GLU:N	2.32	0.57
1:A:512:PHE:HB2	1:A:547:LEU:HG	1.87	0.57
1:C:611:CYS:HB2	1:C:614:ALA:HB2	1.86	0.57
1:C:295:VAL:HG23	1:C:297:MET:HA	1.86	0.57
1:D:194:ILE:HD11	1:D:226:LYS:HE3	1.86	0.57
1:D:326:ASP:HB3	1:D:651:PHE:HZ	1.69	0.57
1:B:412:VAL:HG11	1:B:418:LYS:HA	1.86	0.56
1:B:665:GLY:O	1:B:813:LYS:NZ	2.32	0.56
1:D:741:CYS:HB3	1:D:746:CYS:SG	2.45	0.56
1:D:756:ASN:O	1:D:760:GLU:HG2	2.06	0.56
1:A:511:ILE:HA	1:A:546:TYR:O	2.06	0.56
1:B:483:MET:HA	1:B:486:LEU:HD12	1.88	0.56
1:B:696:VAL:HG23	1:B:698:GLY:H	1.69	0.56
1:C:253:GLY:HA3	1:C:263:LEU:HD22	1.87	0.56
1:C:349:LEU:HG	1:C:358:LEU:HD23	1.88	0.56
1:D:266:LEU:HD13	1:D:322:TYR:HA	1.86	0.56
1:C:806:ALA:HB1	1:C:811:VAL:O	2.06	0.56
1:A:476:LYS:HE2	1:B:476:LYS:HE3	1.86	0.56
1:C:521:TRP:HE1	1:C:559:MET:HB3	1.70	0.56
1:A:330:ARG:CZ	1:A:593:ALA:HB2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:LYS:HD2	1:B:489:ARG:O	2.06	0.55
1:C:582:TRP:HE3	1:C:587:GLU:HG3	1.71	0.55
1:C:688:LEU:HD21	1:C:727:ALA:HA	1.87	0.55
1:D:712:ILE:HG23	1:D:719:VAL:HG11	1.87	0.55
1:D:293:ILE:O	1:D:311:THR:HG22	2.06	0.55
1:D:688:LEU:HD21	1:D:727:ALA:HA	1.87	0.55
1:A:616:GLN:HB3	1:A:620:LYS:HD2	1.88	0.55
1:D:326:ASP:HB3	1:D:651:PHE:CZ	2.41	0.55
1:D:384:PRO:HB2	1:D:395:LEU:HD21	1.88	0.55
1:D:436:GLN:H	1:D:436:GLN:NE2	2.05	0.55
1:A:611:CYS:HB2	1:A:614:ALA:HB2	1.87	0.55
1:C:326:ASP:HB3	1:C:651:PHE:CZ	2.41	0.55
1:A:295:VAL:HG12	1:A:321:THR:HG23	1.88	0.55
1:D:291:VAL:HG22	1:D:317:ILE:HD12	1.87	0.55
1:A:756:ASN:O	1:A:760:GLU:HG2	2.07	0.55
1:A:592:LEU:HG	1:A:648:SER:HB2	1.88	0.54
1:A:737:GLU:OE2	1:A:753:ARG:NH2	2.39	0.54
1:C:241:THR:HG23	1:C:379:ALA:HB2	1.89	0.54
1:B:484:GLU:HG2	1:B:489:ARG:HD2	1.88	0.54
1:C:196:VAL:HG23	1:C:215:ARG:O	2.08	0.54
1:C:621:VAL:HA	1:C:624:LYS:HD2	1.89	0.54
1:A:435:LYS:NZ	1:B:285:SER:O	2.41	0.54
1:B:295:VAL:HG12	1:B:321:THR:HG23	1.89	0.54
1:D:419:TRP:HB3	1:D:458:TYR:CE2	2.43	0.54
1:D:554:LYS:HG3	1:D:562:THR:HG22	1.89	0.54
1:D:703:ASN:OD1	1:D:704:VAL:N	2.35	0.54
1:D:295:VAL:HG12	1:D:321:THR:HG23	1.89	0.54
1:D:696:VAL:HG23	1:D:698:GLY:H	1.72	0.54
1:B:217:LEU:HD13	1:B:222:SER:HA	1.90	0.54
1:B:521:TRP:CD2	1:B:566:VAL:HG21	2.43	0.54
1:B:720:ILE:O	1:B:722:GLU:N	2.38	0.54
1:D:262:LYS:N	1:D:337:ASN:O	2.40	0.54
1:D:439:LYS:HD2	1:D:488:GLN:HB3	1.89	0.54
1:D:439:LYS:NZ	1:D:488:GLN:O	2.32	0.54
1:A:761:LEU:HD12	1:A:771:ILE:HG23	1.90	0.54
1:C:541:GLU:HG2	1:C:542:LYS:H	1.73	0.54
1:C:720:ILE:O	1:C:722:GLU:N	2.35	0.54
1:B:246:THR:HG21	1:B:276:LYS:HE3	1.89	0.53
1:C:237:VAL:HG21	1:C:248:ILE:HD13	1.89	0.53
1:C:584:ASP:OD1	1:C:584:ASP:N	2.41	0.53
1:C:616:GLN:HB3	1:C:620:LYS:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:673:ALA:HA	1:C:676:LEU:HD12	1.88	0.53
1:A:238:VAL:HG12	1:A:380:THR:HA	1.90	0.53
1:C:475:TYR:CZ	1:C:479:LYS:HG3	2.43	0.53
1:B:798:LYS:O	1:B:802:ILE:HG13	2.08	0.53
1:C:229:LEU:HD13	1:C:235:LEU:HD12	1.91	0.53
1:D:672:ILE:O	1:D:676:LEU:HG	2.08	0.53
1:A:433:LYS:HE3	1:A:437:GLY:HA2	1.89	0.53
1:C:432:ARG:NH1	1:C:439:LYS:O	2.41	0.53
1:B:521:TRP:NE1	1:B:559:MET:HB3	2.23	0.53
1:C:521:TRP:NE1	1:C:559:MET:HB3	2.23	0.53
1:A:564:ASP:OD1	1:A:564:ASP:N	2.41	0.53
1:C:387:LEU:O	1:C:391:LEU:HG	2.08	0.53
1:D:473:LEU:HB2	1:D:478:ARG:HG3	1.91	0.53
1:B:592:LEU:HG	1:B:648:SER:HB2	1.91	0.53
1:C:591:VAL:HA	1:C:594:HIS:CD2	2.43	0.53
1:B:670:ARG:HD3	1:B:756:ASN:OD1	2.09	0.53
1:D:229:LEU:HD13	1:D:235:LEU:HD12	1.92	0.52
1:B:410:ILE:HD11	1:B:546:TYR:HD2	1.74	0.52
1:C:383:ASN:N	1:C:383:ASN:OD1	2.42	0.52
1:B:302:THR:HB	1:B:767:HIS:NE2	2.25	0.52
1:B:582:TRP:HE3	1:B:587:GLU:HG3	1.73	0.52
1:C:367:LYS:NZ	1:C:606:GLU:OE2	2.40	0.52
1:D:253:GLY:HA3	1:D:263:LEU:HD22	1.92	0.52
1:A:521:TRP:CE2	1:A:566:VAL:HG21	2.45	0.52
1:A:247:LEU:HG	1:A:251:LEU:HD21	1.90	0.52
1:D:221:GLN:NE2	1:D:244:GLY:O	2.42	0.52
1:D:295:VAL:HG22	1:D:308:VAL:HG11	1.92	0.52
1:C:250:GLU:O	1:C:254:VAL:HG23	2.10	0.52
1:C:268:PRO:O	1:C:354:ARG:NH2	2.42	0.52
1:C:812:ARG:HA	1:C:815:GLU:HB3	1.91	0.52
1:B:511:ILE:HA	1:B:546:TYR:O	2.09	0.52
1:D:247:LEU:HG	1:D:251:LEU:HD21	1.92	0.52
1:D:405:LEU:HD11	1:D:534:ALA:HB3	1.92	0.52
1:D:521:TRP:NE1	1:D:559:MET:HB3	2.24	0.52
1:B:591:VAL:HA	1:B:594:HIS:CD2	2.44	0.52
1:C:591:VAL:HA	1:C:594:HIS:HD2	1.74	0.52
1:C:712:ILE:HG23	1:C:719:VAL:HG11	1.92	0.52
1:C:262:LYS:N	1:C:337:ASN:O	2.42	0.52
1:C:622:LEU:HD22	1:C:638:VAL:HG11	1.90	0.52
1:B:439:LYS:NZ	1:B:488:GLN:HA	2.25	0.51
1:D:523:SER:HB3	1:D:526:GLU:CD	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:TRP:CD2	1:A:566:VAL:HG21	2.45	0.51
1:A:716:LEU:O	1:A:720:ILE:HB	2.10	0.51
1:B:383:ASN:OD1	1:B:383:ASN:N	2.44	0.51
1:C:427:ARG:O	1:C:431:MET:HG2	2.09	0.51
1:A:591:VAL:HA	1:A:594:HIS:CD2	2.45	0.51
1:C:450:LYS:HZ2	1:C:686:GLY:HA2	1.75	0.51
1:D:387:LEU:O	1:D:391:LEU:HG	2.10	0.51
1:B:767:HIS:ND1	1:B:768:PRO:HD2	2.26	0.51
1:C:820:ILE:HG23	1:C:831:ILE:HD12	1.92	0.51
1:A:208:VAL:HG21	1:A:287:LEU:HG	1.91	0.51
1:B:239:SER:O	1:B:379:ALA:HA	2.11	0.51
1:C:276:LYS:HB3	1:C:280:PHE:CE2	2.45	0.51
1:C:291:VAL:HG22	1:C:317:ILE:HD12	1.92	0.51
1:D:229:LEU:HD21	1:D:251:LEU:HB2	1.93	0.51
1:A:268:PRO:O	1:A:354:ARG:NH2	2.41	0.51
1:A:798:LYS:O	1:A:802:ILE:HG13	2.11	0.51
1:B:509:GLN:HA	1:B:544:LYS:O	2.10	0.51
1:B:626:GLU:HA	1:B:631:VAL:O	2.10	0.51
1:C:290:ARG:HG2	1:D:435:LYS:O	2.10	0.51
1:B:482:GLU:HA	1:B:505:PHE:CZ	2.46	0.51
1:B:682:ILE:HD11	1:B:781:LEU:HD13	1.93	0.51
1:C:285:SER:HB3	1:D:436:GLN:HB2	1.91	0.51
1:D:465:LYS:HD2	1:D:489:ARG:O	2.11	0.51
1:A:720:ILE:O	1:A:722:GLU:N	2.41	0.51
1:C:672:ILE:O	1:C:676:LEU:HG	2.11	0.51
1:D:723:LEU:HD12	1:D:728:ALA:HA	1.92	0.51
1:C:344:ASP:HA	1:C:377:LEU:HB2	1.93	0.51
1:C:765:GLY:HA2	1:C:828:GLY:O	2.11	0.51
1:D:591:VAL:HA	1:D:594:HIS:HD2	1.76	0.51
1:B:441:GLN:HB3	1:B:485:PHE:CZ	2.46	0.50
1:B:475:TYR:CZ	1:B:479:LYS:HG3	2.46	0.50
1:C:277:TYR:HA	1:C:319:VAL:HG21	1.92	0.50
1:C:415:GLU:O	1:C:418:LYS:HB3	2.11	0.50
1:C:511:ILE:HA	1:C:546:TYR:O	2.11	0.50
1:D:434:SER:HB2	1:D:436:GLN:O	2.11	0.50
1:A:215:ARG:HH22	1:B:207:GLU:HG2	1.75	0.50
1:A:682:ILE:HD11	1:A:781:LEU:HD13	1.93	0.50
1:A:429:GLU:O	1:A:440:GLY:HA3	2.12	0.50
1:A:539:TYR:CD1	1:A:539:TYR:N	2.78	0.50
1:B:206:LYS:HA	1:B:209:LEU:HD12	1.94	0.50
1:B:256:LYS:HB3	1:B:261:LYS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:SER:O	1:C:379:ALA:HA	2.11	0.50
1:B:521:TRP:CG	1:B:566:VAL:HG21	2.46	0.50
1:C:203:GLU:OE1	1:C:206:LYS:HD2	2.10	0.50
1:D:362:ILE:O	1:D:366:ARG:HG3	2.12	0.50
1:D:509:GLN:HA	1:D:544:LYS:O	2.11	0.50
1:A:671:TRP:CZ2	1:A:675:LYS:HE3	2.46	0.50
1:D:330:ARG:HD3	1:D:648:SER:O	2.11	0.50
1:D:436:GLN:H	1:D:436:GLN:CD	2.15	0.50
1:A:344:ASP:HA	1:A:377:LEU:HB2	1.92	0.50
1:C:510:VAL:CG2	1:C:534:ALA:HB2	2.41	0.50
1:C:295:VAL:HG22	1:C:308:VAL:HG11	1.94	0.50
1:C:521:TRP:CD2	1:C:566:VAL:HG21	2.47	0.50
1:C:592:LEU:HG	1:C:648:SER:HB2	1.93	0.50
1:D:799:LEU:HD23	1:D:802:ILE:HD12	1.94	0.50
1:C:605:GLU:OE1	1:C:618:ALA:HB3	2.12	0.50
1:B:410:ILE:HD11	1:B:546:TYR:CD2	2.45	0.50
1:B:439:LYS:HZ3	1:B:488:GLN:HA	1.77	0.50
1:C:297:MET:SD	1:C:311:THR:HG21	2.52	0.49
1:D:256:LYS:HB3	1:D:261:LYS:HB2	1.93	0.49
1:D:591:VAL:HA	1:D:594:HIS:CD2	2.47	0.49
1:D:297:MET:HG2	1:D:308:VAL:HG11	1.94	0.49
1:C:217:LEU:HD22	1:C:221:GLN:HB3	1.94	0.49
1:D:611:CYS:HB2	1:D:614:ALA:HB2	1.93	0.49
1:A:294:ARG:O	1:A:320:GLY:HA2	2.13	0.49
1:A:510:VAL:CG2	1:A:534:ALA:HB2	2.42	0.49
1:A:591:VAL:HA	1:A:594:HIS:HD2	1.76	0.49
1:C:236:LEU:HD23	1:C:388:ALA:HB2	1.93	0.49
1:C:483:MET:HA	1:C:486:LEU:HD12	1.94	0.49
1:D:217:LEU:HD13	1:D:222:SER:HA	1.95	0.49
1:D:682:ILE:HD11	1:D:781:LEU:HB3	1.94	0.49
1:D:682:ILE:HD11	1:D:781:LEU:HD13	1.93	0.49
1:A:206:LYS:HA	1:A:209:LEU:HD12	1.95	0.49
1:B:229:LEU:HD13	1:B:235:LEU:HD12	1.93	0.49
1:C:696:VAL:HG23	1:C:698:GLY:H	1.77	0.49
1:D:346:ILE:HG22	1:D:378:SER:HB2	1.95	0.49
1:D:521:TRP:HE1	1:D:559:MET:HB3	1.78	0.49
1:C:809:PHE:HB2	1:C:811:VAL:HG23	1.94	0.49
1:D:267:VAL:HG12	1:D:344:ASP:HB3	1.94	0.49
1:C:757:LEU:O	1:C:761:LEU:HG	2.12	0.49
1:A:477:GLN:HA	1:A:480:LEU:HB3	1.94	0.49
1:A:521:TRP:NE1	1:A:559:MET:HB3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ASN:OD1	1:B:427:ARG:NH1	2.44	0.49
1:B:510:VAL:CG2	1:B:534:ALA:HB2	2.42	0.49
1:C:321:THR:O	1:C:325:ILE:HG12	2.13	0.49
1:C:473:LEU:HB2	1:C:478:ARG:HG3	1.95	0.49
1:A:265:PHE:CZ	1:A:344:ASP:HB2	2.48	0.49
1:C:583:SER:HB3	1:C:586:LEU:HD12	1.95	0.49
1:D:429:GLU:OE2	1:D:508:SER:OG	2.18	0.48
1:A:239:SER:O	1:A:379:ALA:HA	2.13	0.48
1:B:238:VAL:HG12	1:B:380:THR:HA	1.95	0.48
1:B:401:ARG:HH21	1:B:402:PRO:HG2	1.78	0.48
1:D:322:TYR:OH	1:D:344:ASP:O	2.31	0.48
1:A:748:GLU:HA	1:A:751:MET:SD	2.53	0.48
1:B:527:PHE:CZ	1:B:531:LEU:HD11	2.47	0.48
1:A:383:ASN:N	1:A:383:ASN:OD1	2.46	0.48
1:B:265:PHE:CZ	1:B:344:ASP:HB2	2.49	0.48
1:D:383:ASN:O	1:D:387:LEU:HB2	2.14	0.48
1:D:757:LEU:O	1:D:761:LEU:HG	2.13	0.48
1:C:256:LYS:HB3	1:C:261:LYS:HD2	1.95	0.48
1:C:401:ARG:HH12	1:C:535:GLY:HA3	1.77	0.48
1:B:470:HIS:O	1:B:478:ARG:HD3	2.14	0.48
1:B:591:VAL:HA	1:B:594:HIS:HD2	1.77	0.48
1:C:470:HIS:H	1:C:473:LEU:HD12	1.78	0.48
1:C:510:VAL:HG23	1:C:534:ALA:HB2	1.95	0.48
1:C:527:PHE:O	1:C:531:LEU:HG	2.14	0.48
1:D:414:ASN:ND2	1:D:417:GLU:H	2.12	0.48
1:D:511:ILE:HA	1:D:546:TYR:O	2.14	0.48
1:A:215:ARG:HH21	1:B:210:LYS:HB2	1.78	0.48
1:A:266:LEU:HD21	1:A:325:ILE:HG13	1.95	0.48
1:A:290:ARG:HD3	1:B:433:LYS:HE3	1.96	0.48
1:B:253:GLY:HA3	1:B:263:LEU:HD22	1.96	0.48
1:C:441:GLN:OE1	1:C:488:GLN:HA	2.14	0.48
1:C:551:PRO:HA	1:C:564:ASP:OD1	2.13	0.48
1:D:723:LEU:HB2	1:D:728:ALA:HB2	1.96	0.48
1:B:604:ILE:HG22	1:B:618:ALA:HB1	1.96	0.47
1:C:505:PHE:H	1:C:536:ARG:NH2	2.12	0.47
1:C:723:LEU:HB2	1:C:728:ALA:HB2	1.95	0.47
1:D:410:ILE:HD11	1:D:546:TYR:HD2	1.79	0.47
1:D:533:ARG:HA	1:D:536:ARG:CD	2.43	0.47
1:A:403:VAL:HG21	1:A:536:ARG:HA	1.96	0.47
1:C:682:ILE:HD11	1:C:781:LEU:HD13	1.97	0.47
1:D:266:LEU:HB3	1:D:322:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:LYS:CE	1:B:488:GLN:HA	2.45	0.47
1:C:741:CYS:HB3	1:C:746:CYS:SG	2.54	0.47
1:D:349:LEU:HG	1:D:358:LEU:HD23	1.96	0.47
1:A:383:ASN:O	1:A:387:LEU:HB2	2.14	0.47
1:A:387:LEU:HD12	1:A:387:LEU:HA	1.76	0.47
1:B:299:ARG:HD3	1:B:796:VAL:HG12	1.97	0.47
1:C:367:LYS:HD2	1:C:367:LYS:HA	1.74	0.47
1:C:767:HIS:CG	1:C:768:PRO:HD2	2.50	0.47
1:D:239:SER:O	1:D:379:ALA:HA	2.15	0.47
1:D:387:LEU:HD12	1:D:387:LEU:HA	1.76	0.47
1:A:773:GLU:O	1:A:777:LYS:HG3	2.15	0.47
1:C:527:PHE:CZ	1:C:531:LEU:HD11	2.50	0.47
1:D:383:ASN:OD1	1:D:383:ASN:N	2.46	0.47
1:D:432:ARG:HG2	1:D:433:LYS:N	2.29	0.47
1:D:600:ARG:HB2	1:D:603:VAL:HG23	1.96	0.47
1:A:501:ALA:HA	1:A:533:ARG:HH22	1.79	0.47
1:A:533:ARG:O	1:A:537:PRO:HG2	2.15	0.47
1:A:626:GLU:HA	1:A:631:VAL:O	2.14	0.47
1:B:272:LEU:HD22	1:B:501:ALA:HB3	1.95	0.47
1:B:475:TYR:HD1	1:B:478:ARG:HH12	1.63	0.47
1:B:624:LYS:HA	1:B:627:GLU:CD	2.35	0.47
1:C:367:LYS:HZ3	1:C:606:GLU:CD	2.16	0.47
1:D:664:LEU:HD11	1:D:805:ILE:HG22	1.97	0.47
1:D:670:ARG:HD3	1:D:756:ASN:OD1	2.14	0.47
1:D:673:ALA:HA	1:D:676:LEU:HD12	1.95	0.47
1:C:245:LYS:HB2	1:C:245:LYS:HE2	1.79	0.47
1:A:497:ALA:HB2	1:A:530:MET:HE3	1.97	0.47
1:B:434:SER:OG	1:B:435:LYS:HG3	2.14	0.47
1:B:266:LEU:HD13	1:B:322:TYR:HA	1.97	0.47
1:C:360:GLY:HA3	1:C:590:ASN:OD1	2.15	0.47
1:A:433:LYS:HA	1:A:438:TYR:HB2	1.97	0.46
1:A:525:ARG:HB2	1:A:575:ILE:HG23	1.97	0.46
1:B:387:LEU:O	1:B:391:LEU:HG	2.15	0.46
1:B:436:GLN:C	1:B:438:TYR:N	2.68	0.46
1:C:436:GLN:HG2	1:D:285:SER:O	2.15	0.46
1:C:682:ILE:HD11	1:C:781:LEU:HB3	1.96	0.46
1:D:537:PRO:O	1:D:539:TYR:N	2.41	0.46
1:B:804:ARG:O	1:B:808:VAL:HG23	2.15	0.46
1:C:406:GLU:HB2	1:C:542:LYS:HD2	1.97	0.46
1:C:450:LYS:HE3	1:C:686:GLY:HA2	1.97	0.46
1:D:500:GLY:O	1:D:533:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:781:LEU:HA	1:D:781:LEU:HD23	1.78	0.46
1:A:282:ARG:HA	1:B:539:TYR:OH	2.16	0.46
1:C:364:ARG:HD2	1:C:597:VAL:HG21	1.97	0.46
1:D:449:ARG:HA	1:D:452:THR:HG23	1.98	0.46
1:A:327:TYR:HB2	1:A:651:PHE:HE2	1.79	0.46
1:A:470:HIS:O	1:A:478:ARG:HD3	2.15	0.46
1:A:507:ALA:H	1:A:537:PRO:HB2	1.79	0.46
1:C:509:GLN:HA	1:C:544:LYS:O	2.15	0.46
1:B:604:ILE:HG21	1:B:622:LEU:HD11	1.97	0.46
1:A:527:PHE:CE2	1:A:531:LEU:HD11	2.51	0.46
1:B:542:LYS:O	1:B:544:LYS:HE2	2.16	0.46
1:C:538:LEU:HD23	1:C:538:LEU:HA	1.75	0.46
1:C:761:LEU:O	1:C:764:SER:OG	2.33	0.46
1:A:622:LEU:HD13	1:A:638:VAL:HG21	1.97	0.46
1:B:418:LYS:HG3	1:B:548:LEU:HB3	1.98	0.46
1:B:436:GLN:O	1:B:438:TYR:N	2.48	0.46
1:B:773:GLU:O	1:B:777:LYS:HG3	2.15	0.46
1:D:414:ASN:HD21	1:D:417:GLU:H	1.64	0.46
1:B:748:GLU:HA	1:B:751:MET:SD	2.56	0.46
1:C:196:VAL:HG11	1:C:210:LYS:HE2	1.98	0.46
1:C:267:VAL:HG12	1:C:344:ASP:HB3	1.98	0.46
1:C:414:ASN:HD21	1:C:417:GLU:H	1.64	0.46
1:C:438:TYR:HB2	1:C:539:TYR:CE1	2.51	0.46
1:D:241:THR:HG23	1:D:379:ALA:HB2	1.98	0.46
1:D:429:GLU:O	1:D:440:GLY:HA3	2.16	0.46
1:A:527:PHE:CZ	1:A:531:LEU:HD11	2.50	0.46
1:A:507:ALA:O	1:A:537:PRO:HB2	2.15	0.45
1:B:268:PRO:O	1:B:354:ARG:NH2	2.50	0.45
1:B:281:LYS:HA	1:B:291:VAL:HG21	1.97	0.45
1:B:473:LEU:HB2	1:B:478:ARG:HG3	1.96	0.45
1:B:809:PHE:HB2	1:B:811:VAL:HG23	1.97	0.45
1:D:495:THR:OG1	1:D:496:THR:N	2.49	0.45
1:B:401:ARG:HD3	1:B:403:VAL:O	2.16	0.45
1:B:505:PHE:HD1	1:B:505:PHE:HA	1.64	0.45
1:C:523:SER:HB3	1:C:526:GLU:CD	2.37	0.45
1:C:669:ALA:HB1	1:C:799:LEU:HD21	1.97	0.45
1:C:700:LEU:HD12	1:C:708:SER:HB2	1.98	0.45
1:A:414:ASN:HD21	1:A:417:GLU:H	1.63	0.45
1:A:462:LYS:HA	1:A:462:LYS:HD3	1.62	0.45
1:A:591:VAL:HG11	1:A:621:VAL:HB	1.98	0.45
1:B:255:PRO:O	1:B:258:MET:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:739:PHE:HD2	1:D:746:CYS:HB2	1.81	0.45
1:A:500:GLY:O	1:A:533:ARG:NH2	2.50	0.45
1:B:294:ARG:O	1:B:320:GLY:HA2	2.16	0.45
1:B:462:LYS:HA	1:B:462:LYS:HD3	1.67	0.45
1:C:495:THR:OG1	1:C:496:THR:N	2.50	0.45
1:C:688:LEU:HD13	1:C:688:LEU:HA	1.81	0.45
1:C:800:GLU:HB3	1:C:804:ARG:HH21	1.81	0.45
1:A:432:ARG:HH21	1:A:540:HIS:HB2	1.81	0.45
1:A:441:GLN:OE1	1:A:488:GLN:HA	2.17	0.45
1:C:266:LEU:HD13	1:C:322:TYR:HD1	1.82	0.45
1:C:759:ILE:HG23	1:C:825:ILE:HD11	1.97	0.45
1:D:541:GLU:OE1	1:D:542:LYS:N	2.50	0.45
1:D:674:VAL:HG11	1:D:752:GLU:HG3	1.98	0.45
1:B:564:ASP:OD1	1:B:564:ASP:N	2.33	0.45
1:D:686:GLY:C	1:D:690:ARG:HH21	2.19	0.45
1:D:688:LEU:HD13	1:D:688:LEU:HA	1.85	0.45
1:A:415:GLU:O	1:A:418:LYS:HB3	2.17	0.45
1:B:757:LEU:O	1:B:761:LEU:HG	2.16	0.45
1:C:414:ASN:ND2	1:C:417:GLU:H	2.15	0.45
1:A:302:THR:HB	1:A:767:HIS:HE2	1.82	0.45
1:A:407:ARG:HH12	1:D:413:ARG:HG2	1.81	0.45
1:A:410:ILE:O	1:A:411:ILE:HD13	2.17	0.45
1:D:700:LEU:HD12	1:D:708:SER:HB2	1.98	0.45
1:A:692:LEU:HB2	1:A:700:LEU:HD22	1.99	0.44
1:B:692:LEU:HD22	1:B:712:ILE:HD13	1.99	0.44
1:C:475:TYR:OH	1:C:479:LYS:HE3	2.17	0.44
1:A:349:LEU:HA	1:A:355:GLY:HA2	1.98	0.44
1:B:432:ARG:NE	1:B:540:HIS:CD2	2.85	0.44
1:C:250:GLU:OE1	1:C:284:TYR:OH	2.27	0.44
1:C:664:LEU:HD11	1:C:805:ILE:HG22	1.99	0.44
1:D:759:ILE:HG23	1:D:825:ILE:HD11	1.98	0.44
1:A:508:SER:HA	1:A:538:LEU:HG	1.99	0.44
1:B:367:LYS:HD2	1:B:367:LYS:HA	1.80	0.44
1:B:414:ASN:HD21	1:B:417:GLU:H	1.65	0.44
1:A:418:LYS:HG3	1:A:548:LEU:HB3	1.98	0.44
1:B:292:ALA:HB1	1:B:310:ASP:O	2.17	0.44
1:C:265:PHE:CZ	1:C:344:ASP:HB2	2.53	0.44
1:D:265:PHE:CZ	1:D:344:ASP:HB2	2.53	0.44
1:D:349:LEU:HA	1:D:355:GLY:HA2	1.99	0.44
1:A:250:GLU:O	1:A:254:VAL:HG23	2.17	0.44
1:C:349:LEU:HD23	1:C:355:GLY:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:LEU:O	1:C:522:LEU:HG	2.17	0.44
1:A:384:PRO:HB2	1:A:395:LEU:HD21	2.00	0.44
1:B:508:SER:HA	1:B:537:PRO:HG3	2.00	0.44
1:D:292:ALA:HB1	1:D:310:ASP:O	2.18	0.44
1:D:660:ILE:HD13	1:D:802:ILE:HG12	1.99	0.44
1:A:571:LEU:HD23	1:A:571:LEU:HA	1.70	0.44
1:D:536:ARG:N	1:D:537:PRO:CD	2.80	0.44
1:A:455:LEU:HD12	1:A:455:LEU:HA	1.73	0.44
1:D:767:HIS:CG	1:D:768:PRO:HD2	2.53	0.44
1:A:432:ARG:NH2	1:A:540:HIS:HB2	2.32	0.44
1:A:495:THR:OG1	1:A:496:THR:N	2.51	0.44
1:A:739:PHE:HD1	1:A:746:CYS:HB2	1.83	0.44
1:A:804:ARG:O	1:A:808:VAL:HG23	2.18	0.44
1:C:450:LYS:HZ2	1:C:689:GLN:HB3	1.83	0.44
1:C:799:LEU:HD23	1:C:799:LEU:HA	1.84	0.44
1:D:768:PRO:HB2	1:D:785:PRO:HB3	1.99	0.44
1:B:266:LEU:HD13	1:B:322:TYR:HD1	1.83	0.43
1:B:346:ILE:HG22	1:B:377:LEU:O	2.18	0.43
1:C:450:LYS:NZ	1:C:689:GLN:HB3	2.33	0.43
1:C:550:GLU:HB3	1:C:553:ARG:HB2	2.00	0.43
1:B:367:LYS:HB3	1:B:598:PHE:CZ	2.54	0.43
1:C:208:VAL:HG21	1:C:287:LEU:HG	2.00	0.43
1:C:455:LEU:HD12	1:C:455:LEU:HA	1.70	0.43
1:D:250:GLU:O	1:D:254:VAL:HG23	2.18	0.43
1:D:508:SER:O	1:D:543:GLY:HA2	2.19	0.43
1:A:521:TRP:HE1	1:A:559:MET:HB3	1.82	0.43
1:B:362:ILE:O	1:B:366:ARG:HG3	2.17	0.43
1:B:467:LYS:HD3	1:B:467:LYS:HA	1.90	0.43
1:C:642:PRO:HB2	1:C:808:VAL:HG13	1.99	0.43
1:C:692:LEU:HB2	1:C:700:LEU:HD22	1.99	0.43
1:B:660:ILE:HD13	1:B:802:ILE:HG12	2.00	0.43
1:C:500:GLY:O	1:C:533:ARG:NH2	2.52	0.43
1:C:571:LEU:HD23	1:C:571:LEU:HA	1.76	0.43
1:D:282:ARG:O	1:D:286:LYS:HE3	2.17	0.43
1:D:364:ARG:HG2	1:D:598:PHE:HE2	1.83	0.43
1:A:295:VAL:HG23	1:A:297:MET:HA	1.99	0.43
1:D:431:MET:HA	1:D:433:LYS:NZ	2.34	0.43
1:A:229:LEU:HD13	1:A:235:LEU:HD12	2.01	0.43
1:B:229:LEU:HD21	1:B:251:LEU:HB2	2.01	0.43
1:B:245:LYS:HE2	1:B:245:LYS:HB2	1.87	0.43
1:B:247:LEU:HG	1:B:251:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:SER:HB3	1:B:526:GLU:CD	2.39	0.43
1:C:330:ARG:NH1	1:C:589:ASP:OD2	2.52	0.43
1:C:523:SER:HB3	1:C:526:GLU:HG3	2.00	0.43
1:D:539:TYR:O	1:D:540:HIS:C	2.57	0.43
1:D:795:ILE:HD13	1:D:795:ILE:HA	1.84	0.43
1:C:433:LYS:HE2	1:C:437:GLY:O	2.18	0.43
1:A:365:LEU:HD23	1:A:368:LEU:HD12	2.01	0.43
1:A:701:SER:HB3	1:A:708:SER:OG	2.19	0.43
1:B:435:LYS:HD2	1:B:436:GLN:N	2.20	0.43
1:B:769:THR:O	1:B:773:GLU:HB2	2.18	0.43
1:D:384:PRO:HB2	1:D:395:LEU:HD11	2.00	0.43
1:D:571:LEU:HD23	1:D:571:LEU:HA	1.74	0.43
1:D:806:ALA:HB1	1:D:811:VAL:O	2.19	0.43
1:A:302:THR:HB	1:A:767:HIS:NE2	2.33	0.43
1:D:217:LEU:HD22	1:D:221:GLN:HB3	2.01	0.43
1:D:390:GLU:HB3	1:D:612:LEU:HD21	2.00	0.43
1:B:741:CYS:HB3	1:B:746:CYS:SG	2.59	0.43
1:C:716:LEU:HD11	1:C:735:TYR:CZ	2.54	0.43
1:D:592:LEU:HG	1:D:648:SER:HB2	2.01	0.43
1:D:809:PHE:HB2	1:D:811:VAL:HG23	2.01	0.43
1:C:437:GLY:O	1:D:281:LYS:NZ	2.37	0.42
1:B:414:ASN:ND2	1:B:417:GLU:H	2.17	0.42
1:B:739:PHE:HD1	1:B:746:CYS:HB2	1.84	0.42
1:C:263:LEU:HD12	1:C:264:LEU:N	2.34	0.42
1:D:245:LYS:HE2	1:D:245:LYS:HB2	1.80	0.42
1:C:554:LYS:HB3	1:C:556:SER:O	2.19	0.42
1:A:330:ARG:NH1	1:A:593:ALA:HB2	2.34	0.42
1:A:410:ILE:HD13	1:A:425:LEU:HD11	2.01	0.42
1:A:670:ARG:HD3	1:A:756:ASN:OD1	2.20	0.42
1:B:200:PRO:HD2	1:B:230:LEU:HD12	2.01	0.42
1:B:591:VAL:HG11	1:B:621:VAL:HB	2.01	0.42
1:C:266:LEU:HB3	1:C:322:TYR:CE1	2.54	0.42
1:C:739:PHE:HD2	1:C:746:CYS:HB2	1.84	0.42
1:D:415:GLU:O	1:D:418:LYS:HB3	2.20	0.42
1:A:196:VAL:HG23	1:A:215:ARG:O	2.20	0.42
1:A:410:ILE:CD1	1:A:546:TYR:HB3	2.49	0.42
1:C:282:ARG:O	1:C:286:LYS:HE3	2.18	0.42
1:C:346:ILE:HG22	1:C:378:SER:HB2	2.02	0.42
1:C:663:ASN:O	1:C:672:ILE:HD11	2.20	0.42
1:D:269:LEU:HB2	1:D:272:LEU:HB3	2.01	0.42
1:D:663:ASN:O	1:D:672:ILE:HD11	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:812:ARG:HA	1:D:815:GLU:HB3	2.02	0.42
1:A:250:GLU:H	1:A:250:GLU:HG3	1.58	0.42
1:A:717:ASP:OD1	1:A:717:ASP:N	2.52	0.42
1:B:290:ARG:HB2	1:B:315:ALA:HA	2.01	0.42
1:B:299:ARG:O	1:B:826:GLU:HG2	2.20	0.42
1:B:435:LYS:HG3	1:B:435:LYS:H	1.52	0.42
1:B:512:PHE:HB2	1:B:547:LEU:HG	2.01	0.42
1:C:781:LEU:HD23	1:C:781:LEU:HA	1.86	0.42
1:D:266:LEU:HB3	1:D:322:TYR:CD1	2.55	0.42
1:D:350:ASP:HB2	1:D:578:VAL:HA	2.02	0.42
1:D:410:ILE:O	1:D:411:ILE:HD13	2.20	0.42
1:D:514:SER:C	1:D:515:LEU:HD23	2.40	0.42
1:A:250:GLU:OE1	1:A:284:TYR:OH	2.24	0.42
1:D:739:PHE:O	1:D:741:CYS:N	2.52	0.42
1:B:405:LEU:HD23	1:B:543:GLY:HA3	2.01	0.42
1:B:433:LYS:NZ	1:B:436:GLN:O	2.50	0.42
1:C:383:ASN:O	1:C:387:LEU:HB2	2.19	0.42
1:D:277:TYR:HA	1:D:319:VAL:HG21	2.02	0.42
1:C:537:PRO:HG2	1:C:540:HIS:HA	2.02	0.42
1:D:535:GLY:HA2	1:D:540:HIS:CE1	2.34	0.42
1:A:256:LYS:HB3	1:A:261:LYS:HB2	2.02	0.41
1:A:367:LYS:HB3	1:A:598:PHE:CZ	2.55	0.41
1:B:423:ALA:O	1:B:427:ARG:HG3	2.19	0.41
1:B:517:MET:O	1:B:520:LYS:HG3	2.20	0.41
1:B:523:SER:HB3	1:B:526:GLU:HG3	2.02	0.41
1:B:665:GLY:HA2	1:B:813:LYS:HD3	2.02	0.41
1:D:297:MET:SD	1:D:311:THR:HG21	2.60	0.41
1:D:583:SER:HB3	1:D:586:LEU:HD12	2.02	0.41
1:A:414:ASN:ND2	1:A:417:GLU:H	2.17	0.41
1:A:455:LEU:HB3	1:A:494:VAL:HG11	2.02	0.41
1:C:290:ARG:HB2	1:C:315:ALA:HA	2.01	0.41
1:D:625:LEU:HB3	1:D:630:PHE:HB2	2.02	0.41
1:D:708:SER:O	1:D:712:ILE:HG13	2.20	0.41
1:B:321:THR:O	1:B:325:ILE:HG12	2.19	0.41
1:C:276:LYS:HA	1:C:276:LYS:HD3	1.70	0.41
1:C:517:MET:O	1:C:520:LYS:HG3	2.21	0.41
1:C:671:TRP:CZ2	1:C:675:LYS:HE3	2.56	0.41
1:D:462:LYS:HA	1:D:462:LYS:HD3	1.58	0.41
1:A:538:LEU:HD22	1:A:541:GLU:N	2.32	0.41
1:A:544:LYS:HE2	1:A:544:LYS:HB2	1.94	0.41
1:B:418:LYS:HD3	1:B:513:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:LEU:HD23	1:B:571:LEU:HA	1.86	0.41
1:C:660:ILE:O	1:C:664:LEU:HG	2.19	0.41
1:C:798:LYS:O	1:C:802:ILE:HG13	2.21	0.41
1:A:503:VAL:HB	1:A:533:ARG:HH12	1.86	0.41
1:A:534:ALA:C	1:A:537:PRO:HD2	2.41	0.41
1:A:544:LYS:HB3	1:A:546:TYR:CE1	2.56	0.41
1:B:262:LYS:HG2	1:B:316:ASP:HA	2.01	0.41
1:D:753:ARG:HD2	1:D:753:ARG:HA	1.84	0.41
1:D:757:LEU:HD23	1:D:775:PHE:HE1	1.84	0.41
1:A:716:LEU:HD22	1:A:720:ILE:HD11	2.03	0.41
1:A:781:LEU:HD23	1:A:781:LEU:HA	1.79	0.41
1:B:781:LEU:HD23	1:B:781:LEU:HA	1.88	0.41
1:C:207:GLU:CA	1:D:215:ARG:HH22	2.29	0.41
1:C:364:ARG:NH1	1:C:593:ALA:HB3	2.36	0.41
1:D:554:LYS:HB3	1:D:556:SER:O	2.21	0.41
1:A:229:LEU:HD21	1:A:251:LEU:HB2	2.02	0.41
1:A:364:ARG:HD2	1:A:597:VAL:HG21	2.02	0.41
1:A:418:LYS:HD3	1:A:513:GLU:HG2	2.02	0.41
1:B:621:VAL:O	1:B:625:LEU:HG	2.21	0.41
1:C:786:GLY:O	1:C:790:THR:OG1	2.28	0.41
1:D:798:LYS:O	1:D:802:ILE:HG13	2.20	0.41
1:A:367:LYS:HE2	1:A:603:VAL:HG13	2.02	0.41
1:A:405:LEU:O	1:D:413:ARG:NH2	2.54	0.41
1:A:484:GLU:HG2	1:A:489:ARG:HD2	2.02	0.41
1:A:739:PHE:CE1	1:A:750:ALA:HB2	2.56	0.41
1:C:649:MET:HB3	1:C:649:MET:HE2	1.94	0.41
1:D:294:ARG:HE	1:D:328:LEU:HD21	1.85	0.41
1:D:365:LEU:HD23	1:D:368:LEU:HD12	2.03	0.41
1:D:475:TYR:CZ	1:D:479:LYS:HG3	2.56	0.41
1:A:507:ALA:N	1:A:537:PRO:HB3	2.32	0.41
1:A:550:GLU:HB3	1:A:553:ARG:HB2	2.03	0.41
1:B:236:LEU:HD23	1:B:388:ALA:HB2	2.02	0.41
1:B:253:GLY:HA2	1:B:340:THR:OG1	2.21	0.41
1:B:535:GLY:C	1:B:537:PRO:HD2	2.40	0.41
1:C:265:PHE:O	1:C:266:LEU:HD23	2.21	0.41
1:C:347:HIS:CE1	1:C:379:ALA:H	2.39	0.41
1:D:265:PHE:O	1:D:266:LEU:HD23	2.20	0.41
1:D:276:LYS:HA	1:D:276:LYS:HD3	1.68	0.41
1:D:305:GLU:HG3	1:D:789:PHE:CE2	2.56	0.41
1:D:350:ASP:HB2	1:D:578:VAL:HG22	2.02	0.41
1:D:622:LEU:HD13	1:D:638:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ASP:HB2	1:B:578:VAL:HG13	2.02	0.41
1:B:700:LEU:HD13	1:B:712:ILE:HD11	2.03	0.41
1:C:410:ILE:HD11	1:C:546:TYR:HD2	1.86	0.41
1:D:441:GLN:OE1	1:D:488:GLN:HA	2.21	0.41
1:A:365:LEU:HD23	1:A:365:LEU:HA	1.76	0.40
1:A:538:LEU:HD13	1:A:541:GLU:HB3	2.01	0.40
1:A:582:TRP:HE3	1:A:587:GLU:HG3	1.85	0.40
1:C:241:THR:HG22	1:C:245:LYS:HE3	2.03	0.40
1:C:515:LEU:C	1:C:522:LEU:HG	2.41	0.40
1:C:685:SER:OG	1:C:688:LEU:HB2	2.21	0.40
1:C:800:GLU:HB3	1:C:804:ARG:NH2	2.36	0.40
1:A:806:ALA:HB1	1:A:811:VAL:O	2.20	0.40
1:B:263:LEU:HD12	1:B:264:LEU:N	2.37	0.40
1:C:294:ARG:O	1:C:320:GLY:HA2	2.21	0.40
1:D:754:VAL:O	1:D:758:ILE:HG13	2.22	0.40
1:A:497:ALA:C	1:A:499:LEU:H	2.24	0.40
1:B:276:LYS:HA	1:B:276:LYS:HD3	1.66	0.40
1:B:477:GLN:HA	1:B:480:LEU:HB3	2.03	0.40
1:C:273:ALA:O	1:C:277:TYR:HB3	2.21	0.40
1:A:290:ARG:HB2	1:A:315:ALA:HA	2.03	0.40
1:A:346:ILE:HG22	1:A:378:SER:HB2	2.02	0.40
1:B:429:GLU:HG2	1:B:509:GLN:HB3	2.03	0.40
1:D:203:GLU:OE1	1:D:206:LYS:HD2	2.21	0.40
1:A:809:PHE:HB2	1:A:811:VAL:HG23	2.02	0.40
1:B:795:ILE:HD13	1:B:795:ILE:HA	1.88	0.40
1:C:401:ARG:HA	1:C:401:ARG:HE	1.86	0.40
1:C:541:GLU:CG	1:C:542:LYS:H	2.34	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	631/639 (99%)	590 (94%)	41 (6%)	0	100	100
1	B	631/639 (99%)	589 (93%)	39 (6%)	3 (0%)	29	67
1	C	637/639 (100%)	597 (94%)	40 (6%)	0	100	100
1	D	636/639 (100%)	589 (93%)	46 (7%)	1 (0%)	47	80
All	All	2535/2556 (99%)	2365 (93%)	166 (6%)	4 (0%)	47	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	434	SER
1	B	437	GLY
1	B	538	LEU
1	D	537	PRO

### 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	541/547 (99%)	524 (97%)	17 (3%)	40	62
1	B	541/547 (99%)	523 (97%)	18 (3%)	38	61
1	C	547/547 (100%)	531 (97%)	16 (3%)	42	63
1	D	546/547 (100%)	527 (96%)	19 (4%)	36	60
All	All	2175/2188 (99%)	2105 (97%)	70 (3%)	39	61

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	266	LEU
1	A	313	ILE
1	A	401	ARG
1	A	414	ASN
1	A	432	ARG
1	A	480	LEU
1	A	505	PHE

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Mol	Chain	Res	Type
1	A	523	SER
1	A	538	LEU
1	A	539	TYR
1	A	564	ASP
1	A	584	ASP
1	A	633	MET
1	A	640	VAL
1	A	688	LEU
1	A	747	THR
1	A	774	HIS
1	B	266	LEU
1	B	313	ILE
1	B	401	ARG
1	B	414	ASN
1	B	433	LYS
1	B	435	LYS
1	B	483	MET
1	B	505	PHE
1	B	539	TYR
1	B	542	LYS
1	B	564	ASP
1	B	584	ASP
1	B	633	MET
1	B	640	VAL
1	B	688	LEU
1	B	747	THR
1	B	774	HIS
1	B	793	ASP
1	C	266	LEU
1	C	313	ILE
1	C	401	ARG
1	C	414	ASN
1	C	435	LYS
1	C	439	LYS
1	C	483	MET
1	C	505	PHE
1	C	539	TYR
1	C	564	ASP
1	C	584	ASP
1	C	633	MET
1	C	640	VAL
1	C	747	THR

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Mol	Chain	Res	Type
1	C	774	HIS
1	C	827	GLU
1	D	266	LEU
1	D	313	ILE
1	D	401	ARG
1	D	414	ASN
1	D	431	MET
1	D	432	ARG
1	D	435	LYS
1	D	436	GLN
1	D	505	PHE
1	D	536	ARG
1	D	539	TYR
1	D	540	HIS
1	D	541	GLU
1	D	545	VAL
1	D	564	ASP
1	D	584	ASP
1	D	633	MET
1	D	747	THR
1	D	827	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	477	GLN
1	C	594	HIS

### 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

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	633/639 (99%)	0.44	41 (6%)	18 15	151, 237, 320, 523	0
1	B	633/639 (99%)	0.43	43 (6%)	17 14	145, 235, 317, 509	0
1	C	639/639 (100%)	0.47	50 (7%)	13 11	151, 240, 326, 399	0
1	D	638/639 (99%)	0.42	36 (5%)	24 20	147, 238, 318, 467	0
All	All	2543/2556 (99%)	0.44	170 (6%)	17 14	145, 237, 320, 523	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	310	ASP	8.4
1	B	310	ASP	7.8
1	C	502	GLY	7.1
1	D	309	VAL	6.2
1	C	309	VAL	6.0
1	A	310	ASP	5.8
1	C	310	ASP	5.8
1	C	307	VAL	5.7
1	C	632	LYS	5.5
1	B	215	ARG	5.3
1	D	307	VAL	5.3
1	A	633	MET	5.2
1	C	235	LEU	5.1
1	C	306	LEU	5.0
1	C	633	MET	5.0
1	B	309	VAL	4.6
1	B	403	VAL	4.5
1	C	580	VAL	4.4
1	B	539	TYR	4.4
1	B	469	TYR	4.3
1	A	235	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	402	PRO	4.1
1	A	469	TYR	4.0
1	C	312	GLY	4.0
1	C	375	ILE	4.0
1	A	700	LEU	4.0
1	C	639	GLU	3.9
1	C	402	PRO	3.8
1	C	236	LEU	3.8
1	C	501	ALA	3.8
1	A	375	ILE	3.7
1	D	538	LEU	3.7
1	D	401	ARG	3.6
1	A	536	ARG	3.6
1	B	311	THR	3.6
1	D	437	GLY	3.6
1	D	306	LEU	3.6
1	B	633	MET	3.5
1	C	302	THR	3.5
1	C	305	GLU	3.5
1	B	536	ARG	3.5
1	A	309	VAL	3.5
1	D	537	PRO	3.5
1	B	375	ILE	3.5
1	C	300	ILE	3.5
1	A	502	GLY	3.4
1	A	632	LYS	3.4
1	A	803	GLU	3.4
1	A	656	GLU	3.3
1	A	237	VAL	3.3
1	A	300	ILE	3.3
1	C	290	ARG	3.3
1	B	396	VAL	3.3
1	A	401	ARG	3.3
1	C	469	TYR	3.3
1	A	403	VAL	3.3
1	D	305	GLU	3.3
1	C	403	VAL	3.2
1	C	291	VAL	3.2
1	D	399	ASP	3.2
1	A	505	PHE	3.2
1	A	215	ARG	3.2
1	D	381	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	717	ASP	3.2
1	D	555	TYR	3.1
1	D	311	THR	3.1
1	D	536	ARG	3.1
1	B	300	ILE	3.1
1	C	299	ARG	3.1
1	A	501	ALA	3.1
1	B	632	LYS	3.0
1	B	237	VAL	3.0
1	B	656	GLU	3.0
1	C	700	LEU	3.0
1	D	580	VAL	3.0
1	D	632	LYS	3.0
1	B	306	LEU	3.0
1	C	451	ARG	3.0
1	C	381	VAL	3.0
1	D	469	TYR	3.0
1	B	216	GLU	3.0
1	B	294	ARG	3.0
1	A	236	LEU	3.0
1	D	717	ASP	2.9
1	A	307	VAL	2.9
1	C	536	ARG	2.9
1	A	252	ALA	2.9
1	C	581	GLU	2.8
1	A	374	PHE	2.8
1	B	376	GLY	2.8
1	B	235	LEU	2.8
1	B	501	ALA	2.8
1	C	638	VAL	2.8
1	A	316	ASP	2.7
1	B	555	TYR	2.7
1	A	312	GLY	2.7
1	C	374	PHE	2.7
1	A	467	LYS	2.7
1	D	579	GLN	2.7
1	B	236	LEU	2.7
1	D	489	ARG	2.7
1	A	304	ASP	2.6
1	C	237	VAL	2.6
1	C	579	GLN	2.6
1	C	252	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	289	LEU	2.6
1	B	553	ARG	2.5
1	C	652	LEU	2.5
1	C	316	ASP	2.5
1	C	465	LYS	2.5
1	C	308	VAL	2.4
1	D	633	MET	2.4
1	B	579	GLN	2.4
1	C	656	GLU	2.4
1	D	300	ILE	2.4
1	B	535	GLY	2.4
1	D	467	LYS	2.4
1	A	634	LYS	2.4
1	C	436	GLN	2.4
1	C	303	LYS	2.4
1	B	506	PRO	2.4
1	D	375	ILE	2.4
1	D	578	VAL	2.4
1	B	374	PHE	2.3
1	B	635	ARG	2.3
1	D	235	LEU	2.3
1	D	402	PRO	2.3
1	A	535	GLY	2.3
1	B	492	VAL	2.3
1	D	374	PHE	2.3
1	D	252	ALA	2.3
1	A	443	ILE	2.3
1	B	814	THR	2.3
1	D	308	VAL	2.3
1	A	489	ARG	2.2
1	A	396	VAL	2.2
1	A	294	ARG	2.2
1	B	307	VAL	2.2
1	A	638	VAL	2.2
1	A	581	GLU	2.2
1	A	619	GLU	2.2
1	B	289	LEU	2.2
1	C	342	VAL	2.2
1	A	636	PRO	2.2
1	C	376	GLY	2.2
1	A	295	VAL	2.1
1	B	214	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	505	PHE	2.1
1	B	598	PHE	2.1
1	D	237	VAL	2.1
1	D	505	PHE	2.1
1	C	285	SER	2.1
1	C	492	VAL	2.1
1	D	403	VAL	2.1
1	A	493	VAL	2.1
1	B	490	LEU	2.1
1	C	304	ASP	2.1
1	C	525	ARG	2.1
1	B	713	LEU	2.1
1	C	401	ARG	2.0
1	D	212	GLU	2.0
1	C	348	THR	2.0
1	A	814	THR	2.0
1	D	798	LYS	2.0
1	B	580	VAL	2.0
1	B	780	GLY	2.0
1	D	604	ILE	2.0
1	B	779	TYR	2.0
1	B	401	ARG	2.0
1	B	815	GLU	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 [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.