



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:58 PM UTC

PDB ID : 7UJB / pdb_00007ujb
Title : N-terminal domain deletion variant of Eta
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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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

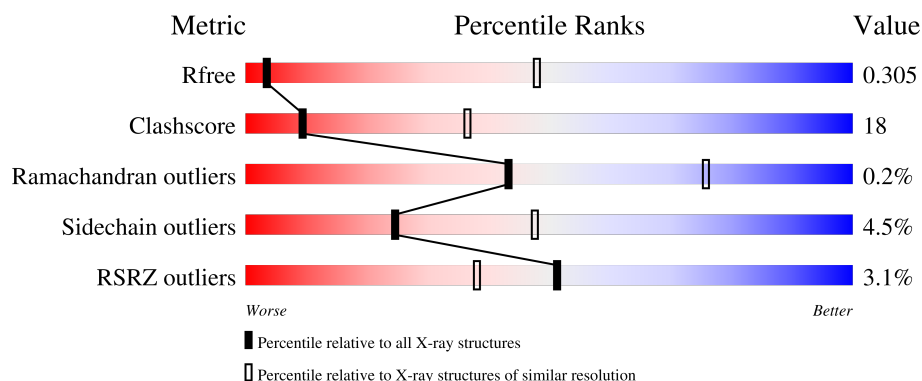
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1249 (4.44-3.80)
Clashscore	190562	1031 (4.42-3.82)
Ramachandran outliers	187476	1211 (4.44-3.80)
Sidechain outliers	187428	1198 (4.44-3.80)
RSRZ outliers	180081	1246 (4.44-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 4% 62% 35% ..
1	B	639	 2% 62% 34% ..
1	C	639	 3% 58% 40% .
1	D	639	 3% 58% 39% .

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.

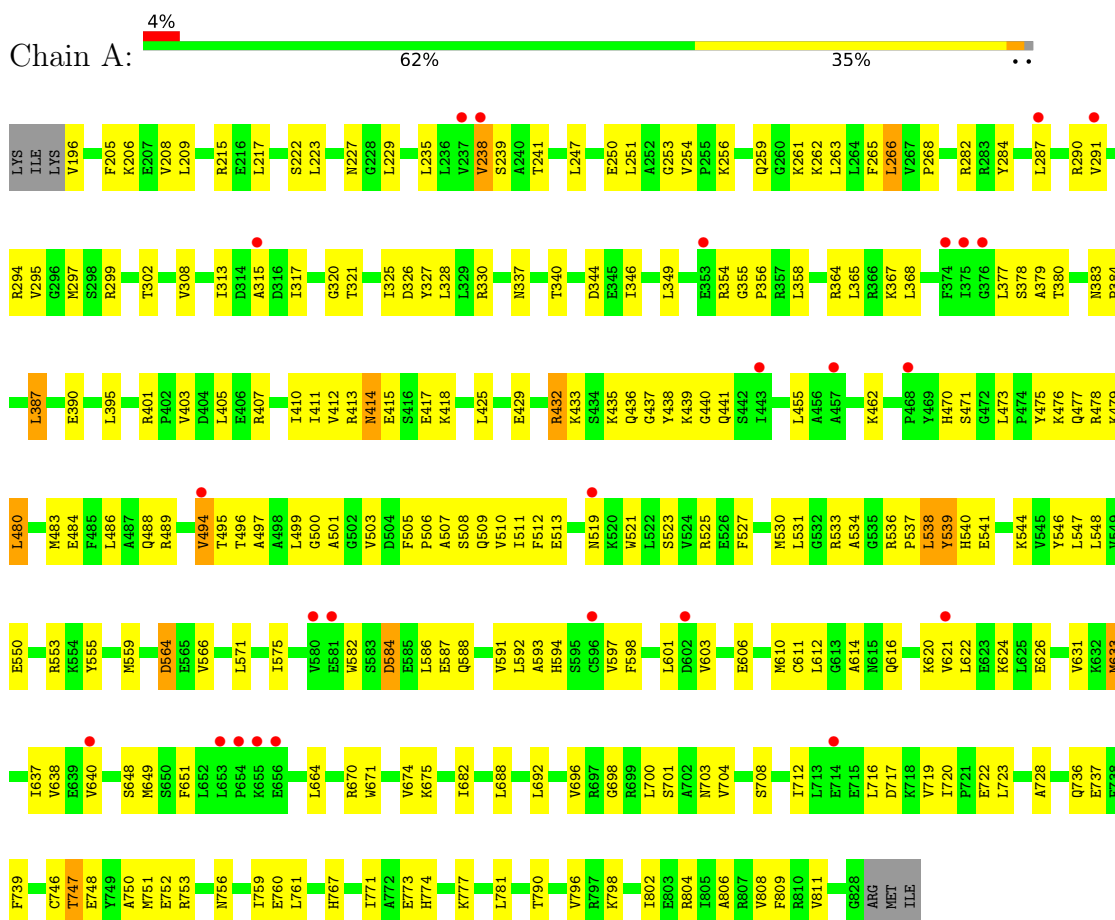
- Molecule 1 is a protein called DEAD/DEAH box RNA helicase.

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			

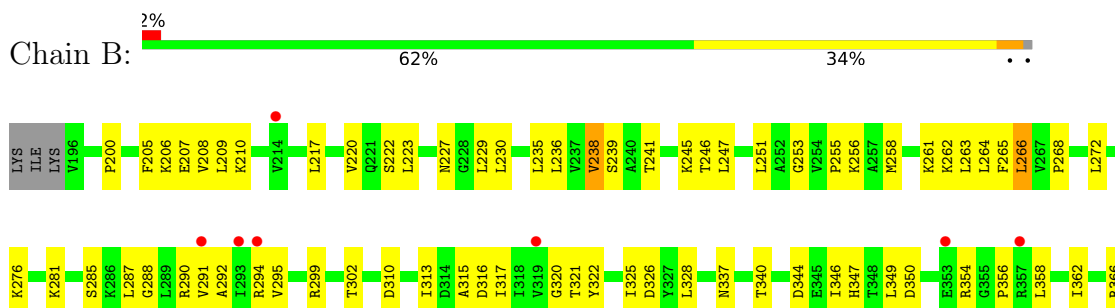
3 Residue-property plots

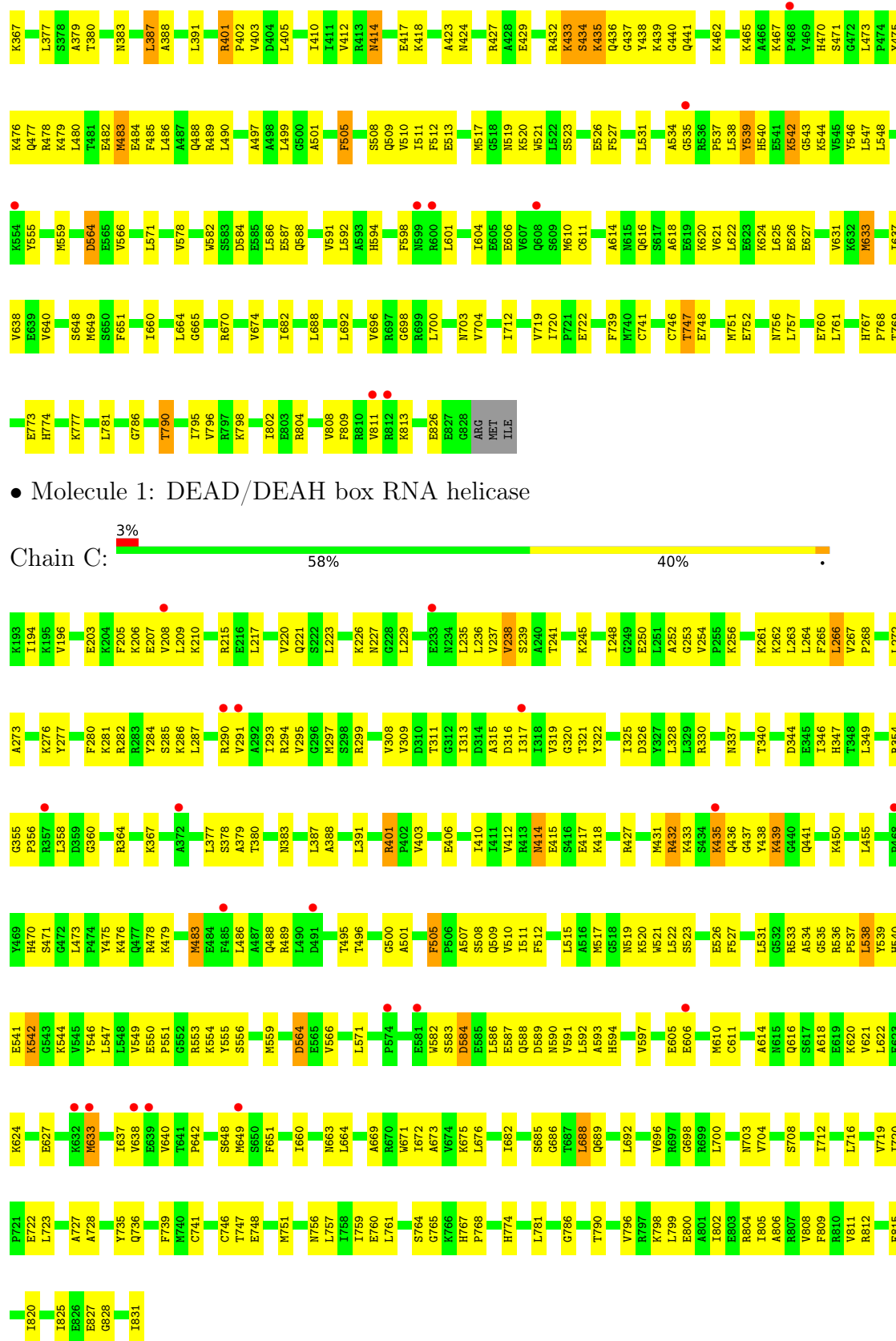
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	135.24Å 135.24Å 262.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.48 – 4.12 43.48 – 4.12	Depositor EDS
% Data completeness (in resolution range)	90.0 (43.48-4.12) 90.3 (43.48-4.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.250 , 0.303 0.256 , 0.305	Depositor DCC
R_{free} test set	1997 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	177.0	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 766.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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	0.87	EDS
Total number of atoms	20234	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.28	0/5123	0.51	0/6907
1	B	0.28	0/5123	0.53	0/6907
1	C	0.28	0/5176	0.52	0/6975
1	D	0.28	0/5168	0.53	0/6964
All	All	0.28	0/20590	0.52	0/27753

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.

There are no bond angle outliers.

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	177	0
1	B	5034	0	5187	177	0
1	C	5087	0	5257	205	0
1	D	5079	0	5246	203	0
All	All	20234	0	20877	739	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 18.

All (739) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:281:LYS:HA	1:D:291:VAL:HG21	1.78	0.66
1:A:606:GLU:HG2	1:A:610:MET:HE3	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:633:MET:HE3	1:D:638:VAL:HG22	1.79	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:497:ALA:HB2	1:A:530:MET:HE3	1.81	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:665:GLY:O	1:B:813:LYS:NZ	2.32	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:C:309:VAL:HG21	1:D:439:LYS:HZ1	1.64	0.62
1:B:510:VAL:HG23	1:B:534:ALA:HB2	1.81	0.61
1:C:606:GLU:HG2	1:C:610:MET:HE3	1.83	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:519:ASN:HA	1:B:559:MET:HE3	1.85	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:497:ALA:HB2	1:D:530:MET:HE3	1.85	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:633:MET:HE3	1:C:638:VAL:HG22	1.86	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:A:633:MET:HE3	1:A:638:VAL:HG22	1.87	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:434:SER:OG	1:B:435:LYS:N	2.33	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:D:523:SER:HB3	1:D:526:GLU:CD	2.30	0.56
1:A:476:LYS:HE2	1:B:476:LYS:HE3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:TRP:HE1	1:C:559:MET:HB3	1.70	0.56
1:B:649:MET:HE2	1:B:804:ARG:HH11	1.70	0.55
1:A:330:ARG:CZ	1:A:593:ALA:HB2	2.37	0.55
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:D:436:GLN:H	1:D:436:GLN:CD	2.15	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:B:601:LEU:HD22	1:B:633:MET:HE1	1.89	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:747:THR:HG22	1:B:751:MET:HE3	1.90	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:606:GLU:HG2	1:B:610:MET:HE3	1.91	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:B:633:MET:HE3	1:B:638:VAL:HG22	1.89	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:367:LYS:NZ	1:C:606:GLU:OE2	2.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:649:MET:HE2	1:D:804:ARG:HH11	1.75	0.52
1:B:624:LYS:HA	1:B:627:GLU:CD	2.35	0.52
1:C:622:LEU:HD22	1:C:638:VAL:HG11	1.90	0.52
1:D:519:ASN:HA	1:D:559:MET:HE3	1.91	0.52
1:B:439:LYS:NZ	1:B:488:GLN:HA	2.25	0.51
1:D:439:LYS:NZ	1:D:488:GLN:O	2.32	0.51
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:436:GLN:C	1:B:438:TYR:N	2.68	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:A:649:MET:HE2	1:A:804:ARG:HH11	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:519:ASN:HA	1:A:559:MET:HE3	1.92	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
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: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:D:686:GLY:C	1:D:690:ARG:HH21	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:523:SER:HB3	1:C:526:GLU:CD	2.37	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
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:C:483:MET:HE1	1:C:489:ARG:NH2	2.28	0.48
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:B:523:SER:HB3	1:B:526:GLU:CD	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:HH21	1:B:210:LYS:HB2	1.78	0.48
1:D:539:TYR:O	1:D:540:HIS:C	2.57	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:C:786:GLY:O	1:C:790:THR:OG1	2.28	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:523:SER:OG	1:D:576:GLU:OE2	2.23	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
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:A:747:THR:HG22	1:A:751:MET:HE3	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:434:SER:OG	1:B:435:LYS:HG3	2.14	0.47
1:D:514:SER:C	1:D:515:LEU:HD23	2.40	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: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
1:D:606:GLU:HG2	1:D:610:MET:HE3	1.98	0.46
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:A:534:ALA:C	1:A:537:PRO:HD2	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:535:GLY:C	1:B:537:PRO:HD2	2.40	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: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
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:515:LEU:C	1:C:522:LEU:HG	2.41	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:A:497:ALA:C	1:A:499:LEU:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:THR:OG1	1:C:496:THR:N	2.50	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:285:SER:C	1:D:287:LEU:H	2.25	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
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:C:326:ASP:CG	1:C:330:ARG:HE	2.26	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:A:471:SER:C	1:A:473:LEU:H	2.26	0.43
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:B:649:MET:HE2	1:B:804:ARG:NH1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:471:SER:C	1:B:473:LEU:H	2.26	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:C:649:MET:HE2	1:C:804:ARG:HH11	1.82	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:471:SER:C	1:C:473:LEU:H	2.27	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:519:ASN:HA	1:C:559:MET:HE3	1.99	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
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:A:250:GLU:OE1	1:A:284:TYR:OH	2.24	0.42
1:C:433:LYS:HZ3	1:D:290:ARG:HB3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:497:ALA:C	1:B:499:LEU:H	2.28	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:471:SER:C	1:D:473:LEU:H	2.28	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:B:436:GLN:C	1:B:438:TYR:H	2.28	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
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:544:LYS:HB3	1:A:546:TYR:CE1	2.56	0.41
1:A:601:LEU:HD22	1:A:633:MET:HE1	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:716:LEU:C	1:D:718:LYS:H	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: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: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
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: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:C:624:LYS:HA	1:C:627:GLU:CD	2.46	0.40
1:D:754:VAL:O	1:D:758:ILE:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:347:HIS:C	1:B:349:LEU:N	2.79	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%)	24	61
1	C	637/639 (100%)	597 (94%)	40 (6%)	0	100	100
1	D	636/639 (100%)	589 (93%)	46 (7%)	1 (0%)	43	76
All	All	2535/2556 (99%)	2365 (93%)	166 (6%)	4 (0%)	43	76

All (4) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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%)	516 (95%)	25 (5%)	24	47
1	B	541/547 (99%)	519 (96%)	22 (4%)	27	50
1	C	547/547 (100%)	524 (96%)	23 (4%)	26	49
1	D	546/547 (100%)	519 (95%)	27 (5%)	22	46
All	All	2175/2188 (99%)	2078 (96%)	97 (4%)	24	47

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	VAL
1	A	259	GLN
1	A	266	LEU
1	A	313	ILE
1	A	387	LEU
1	A	401	ARG
1	A	414	ASN
1	A	432	ARG
1	A	480	LEU
1	A	494	VAL
1	A	505	PHE
1	A	509	GLN
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	637	ILE
1	A	640	VAL

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Mol	Chain	Res	Type
1	A	688	LEU
1	A	736	GLN
1	A	747	THR
1	A	774	HIS
1	A	790	THR
1	B	220	VAL
1	B	238	VAL
1	B	266	LEU
1	B	313	ILE
1	B	387	LEU
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	637	ILE
1	B	640	VAL
1	B	688	LEU
1	B	747	THR
1	B	774	HIS
1	B	790	THR
1	C	220	VAL
1	C	238	VAL
1	C	266	LEU
1	C	313	ILE
1	C	401	ARG
1	C	414	ASN
1	C	432	ARG
1	C	435	LYS
1	C	439	LYS
1	C	483	MET
1	C	505	PHE
1	C	542	LYS
1	C	549	VAL
1	C	564	ASP
1	C	584	ASP

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Mol	Chain	Res	Type
1	C	633	MET
1	C	637	ILE
1	C	640	VAL
1	C	688	LEU
1	C	736	GLN
1	C	747	THR
1	C	774	HIS
1	C	827	GLU
1	D	238	VAL
1	D	266	LEU
1	D	313	ILE
1	D	387	LEU
1	D	401	ARG
1	D	414	ASN
1	D	431	MET
1	D	435	LYS
1	D	436	GLN
1	D	484	GLU
1	D	505	PHE
1	D	536	ARG
1	D	539	TYR
1	D	540	HIS
1	D	541	GLU
1	D	542	LYS
1	D	545	VAL
1	D	549	VAL
1	D	564	ASP
1	D	584	ASP
1	D	633	MET
1	D	640	VAL
1	D	688	LEU
1	D	736	GLN
1	D	747	THR
1	D	774	HIS
1	D	827	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	421	HIS
1	A	453	HIS
1	A	477	GLN

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Mol	Chain	Res	Type
1	C	421	HIS
1	C	436	GLN
1	C	477	GLN
1	C	594	HIS
1	C	615	ASN
1	C	616	GLN
1	D	408	HIS
1	D	774	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	633/639 (99%)	0.15	25 (3%) 43 34	151, 237, 320, 523	0
1	B	633/639 (99%)	0.12	15 (2%) 59 45	145, 235, 317, 509	0
1	C	639/639 (100%)	0.15	19 (2%) 52 39	151, 240, 326, 399	0
1	D	638/639 (99%)	0.15	21 (3%) 49 37	147, 238, 318, 467	0
All	All	2543/2556 (99%)	0.14	80 (3%) 51 38	145, 237, 320, 523	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	311	THR	6.6
1	D	555	TYR	5.3
1	A	376	GLY	4.7
1	A	596	CYS	4.5
1	C	639	GLU	4.4
1	B	357	ARG	4.4
1	D	554	LYS	4.3
1	D	582	TRP	4.1
1	C	291	VAL	3.9
1	A	238	VAL	3.9
1	D	607	VAL	3.8
1	D	400	GLU	3.4
1	B	811	VAL	3.3
1	D	320	GLY	3.3
1	C	485	PHE	3.3
1	A	655	LYS	3.2
1	C	632	LYS	3.0
1	B	214	VAL	3.0
1	A	468	PRO	3.0
1	A	237	VAL	3.0
1	A	581	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	653	LEU	2.9
1	A	580	VAL	2.9
1	C	581	GLU	2.9
1	D	639	GLU	2.8
1	B	599	ASN	2.8
1	B	600	ARG	2.8
1	C	574	PRO	2.8
1	C	233	GLU	2.8
1	D	357	ARG	2.7
1	C	633	MET	2.7
1	A	287	LEU	2.7
1	A	315	ALA	2.7
1	B	812	ARG	2.7
1	A	621	VAL	2.6
1	C	435	LYS	2.6
1	A	375	ILE	2.5
1	A	291	VAL	2.5
1	D	606	GLU	2.5
1	D	231	ASP	2.5
1	A	374	PHE	2.5
1	D	294	ARG	2.5
1	A	714	GLU	2.5
1	A	519	ASN	2.5
1	B	608	GLN	2.5
1	D	742	PRO	2.5
1	B	554	LYS	2.5
1	B	468	PRO	2.4
1	D	603	VAL	2.4
1	B	294	ARG	2.4
1	D	319	VAL	2.4
1	B	293	ILE	2.4
1	D	638	VAL	2.4
1	D	624	LYS	2.4
1	C	468	PRO	2.3
1	A	353	GLU	2.3
1	B	353	GLU	2.3
1	A	602	ASP	2.3
1	A	656	GLU	2.2
1	D	324	GLY	2.2
1	A	457	ALA	2.2
1	C	290	ARG	2.2
1	C	317	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	638	VAL	2.2
1	A	443	ILE	2.2
1	C	208	VAL	2.2
1	C	649	MET	2.2
1	B	291	VAL	2.1
1	C	491	ASP	2.1
1	C	606	GLU	2.1
1	C	372	ALA	2.1
1	A	640	VAL	2.1
1	B	319	VAL	2.1
1	D	309	VAL	2.1
1	B	535	GLY	2.0
1	D	600	ARG	2.0
1	D	602	ASP	2.0
1	A	494	VAL	2.0
1	A	654	PRO	2.0
1	C	357	ARG	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 oligosaccharides 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.