



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:53 am GMT

PDB ID : 1ZM4
Title : Structure of the eEF2-ETA-bTAD complex
Authors : Joergensen, R.; Merrill, A.R.; Yates, S.P.; Marquez, V.E.; Schwan, A.L.; Boesen, T.; Andersen, G.R.
Deposited on : 2005-05-10
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

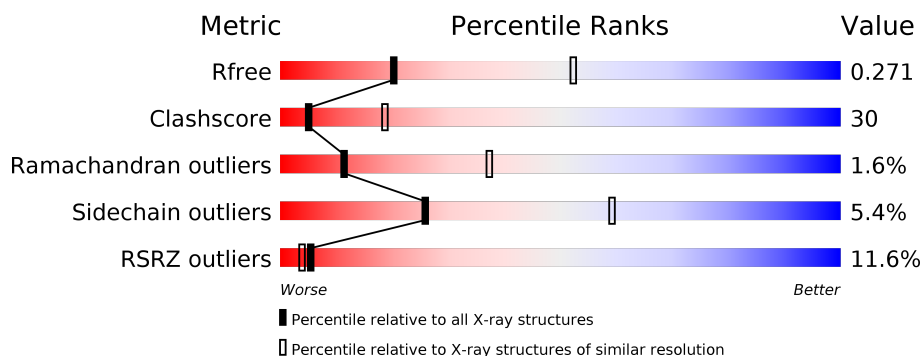
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	842	<div> <div>3%</div> <div> <div>50%</div> <div>45%</div> <div>..</div> </div> </div>
1	C	842	<div> <div>10%</div> <div> <div>50%</div> <div>44%</div> <div>..</div> </div> </div>
1	E	842	<div> <div>29%</div> <div> <div>46%</div> <div>49%</div> <div>..</div> </div> </div>
2	B	207	<div> <div>57%</div> <div>37%</div> <div>5%</div> </div>
2	D	207	<div> <div>%</div> <div> <div>60%</div> <div>37%</div> <div>.</div> </div> </div>
2	F	207	<div> <div>%</div> <div> <div>54%</div> <div>40%</div> <div>7%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24125 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			
1	C	823	Total	C	N	O	S	0	0	0
			6415	4082	1095	1208	30			
1	E	823	Total	C	N	O	S	0	0	0
			6415	4082	1095	1208	30			

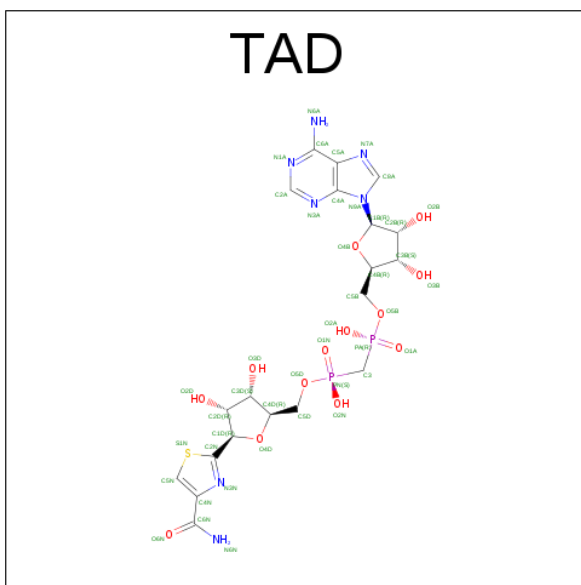
There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called exotoxin A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	0	0	0
			1587	1001	283	303			
2	D	207	Total	C	N	O	0	0	0
			1587	1001	283	303			
2	F	207	Total	C	N	O	0	0	0
			1587	1001	283	303			

- Molecule 3 is BETA-METHYLENE-THIAZOLE-4-CARBOXYAMIDE-ADENINE DINUCLEOTIDE (three-letter code: TAD) (formula: C₂₀H₂₇N₇O₁₃P₂S).

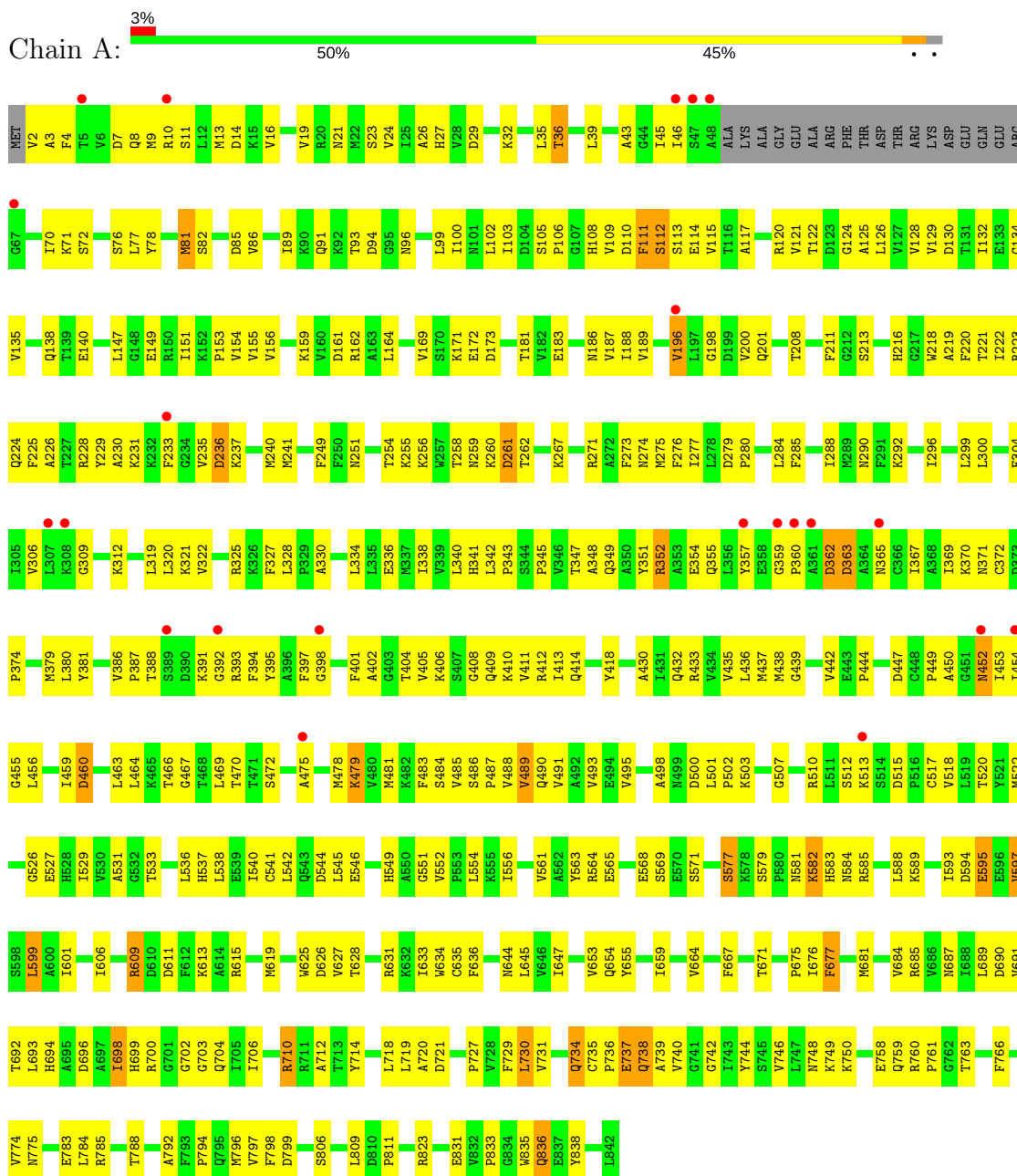


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total 43	C 20	N 7	O 13	P 2	S 1	0	0
3	D	1	Total 43	C 20	N 7	O 13	P 2	S 1	0	0
3	F	1	Total 43	C 20	N 7	O 13	P 2	S 1	0	0

3 Residue-property plots

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

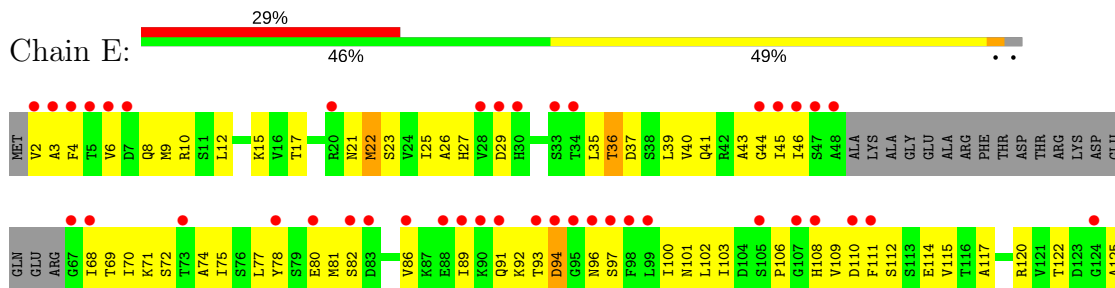
• Molecule 1: Elongation factor 2

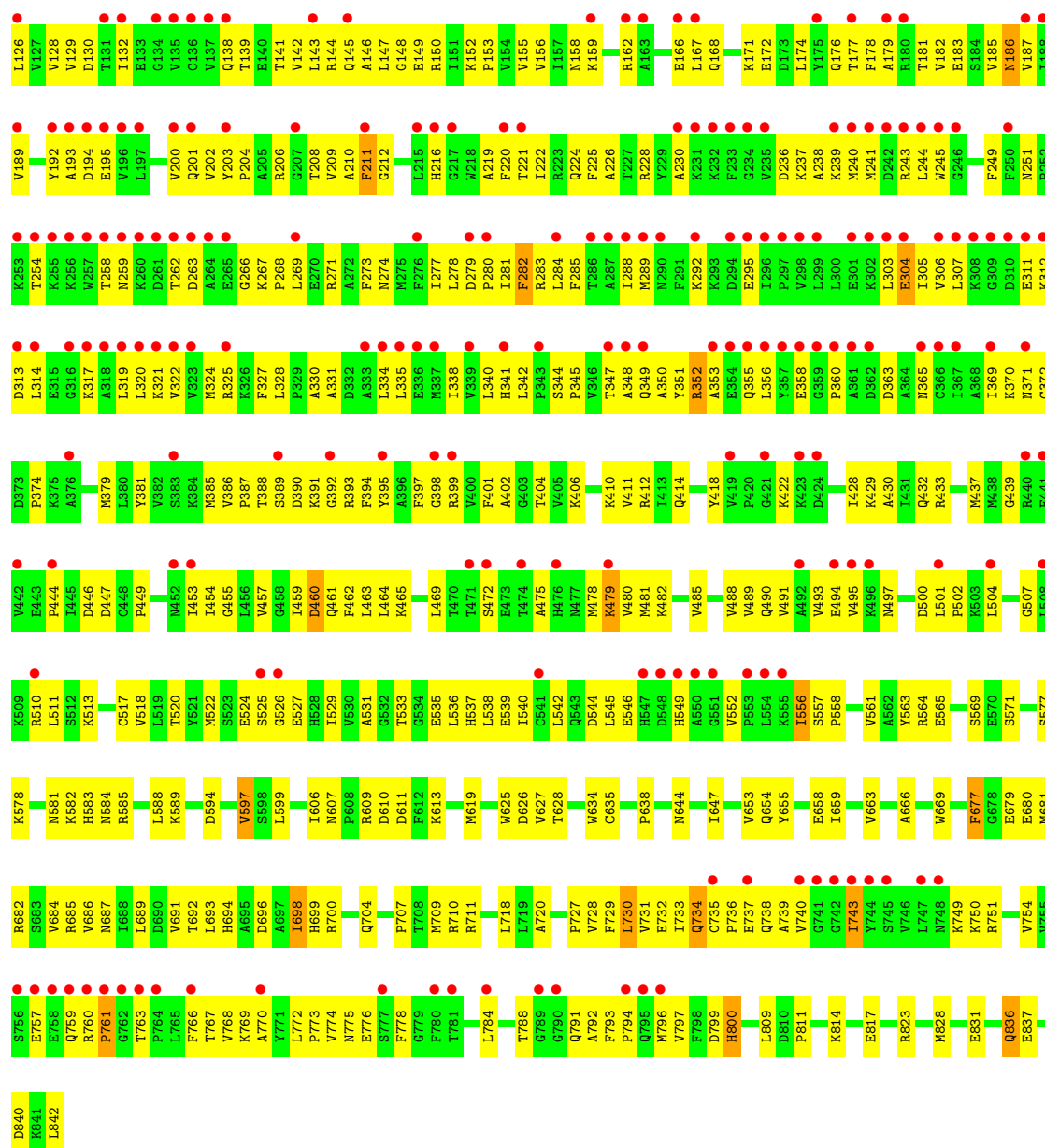


Chain C:



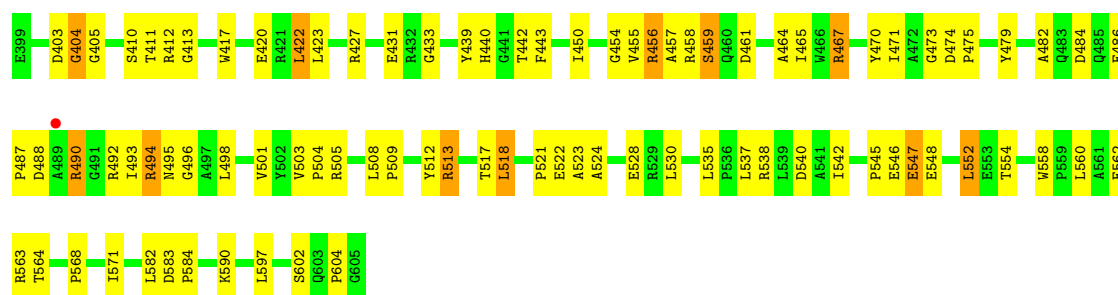
Chain E:



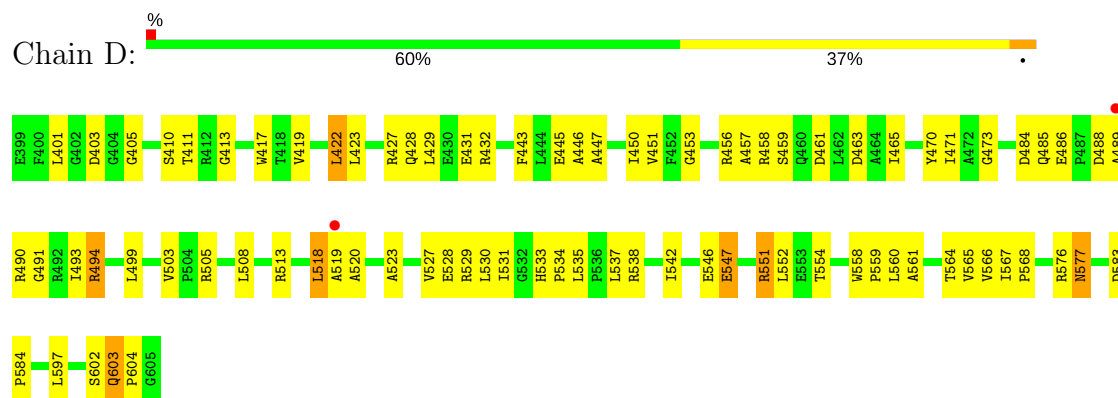


• Molecule 2: exotoxin A

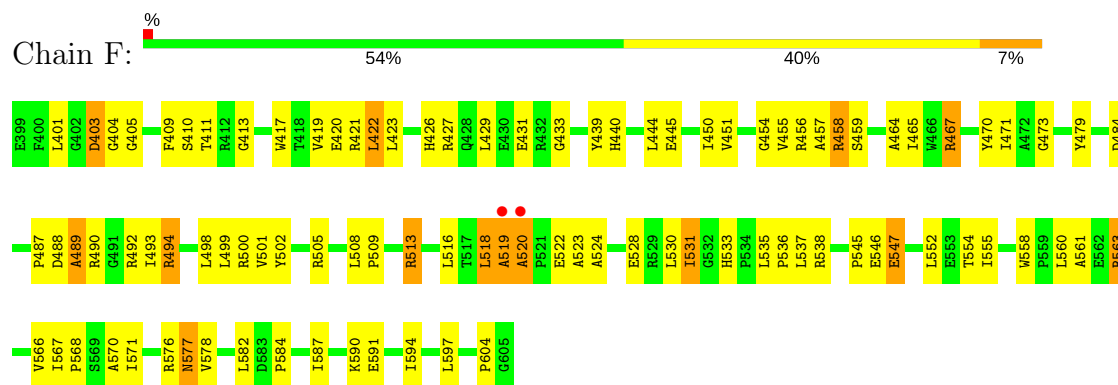
Chain B: 57% 37% 5%



• Molecule 2: exotoxin A



• Molecule 2: exotoxin A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	326.95Å 68.58Å 190.20Å 90.00° 103.42° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.90) 99.8 (29.97-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.99 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.276 0.246 , 0.271	Depositor DCC
R_{free} test set	1849 reflections (2.02%)	DCC
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	24125	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.77 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2606e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/6517	0.66	1/8823 (0.0%)
1	C	0.42	0/6517	0.66	2/8823 (0.0%)
1	E	0.41	0/6517	0.62	0/8823
2	B	0.58	0/1626	0.82	0/2216
2	D	0.57	0/1626	0.80	0/2216
2	F	0.57	0/1626	0.83	0/2216
All	All	0.45	0/24429	0.69	3/33117 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	820	LEU	CA-CB-CG	6.18	129.51	115.30
1	A	236	ASP	N-CA-C	-5.56	95.98	111.00
1	C	711	ARG	NE-CZ-NH2	-5.05	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6405	0	6472	394	1
1	C	6415	0	6488	407	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	6415	0	6488	425	0
2	B	1587	0	1539	75	0
2	D	1587	0	1539	75	0
2	F	1587	0	1539	83	1
3	B	43	0	25	2	0
3	D	43	0	25	2	0
3	F	43	0	25	3	0
All	All	24125	0	24140	1434	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (1434) 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)
2:B:552:LEU:HD12	2:B:552:LEU:H	1.10	1.15
1:E:71:LYS:HE3	1:E:387:PRO:HD2	1.32	1.11
1:E:556:ILE:HG22	1:E:557:SER:H	1.08	1.09
1:E:699:DDE:HAC2	1:E:699:DDE:HAD2	1.12	1.08
1:C:699:DDE:HAC2	1:C:699:DDE:HAD2	1.09	1.08
1:A:464:LEU:HD21	1:A:485:VAL:HB	1.32	1.07
1:C:759:GLN:HG2	1:C:760:ARG:H	1.12	1.06
1:C:231:LYS:HG3	1:C:232:LYS:H	1.18	1.04
1:E:68:ILE:HD12	1:E:390:ASP:HB2	1.39	1.03
1:C:542:LEU:HD13	1:C:556:ILE:HD11	1.41	1.02
1:E:147:LEU:HD13	1:E:192:TYR:HB2	1.42	1.01
1:E:522:MET:HB2	2:F:490:ARG:NH2	1.77	0.98
2:B:546:GLU:HG3	2:B:547:GLU:HG3	1.42	0.98
1:E:694:HIS:CD2	1:E:696:ASP:H	1.81	0.97
1:A:784:LEU:HD23	1:A:794:PRO:HG3	1.47	0.97
1:E:581:ASN:HD21	1:E:704:GLN:HG3	1.26	0.96
1:C:404:THR:HG22	1:C:449:PRO:HA	1.49	0.95
2:B:405:GLY:HA2	1:C:627:VAL:HG12	1.49	0.94
1:E:27:HIS:HD2	1:E:29:ASP:H	1.14	0.94
1:A:694:HIS:HD2	1:A:696:ASP:H	1.01	0.93
1:E:391:LYS:HG3	1:E:392:GLY:H	1.34	0.93
1:E:91:GLN:HE22	1:E:344:SER:H	1.15	0.92
1:C:694:HIS:HD2	1:C:696:ASP:H	1.17	0.92
2:B:457:ALA:HB2	2:B:558:TRP:CD2	2.05	0.92
1:C:784:LEU:HD23	1:C:794:PRO:HG3	1.49	0.92
1:C:578:LYS:HE3	1:C:840:ASP:OD1	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:HG21	1:A:138:GLN:HG3	1.53	0.90
1:A:254:THR:HB	1:A:256:LYS:HE3	1.52	0.90
1:C:186:ASN:HB3	1:C:201:GLN:HE21	1.37	0.89
1:A:710:ARG:HG3	1:A:710:ARG:HH11	1.36	0.89
1:A:510:ARG:HD2	1:A:549:HIS:HA	1.53	0.89
1:A:533:THR:H	1:A:537:HIS:HD2	1.14	0.89
1:A:836:GLN:H	1:A:836:GLN:HE21	1.18	0.88
1:C:836:GLN:HE21	1:C:836:GLN:H	1.21	0.88
1:E:556:ILE:HG22	1:E:557:SER:N	1.88	0.87
1:C:699:DDE:CAC	1:C:699:DDE:HAD2	1.87	0.87
1:E:694:HIS:HD2	1:E:696:ASP:H	0.90	0.87
1:C:391:LYS:HD2	1:C:392:GLY:H	1.36	0.87
1:E:784:LEU:HD23	1:E:794:PRO:HG3	1.57	0.86
1:A:186:ASN:HB3	1:A:201:GLN:HE21	1.40	0.86
1:C:256:LYS:HE3	1:C:257:TRP:H	1.41	0.86
1:A:277:ILE:O	1:A:280:PRO:HD2	1.75	0.86
1:E:694:HIS:HD2	1:E:696:ASP:N	1.73	0.85
1:A:694:HIS:O	1:A:700:ARG:HD3	1.76	0.85
1:A:391:LYS:HG2	1:A:392:GLY:H	1.41	0.85
1:A:694:HIS:CD2	1:A:696:ASP:H	1.91	0.85
1:C:759:GLN:HG2	1:C:760:ARG:N	1.91	0.85
1:E:545:LEU:HD12	1:E:549:HIS:HB2	1.59	0.85
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.59	0.84
2:B:552:LEU:HD12	2:B:552:LEU:N	1.93	0.84
1:A:109:VAL:CG2	1:A:138:GLN:HG3	2.07	0.84
1:C:759:GLN:CG	1:C:760:ARG:H	1.89	0.84
2:F:488:ASP:HB3	2:F:492:ARG:CB	2.08	0.84
1:E:204:PRO:HA	1:E:209:VAL:HB	1.58	0.83
1:C:226:ALA:O	1:C:230:ALA:HB2	1.78	0.83
1:E:699:DDE:HAD2	1:E:699:DDE:CAC	1.92	0.83
1:A:45:ILE:HD12	1:A:76:SER:HB2	1.60	0.83
1:A:513:LYS:HE2	1:A:513:LYS:HA	1.59	0.83
2:B:455:VAL:O	2:B:456:ARG:HD2	1.79	0.83
1:C:231:LYS:HG3	1:C:232:LYS:N	1.93	0.83
1:E:522:MET:HB2	2:F:490:ARG:HH22	1.44	0.83
1:E:147:LEU:CD1	1:E:192:TYR:HB2	2.10	0.82
1:E:699:DDE:HAC2	1:E:699:DDE:NAD	1.94	0.82
1:E:536:LEU:HG	1:E:540:ILE:CD1	2.09	0.82
1:E:45:ILE:HD11	1:E:78:TYR:CB	2.09	0.82
1:A:391:LYS:CE	1:A:393:ARG:HD3	2.09	0.82
1:A:533:THR:H	1:A:537:HIS:CD2	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.61	0.81
1:E:155:VAL:HG21	1:E:202:VAL:HG21	1.60	0.81
1:E:694:HIS:O	1:E:700:ARG:HD3	1.79	0.81
1:C:699:DDE:HAC2	1:C:699:DDE:NAD	1.92	0.81
1:A:644:ASN:HD22	1:A:684:VAL:HB	1.46	0.81
1:C:25:ILE:CD1	1:C:125:ALA:HB1	2.12	0.80
1:E:117:ALA:HA	1:E:481:MET:SD	2.21	0.80
2:B:490:ARG:HB2	2:B:490:ARG:NH1	1.96	0.80
1:C:391:LYS:CD	1:C:392:GLY:H	1.95	0.80
1:E:685:ARG:HE	1:E:687:ASN:HD21	1.27	0.80
1:A:433:ARG:HH11	1:A:433:ARG:HG2	1.45	0.80
2:B:552:LEU:CD1	2:B:552:LEU:H	1.91	0.79
1:E:26:ALA:HB2	1:E:128:VAL:HB	1.62	0.79
1:E:45:ILE:HD11	1:E:78:TYR:HB3	1.63	0.79
1:C:581:ASN:ND2	1:C:704:GLN:HG3	1.97	0.78
2:F:546:GLU:CG	2:F:547:GLU:HG3	2.13	0.78
2:F:546:GLU:HG3	2:F:547:GLU:HG3	1.64	0.78
2:B:490:ARG:HH11	2:B:490:ARG:HB2	1.47	0.78
1:E:814:LYS:O	1:E:817:GLU:HG2	1.83	0.78
2:D:527:VAL:HG22	2:D:542:ILE:HD13	1.66	0.78
1:E:77:LEU:HB2	1:E:100:ILE:HB	1.66	0.78
2:D:551:ARG:HH11	2:D:551:ARG:CG	1.97	0.78
1:C:132:ILE:H	1:C:132:ILE:HD12	1.49	0.78
1:C:140:GLU:HG3	1:C:188:ILE:CD1	2.14	0.77
1:C:225:PHE:CE2	1:C:277:ILE:HA	2.18	0.77
1:C:703:GLY:HA2	2:D:493:ILE:HD13	1.66	0.77
1:E:647:ILE:HB	1:E:687:ASN:HD22	1.50	0.77
1:A:836:GLN:NE2	1:A:836:GLN:H	1.82	0.77
2:F:488:ASP:HB3	2:F:492:ARG:HB2	1.67	0.77
1:A:464:LEU:HD23	1:A:483:PHE:HE1	1.50	0.77
1:A:464:LEU:HD23	1:A:483:PHE:CE1	2.20	0.77
1:E:288:ILE:HG23	1:E:319:LEU:HD23	1.67	0.77
1:A:410:LYS:HG2	1:A:430:ALA:HB2	1.67	0.77
2:D:527:VAL:HG22	2:D:542:ILE:CD1	2.14	0.77
1:E:71:LYS:HB3	1:E:386:VAL:HG23	1.67	0.77
1:E:281:ILE:HG12	1:E:327:PHE:HE2	1.50	0.76
1:E:581:ASN:ND2	1:E:704:GLN:HG3	1.98	0.76
2:D:432:ARG:NE	2:D:432:ARG:HA	2.00	0.76
1:A:149:GLU:HA	1:A:355:GLN:HE22	1.48	0.76
1:C:277:ILE:O	1:C:280:PRO:HD2	1.86	0.76
1:A:589:LYS:HE3	1:A:689:LEU:HD11	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:NZ	1:A:105:SER:HB2	2.01	0.76
1:A:35:LEU:HD22	1:A:334:LEU:HD11	1.68	0.76
1:A:710:ARG:NH1	1:A:710:ARG:HG3	1.99	0.76
1:E:237:LYS:HA	1:E:240:MET:HB3	1.67	0.76
1:E:338:ILE:O	1:E:342:LEU:HB2	1.86	0.75
1:A:569:SER:O	1:A:720:ALA:HB1	1.85	0.75
1:C:694:HIS:O	1:C:700:ARG:HD3	1.87	0.75
1:E:26:ALA:CB	1:E:128:VAL:HB	2.16	0.75
1:C:391:LYS:HG3	1:C:393:ARG:HG2	1.68	0.75
1:E:331:ALA:O	1:E:335:LEU:HG	1.87	0.75
1:C:228:ARG:C	1:C:230:ALA:H	1.91	0.74
1:E:836:GLN:NE2	1:E:836:GLN:H	1.84	0.74
1:E:91:GLN:HE22	1:E:344:SER:N	1.85	0.74
2:D:546:GLU:HG3	2:D:547:GLU:HG2	1.69	0.74
2:F:552:LEU:HD12	2:F:552:LEU:N	2.03	0.74
1:E:698:ILE:H	1:E:698:ILE:HD13	1.51	0.74
2:B:427:ARG:O	2:B:431:GLU:HG3	1.86	0.74
1:A:322:VAL:HG22	1:A:325:ARG:HH21	1.53	0.74
1:E:381:TYR:OH	1:E:481:MET:HG3	1.88	0.74
1:C:464:LEU:HD23	1:C:483:PHE:CE1	2.22	0.73
1:E:78:TYR:HE1	1:E:97:SER:HB3	1.53	0.73
1:C:542:LEU:HD13	1:C:556:ILE:CD1	2.18	0.73
2:F:470:TYR:CD2	3:F:702:TAD:H3D	2.23	0.73
1:E:578:LYS:HE3	1:E:840:ASP:OD1	1.89	0.73
1:E:536:LEU:HG	1:E:540:ILE:HD11	1.69	0.73
2:F:513:ARG:HH11	2:F:513:ARG:HB2	1.54	0.73
2:B:524:ALA:O	2:B:528:GLU:HG3	1.88	0.73
1:E:379:MET:HB2	1:E:402:ALA:HB3	1.70	0.73
2:F:410:SER:HB3	2:F:413:GLY:O	1.89	0.73
1:C:836:GLN:NE2	1:C:836:GLN:H	1.86	0.72
1:E:258:THR:HG22	1:E:259:ASN:H	1.53	0.72
1:E:556:ILE:CG2	1:E:557:SER:H	1.90	0.72
2:D:546:GLU:HG3	2:D:547:GLU:CG	2.18	0.72
1:C:472:SER:HB3	1:C:475:ALA:HB2	1.71	0.72
1:C:495:VAL:HG11	1:C:501:LEU:HG	1.72	0.72
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.71	0.72
2:F:433:GLY:O	2:F:505:ARG:HB2	1.89	0.72
1:C:545:LEU:HD12	1:C:549:HIS:CD2	2.24	0.72
1:E:594:ASP:HB2	1:E:597:VAL:HG23	1.72	0.72
1:A:406:LYS:HG2	1:A:447:ASP:HB3	1.72	0.71
2:B:410:SER:HB3	2:B:413:GLY:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:757:GLU:HG3	1:E:768:VAL:HG22	1.70	0.71
1:C:533:THR:H	1:C:537:HIS:CD2	2.08	0.71
1:E:404:THR:HG22	1:E:449:PRO:HA	1.71	0.71
1:E:464:LEU:HD21	1:E:485:VAL:HB	1.72	0.71
2:D:485:GLN:O	2:D:486:GLU:HG2	1.90	0.71
2:D:531:ILE:HD12	2:D:537:LEU:HD23	1.73	0.71
1:C:694:HIS:CD2	1:C:696:ASP:H	2.03	0.71
1:E:728:VAL:HB	1:E:800:HIS:CD2	2.26	0.71
2:B:455:VAL:C	2:B:456:ARG:HD2	2.10	0.71
1:E:465:LYS:HD2	1:E:517:CYS:SG	2.31	0.71
1:C:454:ILE:HG13	1:C:455:GLY:H	1.56	0.71
1:A:694:HIS:HD2	1:A:696:ASP:N	1.83	0.70
1:C:391:LYS:CG	1:C:393:ARG:HG2	2.21	0.70
1:E:186:ASN:CG	1:E:201:GLN:HE21	1.93	0.70
1:A:452:ASN:N	1:A:452:ASN:HD22	1.88	0.70
1:C:169:VAL:HG22	1:C:173:ASP:HB2	1.73	0.70
1:C:189:VAL:CG1	1:C:200:VAL:HG12	2.20	0.70
1:A:71:LYS:HB3	1:A:386:VAL:HG23	1.72	0.70
1:E:348:ALA:HA	1:E:351:TYR:CE2	2.27	0.70
1:C:192:TYR:HA	1:C:763:THR:HG22	1.72	0.70
1:C:231:LYS:CG	1:C:232:LYS:H	2.02	0.70
1:C:484:SER:HB3	1:C:797:VAL:CG2	2.21	0.70
1:A:510:ARG:HG2	1:A:549:HIS:ND1	2.06	0.70
1:C:192:TYR:HA	1:C:763:THR:CG2	2.20	0.70
1:E:155:VAL:CG2	1:E:202:VAL:HG21	2.20	0.70
1:E:738:GLN:NE2	1:E:791:GLN:HE22	1.90	0.70
1:A:693:LEU:HB3	1:A:700:ARG:HD2	1.73	0.70
1:E:533:THR:H	1:E:537:HIS:CD2	2.09	0.70
2:F:531:ILE:HG22	2:F:533:HIS:H	1.57	0.69
2:F:537:LEU:O	2:F:538:ARG:HD2	1.92	0.69
1:C:348:ALA:HA	1:C:351:TYR:CE2	2.27	0.69
1:C:410:LYS:HA	1:C:430:ALA:HA	1.74	0.69
1:C:584:ASN:HD22	1:C:693:LEU:HA	1.56	0.69
1:E:27:HIS:CD2	1:E:29:ASP:H	2.04	0.69
1:C:743:ILE:HD13	1:C:784:LEU:HD11	1.72	0.69
2:B:513:ARG:HH11	2:B:513:ARG:HB2	1.57	0.69
1:C:140:GLU:HG3	1:C:188:ILE:HD13	1.74	0.69
1:C:374:PRO:O	1:C:404:THR:HG23	1.93	0.69
1:E:186:ASN:HB2	1:E:201:GLN:HG2	1.72	0.69
1:C:321:LYS:O	1:C:325:ARG:HG3	1.93	0.69
1:E:734:GLN:N	1:E:734:GLN:HE21	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:427:ARG:O	2:D:431:GLU:HG3	1.93	0.69
1:E:155:VAL:HG23	1:E:202:VAL:HG11	1.74	0.69
1:A:644:ASN:ND2	1:A:684:VAL:HB	2.08	0.69
1:E:334:LEU:O	1:E:338:ILE:HG12	1.93	0.68
1:E:545:LEU:HD12	1:E:549:HIS:CB	2.24	0.68
1:A:486:SER:O	1:A:488:VAL:HG13	1.94	0.68
1:C:552:VAL:HG13	1:C:553:PRO:HD2	1.75	0.68
1:C:244:LEU:HD22	1:C:277:ILE:HD11	1.76	0.68
2:B:440:HIS:HB2	2:B:471:ILE:HG22	1.74	0.68
1:E:410:LYS:HA	1:E:430:ALA:HA	1.76	0.68
1:C:581:ASN:HD21	1:C:704:GLN:HG3	1.56	0.68
1:A:169:VAL:HG22	1:A:173:ASP:HB2	1.76	0.68
1:C:220:PHE:HB3	1:C:328:LEU:HD13	1.76	0.68
1:E:220:PHE:HB3	1:E:328:LEU:HD13	1.74	0.68
1:E:693:LEU:HB3	1:E:700:ARG:HD2	1.76	0.68
1:A:130:ASP:OD1	1:A:159:LYS:HD2	1.94	0.67
1:A:140:GLU:HG3	1:A:188:ILE:CD1	2.23	0.67
1:A:533:THR:N	1:A:537:HIS:HD2	1.91	0.67
1:C:584:ASN:HD21	1:C:694:HIS:H	1.42	0.67
1:E:391:LYS:HG3	1:E:392:GLY:N	2.08	0.67
1:C:21:ASN:ND2	1:C:345:PRO:HG3	2.09	0.67
1:C:584:ASN:ND2	1:C:694:HIS:H	1.93	0.67
1:C:237:LYS:HA	1:C:240:MET:HB3	1.76	0.67
1:E:158:ASN:ND2	1:E:159:LYS:HG3	2.09	0.67
1:E:43:ALA:O	1:E:77:LEU:HA	1.95	0.67
2:F:582:LEU:HD21	2:F:587:ILE:HD11	1.77	0.67
1:C:508:LEU:HD23	1:C:545:LEU:HD11	1.74	0.67
1:E:152:LYS:HD2	1:E:200:VAL:CG2	2.25	0.67
1:A:391:LYS:HE2	1:A:393:ARG:HD3	1.77	0.67
1:E:730:LEU:HB2	1:E:799:ASP:HB2	1.76	0.67
1:C:172:GLU:HA	1:C:274:ASN:HD21	1.59	0.67
1:C:509:LYS:HD2	1:C:509:LYS:N	2.09	0.67
2:D:518:LEU:O	2:D:523:ALA:HB3	1.95	0.67
1:A:32:LYS:HZ2	1:A:105:SER:HB2	1.58	0.67
1:C:484:SER:HB3	1:C:797:VAL:HG22	1.77	0.67
1:E:91:GLN:NE2	1:E:344:SER:H	1.89	0.67
1:E:588:LEU:HD12	1:E:588:LEU:C	2.15	0.66
1:C:495:VAL:HG21	1:C:501:LEU:HD12	1.78	0.66
1:E:698:ILE:N	1:E:698:ILE:HD13	2.10	0.66
1:C:820:LEU:O	1:C:824:LYS:HG3	1.93	0.66
1:E:152:LYS:HD2	1:E:200:VAL:HG23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:ASN:HD22	1:A:693:LEU:HA	1.60	0.66
1:C:698:ILE:HD13	1:C:698:ILE:N	2.11	0.66
1:E:204:PRO:C	1:E:222:ILE:HD12	2.16	0.66
1:E:836:GLN:HE21	1:E:836:GLN:H	1.38	0.66
1:C:103:ILE:HD11	1:C:453:ILE:HG12	1.77	0.66
1:C:285:PHE:HE2	1:C:324:MET:SD	2.19	0.66
1:C:734:GLN:HE21	1:C:734:GLN:N	1.92	0.66
1:C:730:LEU:HB2	1:C:799:ASP:HB2	1.75	0.66
2:D:552:LEU:HD12	2:D:552:LEU:N	2.09	0.66
1:E:411:VAL:HG11	1:E:469:LEU:HB3	1.78	0.66
1:A:545:LEU:HD12	1:A:549:HIS:HB2	1.77	0.66
2:B:405:GLY:CA	1:C:627:VAL:HG12	2.25	0.66
1:E:321:LYS:O	1:E:325:ARG:HG3	1.96	0.66
1:E:45:ILE:HD11	1:E:78:TYR:HB2	1.77	0.66
1:E:533:THR:H	1:E:537:HIS:HD2	1.44	0.66
1:C:45:ILE:HD11	1:C:78:TYR:HB2	1.76	0.66
1:A:729:PHE:CE2	1:A:774:VAL:HG22	2.31	0.66
1:E:225:PHE:CZ	1:E:328:LEU:HD11	2.30	0.66
2:B:521:PRO:HG2	2:B:522:GLU:OE2	1.96	0.65
2:D:530:LEU:HA	2:D:604:PRO:HG3	1.78	0.65
1:E:391:LYS:HB3	1:E:393:ARG:HG2	1.78	0.65
1:A:654:GLN:HG2	1:A:655:TYR:CD1	2.31	0.65
1:A:784:LEU:CD2	1:A:794:PRO:HG3	2.24	0.65
1:C:162:ARG:O	1:C:166:GLU:HB2	1.97	0.65
1:C:72:SER:HA	1:C:439:GLY:O	1.95	0.65
1:E:10:ARG:HG3	1:E:10:ARG:HH11	1.61	0.65
1:A:126:LEU:HD11	1:A:156:VAL:CG2	2.26	0.65
2:B:405:GLY:HA2	1:C:627:VAL:CG1	2.26	0.65
1:A:698:ILE:HD13	1:A:698:ILE:N	2.11	0.65
1:C:588:LEU:C	1:C:588:LEU:HD12	2.16	0.65
1:E:141:THR:HA	1:E:144:ARG:NH2	2.11	0.65
1:A:153:PRO:HD2	1:A:200:VAL:CG1	2.27	0.65
1:A:348:ALA:HA	1:A:351:TYR:CE2	2.32	0.65
2:B:457:ALA:HB2	2:B:558:TRP:CE3	2.31	0.65
1:A:500:ASP:HB2	1:A:552:VAL:HG11	1.79	0.65
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.78	0.65
1:A:381:TYR:HB2	1:A:478:MET:HE3	1.78	0.65
1:A:406:LYS:HG2	1:A:447:ASP:CB	2.26	0.65
1:C:132:ILE:N	1:C:132:ILE:HD12	2.11	0.65
1:A:140:GLU:HG3	1:A:188:ILE:HD13	1.78	0.65
1:A:296:ILE:O	1:A:300:LEU:HD13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ASP:O	1:A:10:ARG:HG2	1.97	0.64
1:C:227:THR:O	1:C:230:ALA:HB3	1.97	0.64
1:C:10:ARG:HD3	1:C:445:ILE:HD11	1.78	0.64
1:E:589:LYS:HE3	1:E:689:LEU:HD11	1.79	0.64
1:A:132:ILE:HD12	1:A:162:ARG:NE	2.13	0.64
1:C:191:THR:O	1:C:763:THR:HG22	1.96	0.64
1:A:220:PHE:HB3	1:A:328:LEU:HD13	1.78	0.64
1:C:164:LEU:HD12	1:C:285:PHE:CE1	2.33	0.64
1:E:737:GLU:HG3	1:E:766:PHE:CE1	2.32	0.64
1:E:150:ARG:NH1	1:E:355:GLN:HB2	2.12	0.64
1:E:500:ASP:HB3	1:E:552:VAL:HG21	1.79	0.64
1:A:500:ASP:CB	1:A:552:VAL:HG11	2.27	0.64
1:E:381:TYR:O	1:E:398:GLY:HA3	1.98	0.64
1:E:71:LYS:HE3	1:E:387:PRO:CD	2.20	0.64
1:A:226:ALA:CB	1:A:241:MET:HB3	2.26	0.63
1:A:501:LEU:HB3	1:A:502:PRO:HD3	1.79	0.63
2:D:551:ARG:HH11	2:D:551:ARG:HG2	1.60	0.63
1:E:172:GLU:HA	1:E:274:ASN:HD21	1.63	0.63
1:A:410:LYS:HA	1:A:430:ALA:HA	1.80	0.63
1:A:627:VAL:HG12	2:F:405:GLY:HA2	1.79	0.63
1:A:235:VAL:HG21	1:A:240:MET:HB2	1.81	0.63
1:A:647:ILE:HB	1:A:687:ASN:HD22	1.63	0.63
1:C:226:ALA:CB	1:C:241:MET:HB3	2.29	0.63
1:A:381:TYR:HB2	1:A:478:MET:CE	2.29	0.63
1:E:279:ASP:O	1:E:283:ARG:HG2	1.99	0.63
1:E:285:PHE:CE2	1:E:320:LEU:HD11	2.34	0.63
1:A:647:ILE:HB	1:A:687:ASN:ND2	2.12	0.63
1:E:584:ASN:HD22	1:E:693:LEU:HA	1.64	0.63
1:E:81:MET:O	1:E:96:ASN:HB3	1.98	0.63
2:D:457:ALA:HB2	2:D:558:TRP:CE3	2.34	0.63
1:E:132:ILE:N	1:E:132:ILE:HD12	2.13	0.63
1:E:459:ILE:HG21	1:E:463:LEU:HD12	1.81	0.63
1:E:814:LYS:HA	1:E:817:GLU:OE2	1.99	0.63
1:A:387:PRO:HG3	1:A:394:PHE:CE1	2.34	0.62
1:C:507:GLY:HA3	1:C:549:HIS:HB3	1.81	0.62
1:E:488:VAL:HG23	1:E:489:VAL:HG23	1.81	0.62
1:E:584:ASN:ND2	1:E:694:HIS:H	1.97	0.62
1:A:391:LYS:HB3	1:A:393:ARG:HG2	1.80	0.62
1:C:45:ILE:HD11	1:C:78:TYR:CB	2.29	0.62
1:E:739:ALA:O	1:E:788:THR:HG22	2.00	0.62
2:D:457:ALA:HB2	2:D:558:TRP:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:581:ASN:HB3	1:E:583:HIS:CD2	2.34	0.62
1:A:698:ILE:H	1:A:698:ILE:HD13	1.65	0.62
1:A:510:ARG:HD2	1:A:549:HIS:CA	2.29	0.62
1:C:495:VAL:HG11	1:C:501:LEU:CG	2.29	0.62
1:C:594:ASP:HB2	1:C:597:VAL:HG23	1.81	0.62
1:E:561:VAL:HG21	1:E:775:ASN:HB3	1.80	0.62
2:F:505:ARG:HH11	2:F:505:ARG:HG3	1.64	0.62
1:E:144:ARG:HA	1:E:147:LEU:HD12	1.81	0.62
1:E:204:PRO:CA	1:E:209:VAL:HB	2.30	0.62
1:E:82:SER:O	1:E:86:VAL:HG23	1.99	0.62
1:C:464:LEU:HD23	1:C:483:PHE:HE1	1.61	0.62
2:D:527:VAL:HG13	2:D:542:ILE:HD12	1.81	0.62
1:E:571:SER:HB2	1:E:589:LYS:HG3	1.82	0.62
1:C:236:ASP:O	1:C:240:MET:HB2	1.99	0.61
1:E:348:ALA:HA	1:E:351:TYR:CZ	2.34	0.61
1:A:588:LEU:HD12	1:A:588:LEU:C	2.20	0.61
1:C:220:PHE:HA	1:C:224:GLN:OE1	1.99	0.61
1:C:288:ILE:HG23	1:C:319:LEU:HD23	1.82	0.61
1:C:536:LEU:HD12	1:C:537:HIS:N	2.15	0.61
1:E:71:LYS:HB3	1:E:386:VAL:CG2	2.30	0.61
1:E:644:ASN:ND2	1:E:684:VAL:H	1.98	0.61
1:A:568:GLU:HB3	1:A:721:ASP:OD2	1.99	0.61
1:A:734:GLN:HE21	1:A:734:GLN:N	1.98	0.61
1:C:229:TYR:CE2	1:C:276:PHE:HB3	2.36	0.61
1:C:336:GLU:HG2	1:C:340:LEU:HD12	1.80	0.61
1:E:565:GLU:O	1:E:681:MET:HA	2.01	0.61
1:A:360:PRO:HD2	1:A:363:ASP:HB2	1.83	0.61
1:A:3:ALA:HA	1:A:46:ILE:HG22	1.81	0.61
1:C:270:GLU:OE1	1:C:275:MET:HG3	1.99	0.61
1:C:26:ALA:HB2	1:C:128:VAL:HB	1.83	0.61
1:E:500:ASP:HB2	1:E:552:VAL:HG11	1.81	0.61
2:F:505:ARG:NH1	2:F:505:ARG:HG3	2.15	0.61
1:A:561:VAL:HG21	1:A:775:ASN:HA	1.83	0.61
2:D:445:GLU:OE1	2:D:494:ARG:NH2	2.34	0.61
1:A:510:ARG:HB2	1:A:510:ARG:CZ	2.30	0.61
1:A:520:THR:HA	1:A:529:ILE:O	2.00	0.61
1:A:736:PRO:O	1:A:738:GLN:N	2.34	0.61
1:E:183:GLU:O	1:E:187:VAL:HG23	2.01	0.61
1:A:309:GLY:H	1:A:312:LYS:HZ3	1.46	0.61
1:C:611:ASP:OD2	1:C:613:LYS:HB2	2.00	0.61
1:A:103:ILE:HD13	1:A:121:VAL:HG23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:THR:HG22	1:C:260:LYS:H	1.65	0.60
1:E:39:LEU:HD11	1:E:334:LEU:CD1	2.32	0.60
1:E:536:LEU:HG	1:E:540:ILE:HD12	1.81	0.60
2:F:456:ARG:O	2:F:458:ARG:HD3	2.01	0.60
1:A:200:VAL:O	1:A:200:VAL:HG12	2.00	0.60
1:A:220:PHE:HA	1:A:224:GLN:OE1	2.01	0.60
1:C:569:SER:O	1:C:720:ALA:HB1	2.02	0.60
1:A:381:TYR:O	1:A:398:GLY:HA3	2.01	0.60
1:A:744:TYR:O	1:A:748:ASN:ND2	2.35	0.60
1:C:491:VAL:HG13	1:C:538:LEU:HD21	1.83	0.60
1:C:81:MET:O	1:C:96:ASN:HB3	2.01	0.60
1:E:524:GLU:C	1:E:526:GLY:H	2.05	0.60
1:E:754:VAL:HA	1:E:770:ALA:HB2	1.83	0.60
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.83	0.60
1:E:114:GLU:O	1:E:117:ALA:HB3	2.01	0.60
1:A:345:PRO:O	1:A:349:GLN:HG3	2.00	0.60
1:A:391:LYS:HE3	1:A:393:ARG:HD3	1.83	0.60
1:C:509:LYS:O	1:C:513:LYS:HG3	2.02	0.60
1:C:77:LEU:HB2	1:C:100:ILE:HB	1.82	0.60
1:A:229:TYR:CE2	1:A:276:PHE:HB3	2.37	0.60
1:C:556:ILE:HG23	1:C:556:ILE:O	2.02	0.60
1:E:698:ILE:CD1	1:E:698:ILE:H	2.04	0.60
1:C:256:LYS:HE3	1:C:257:TRP:N	2.16	0.60
1:E:258:THR:HG22	1:E:259:ASN:N	2.17	0.60
2:F:470:TYR:CE2	3:F:702:TAD:H3D	2.37	0.59
1:E:743:ILE:HD13	1:E:784:LEU:HD11	1.83	0.59
2:F:427:ARG:O	2:F:431:GLU:HG3	2.02	0.59
1:A:106:PRO:HG3	1:A:114:GLU:HG3	1.84	0.59
2:B:423:LEU:HD11	2:B:590:LYS:HD3	1.83	0.59
1:A:9:MET:O	1:A:13:MET:HG3	2.02	0.59
1:A:155:VAL:HG12	1:A:156:VAL:N	2.17	0.59
1:A:406:LYS:O	1:A:409:GLN:HB3	2.01	0.59
1:C:784:LEU:CD2	1:C:794:PRO:HG3	2.30	0.59
1:A:472:SER:HB3	1:A:475:ALA:HB2	1.84	0.59
2:D:531:ILE:CD1	2:D:537:LEU:HD23	2.32	0.59
1:E:472:SER:HB3	1:E:475:ALA:HB2	1.84	0.59
1:C:26:ALA:HB3	1:C:32:LYS:HB2	1.84	0.59
1:E:279:ASP:HB3	1:E:280:PRO:HD3	1.85	0.59
1:A:611:ASP:OD2	1:A:613:LYS:HB2	2.02	0.59
1:C:103:ILE:HD13	1:C:121:VAL:HG23	1.84	0.59
1:C:545:LEU:HA	1:C:549:HIS:HD2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:581:ASN:HB3	1:C:583:HIS:CD2	2.38	0.59
1:A:581:ASN:ND2	1:A:699:DDE:O	2.35	0.59
1:A:258:THR:HG22	1:A:260:LYS:H	1.68	0.59
1:A:172:GLU:HA	1:A:274:ASN:HD21	1.68	0.59
1:E:221:THR:OG1	1:E:224:GLN:HG3	2.03	0.59
1:A:126:LEU:HD11	1:A:156:VAL:HG23	1.84	0.58
1:E:21:ASN:ND2	1:E:345:PRO:HG3	2.18	0.58
1:A:251:ASN:HB3	1:A:254:THR:OG1	2.03	0.58
1:A:823:ARG:NH2	1:A:833:PRO:HD3	2.18	0.58
1:C:533:THR:H	1:C:537:HIS:HD2	1.51	0.58
1:A:433:ARG:NH1	1:A:433:ARG:HG2	2.16	0.58
1:E:478:MET:O	1:E:479:LYS:C	2.42	0.58
2:F:457:ALA:HB2	2:F:558:TRP:CD2	2.37	0.58
1:C:110:ASP:C	1:C:112:SER:H	2.07	0.58
1:C:25:ILE:HG22	1:C:139:THR:HG23	1.85	0.58
1:C:685:ARG:HE	1:C:687:ASN:HD21	1.51	0.58
1:C:799:ASP:OD1	1:C:800:HIS:HD2	1.87	0.58
1:C:699:DDE:CAC	1:C:699:DDE:NAD	2.58	0.58
1:C:733:ILE:HG21	1:C:743:ILE:HD11	1.86	0.58
1:C:45:ILE:HB	1:C:76:SER:HB2	1.84	0.58
2:D:518:LEU:H	2:D:518:LEU:HD22	1.67	0.58
1:E:659:ILE:HD13	1:E:693:LEU:HD21	1.85	0.58
1:A:91:GLN:HE22	1:A:343:PRO:HA	1.67	0.58
1:C:524:GLU:C	1:C:526:GLY:H	2.06	0.58
1:C:110:ASP:OD1	1:C:781:THR:HG21	2.04	0.58
1:A:464:LEU:CD2	1:A:485:VAL:HB	2.20	0.58
1:A:171:LYS:HE2	1:A:279:ASP:OD1	2.03	0.58
1:E:186:ASN:HA	1:E:189:VAL:HB	1.86	0.58
1:E:355:GLN:O	1:E:479:LYS:HG3	2.03	0.58
2:F:570:ALA:HB3	2:F:591:GLU:OE1	2.04	0.58
1:C:283:ARG:HB3	1:C:299:LEU:HD21	1.86	0.58
1:C:10:ARG:NH2	1:C:449:PRO:HD3	2.19	0.58
1:E:522:MET:CB	2:F:490:ARG:HH22	2.14	0.58
1:A:27:HIS:HD2	1:A:29:ASP:H	1.50	0.57
1:E:110:ASP:CB	1:E:536:LEU:HD22	2.33	0.57
1:E:571:SER:HB2	1:E:589:LYS:CG	2.34	0.57
1:A:27:HIS:CD2	1:A:29:ASP:H	2.21	0.57
1:E:120:ARG:HE	1:E:356:LEU:HD22	1.69	0.57
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.85	0.57
2:F:488:ASP:HB3	2:F:492:ARG:HB3	1.83	0.57
1:A:26:ALA:HB2	1:A:128:VAL:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:ASN:HB3	1:C:254:THR:OG1	2.04	0.57
1:E:581:ASN:ND2	1:E:704:GLN:CG	2.68	0.57
1:A:36:THR:HG22	1:A:102:LEU:HD21	1.87	0.57
1:A:584:ASN:HD21	1:A:700:ARG:HG2	1.70	0.57
1:C:387:PRO:HG3	1:C:394:PHE:CE1	2.38	0.57
1:C:391:LYS:CG	1:C:392:GLY:N	2.68	0.57
1:C:581:ASN:O	1:C:582:LYS:HB2	2.04	0.57
1:E:3:ALA:HA	1:E:46:ILE:O	2.04	0.57
1:E:699:DDE:CAC	1:E:699:DDE:NAD	2.60	0.57
1:A:290:ASN:HB3	1:A:292:LYS:HE2	1.86	0.57
1:E:374:PRO:O	1:E:404:THR:HG23	2.04	0.57
1:C:406:LYS:HB3	1:C:447:ASP:HB3	1.85	0.57
1:C:727:PRO:HG2	1:C:774:VAL:HB	1.85	0.57
1:C:811:PRO:HB3	1:C:820:LEU:HD22	1.85	0.57
1:E:729:PHE:CE2	1:E:774:VAL:HG22	2.40	0.57
1:A:288:ILE:HG23	1:A:319:LEU:HD23	1.85	0.57
2:B:530:LEU:HD23	2:B:604:PRO:HD3	1.87	0.57
1:C:183:GLU:O	1:C:187:VAL:HG23	2.04	0.57
1:C:703:GLY:HA2	2:D:493:ILE:CD1	2.34	0.57
2:D:528:GLU:OE2	2:D:534:PRO:HA	2.03	0.57
1:E:251:ASN:HB3	1:E:254:THR:OG1	2.05	0.57
1:E:644:ASN:HD22	1:E:684:VAL:H	1.52	0.57
1:A:374:PRO:O	1:A:404:THR:HG23	2.04	0.57
1:C:89:ILE:HG22	1:C:91:GLN:HG2	1.87	0.57
2:D:531:ILE:HG23	2:D:533:HIS:H	1.69	0.57
1:E:249:PHE:CD1	1:E:271:ARG:HA	2.40	0.57
1:A:459:ILE:HG21	1:A:463:LEU:HD12	1.87	0.57
1:E:37:ASP:O	1:E:41:GLN:HG3	2.05	0.57
1:E:728:VAL:HB	1:E:800:HIS:HD2	1.67	0.57
2:F:401:LEU:HD23	2:F:567:ILE:HG22	1.86	0.57
1:A:153:PRO:HD2	1:A:200:VAL:HG12	1.85	0.56
1:A:594:ASP:HB2	1:A:597:VAL:HG23	1.87	0.56
2:D:465:ILE:HD12	2:D:535:LEU:HD12	1.87	0.56
1:A:3:ALA:HA	1:A:46:ILE:O	2.03	0.56
1:A:490:GLN:HB3	1:A:531:ALA:HB2	1.86	0.56
1:E:226:ALA:O	1:E:230:ALA:HB2	2.05	0.56
1:E:338:ILE:HG23	1:E:342:LEU:HD12	1.86	0.56
1:E:222:ILE:HD13	1:E:245:TRP:HB2	1.87	0.56
1:E:219:ALA:HB3	1:E:330:ALA:HA	1.86	0.56
1:E:391:LYS:CG	1:E:392:GLY:H	2.13	0.56
1:A:82:SER:HB2	1:A:85:ASP:OD2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:698:ILE:HD13	1:C:698:ILE:H	1.69	0.56
1:C:733:ILE:HG21	1:C:743:ILE:CD1	2.36	0.56
1:A:258:THR:HG22	1:A:259:ASN:N	2.20	0.56
1:A:225:PHE:CE2	1:A:277:ILE:HG23	2.40	0.56
1:A:485:VAL:O	1:A:487:PRO:HD3	2.06	0.56
1:E:17:THR:HB	1:E:92:LYS:O	2.05	0.56
1:E:237:LYS:HA	1:E:240:MET:CB	2.35	0.56
1:E:237:LYS:O	1:E:241:MET:HG2	2.06	0.56
1:E:607:ASN:HB3	1:E:610:ASP:OD2	2.05	0.56
2:F:487:PRO:HA	2:F:492:ARG:O	2.06	0.56
1:E:189:VAL:HG11	1:E:201:GLN:HA	1.87	0.56
2:F:530:LEU:HA	2:F:604:PRO:HG3	1.87	0.56
1:C:413:ILE:HD13	1:C:459:ILE:HG23	1.87	0.56
1:A:404:THR:HG22	1:A:449:PRO:HA	1.88	0.56
2:B:504:PRO:HD3	2:B:563:ARG:O	2.06	0.56
1:E:185:VAL:O	1:E:189:VAL:HG23	2.05	0.56
1:E:80:GLU:HA	1:E:96:ASN:O	2.05	0.56
1:A:565:GLU:O	1:A:681:MET:HA	2.06	0.56
1:C:132:ILE:H	1:C:132:ILE:CD1	2.18	0.56
1:E:524:GLU:HG3	1:E:669:TRP:CZ3	2.40	0.56
1:A:454:ILE:HG13	1:A:455:GLY:H	1.71	0.56
1:C:24:VAL:HG23	1:C:102:LEU:HD11	1.86	0.56
1:C:501:LEU:C	1:C:501:LEU:HD23	2.26	0.56
1:C:91:GLN:HE22	1:C:343:PRO:HA	1.70	0.56
1:E:167:LEU:H	1:E:167:LEU:HD12	1.70	0.56
1:E:120:ARG:HE	1:E:356:LEU:CD2	2.18	0.56
2:F:546:GLU:HG2	2:F:547:GLU:HG3	1.87	0.56
1:A:223:ARG:HG2	1:A:223:ARG:HH11	1.70	0.55
1:C:171:LYS:HE2	1:C:279:ASP:OD1	2.05	0.55
1:C:494:GLU:HG2	1:C:495:VAL:N	2.21	0.55
2:D:551:ARG:CG	2:D:551:ARG:NH1	2.61	0.55
1:E:204:PRO:HG3	1:E:209:VAL:HG11	1.88	0.55
1:A:196:VAL:HG12	1:A:196:VAL:O	2.06	0.55
1:A:493:VAL:HG12	1:A:554:LEU:HD22	1.89	0.55
1:C:140:GLU:HG3	1:C:188:ILE:HD11	1.84	0.55
1:E:482:LYS:HD3	1:E:797:VAL:HG11	1.88	0.55
1:A:129:VAL:HG13	1:A:134:GLY:O	2.07	0.55
1:A:216:HIS:HB2	1:A:218:TRP:CD1	2.42	0.55
1:C:216:HIS:HB2	1:C:218:TRP:CD1	2.41	0.55
1:C:585:ARG:HD2	1:C:692:THR:OG1	2.07	0.55
1:A:381:TYR:OH	1:A:481:MET:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:PHE:HA	1:C:277:ILE:HD13	1.88	0.55
2:F:519:ALA:O	2:F:520:ALA:HB2	2.06	0.55
2:B:537:LEU:O	2:B:538:ARG:HD3	2.06	0.55
1:C:169:VAL:CG2	1:C:173:ASP:HB2	2.37	0.55
1:A:405:VAL:HA	1:A:409:GLN:OE1	2.07	0.55
1:A:536:LEU:O	1:A:540:ILE:HG23	2.07	0.55
2:D:537:LEU:O	2:D:538:ARG:HD2	2.06	0.55
1:E:292:LYS:HD3	1:E:295:GLU:OE2	2.06	0.55
1:E:491:VAL:HG21	1:E:542:LEU:HD21	1.89	0.55
2:F:524:ALA:O	2:F:528:GLU:HG3	2.07	0.55
1:A:103:ILE:HD11	1:A:453:ILE:HG12	1.89	0.54
1:A:414:GLN:HB3	1:A:418:TYR:CD2	2.41	0.54
1:C:200:VAL:O	1:C:200:VAL:HG13	2.07	0.54
1:C:256:LYS:HA	1:C:256:LYS:CE	2.38	0.54
1:A:452:ASN:N	1:A:452:ASN:ND2	2.56	0.54
1:C:348:ALA:HA	1:C:351:TYR:CZ	2.41	0.54
1:C:659:ILE:HD13	1:C:693:LEU:HD21	1.88	0.54
1:E:72:SER:HA	1:E:439:GLY:O	2.07	0.54
1:E:429:LYS:HG3	1:E:462:PHE:CZ	2.42	0.54
1:A:338:ILE:HG23	1:A:342:LEU:HD12	1.89	0.54
1:A:391:LYS:HG2	1:A:392:GLY:N	2.19	0.54
1:C:545:LEU:HD12	1:C:549:HIS:HD2	1.70	0.54
1:C:542:LEU:CD1	1:C:556:ILE:HD11	2.28	0.54
1:C:760:ARG:HD3	1:C:763:THR:OG1	2.07	0.54
1:E:46:ILE:N	1:E:46:ILE:HD12	2.22	0.54
1:A:285:PHE:CE2	1:A:320:LEU:HD11	2.42	0.54
1:A:736:PRO:HB2	1:A:738:GLN:HG3	1.89	0.54
1:C:538:LEU:O	1:C:542:LEU:HG	2.06	0.54
1:E:381:TYR:HE2	1:E:481:MET:HE2	1.73	0.54
1:A:357:TYR:CE2	1:A:359:GLY:HA3	2.42	0.54
1:C:520:THR:HA	1:C:529:ILE:O	2.08	0.54
1:C:711:ARG:HD2	2:D:577:ASN:HD21	1.73	0.54
1:E:109:VAL:O	1:E:109:VAL:HG12	2.08	0.54
1:E:212:GLY:HA3	1:E:219:ALA:HA	1.89	0.54
2:D:470:TYR:CD2	3:D:701:TAD:H3D	2.42	0.54
1:E:432:GLN:HB2	1:E:457:VAL:O	2.07	0.54
1:E:647:ILE:HB	1:E:687:ASN:ND2	2.19	0.54
1:A:43:ALA:HB1	1:A:78:TYR:O	2.08	0.54
1:C:126:LEU:HD11	1:C:156:VAL:CG2	2.38	0.54
1:C:357:TYR:CD2	1:C:366:CYS:HB2	2.43	0.54
1:E:561:VAL:HG21	1:E:775:ASN:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:THR:HG22	1:A:467:GLY:N	2.23	0.54
2:B:490:ARG:NH1	2:B:492:ARG:HG2	2.22	0.54
1:C:348:ALA:O	1:C:352:ARG:HB2	2.08	0.54
1:A:89:ILE:HG22	1:A:91:GLN:HG2	1.88	0.54
1:C:229:TYR:CZ	1:C:276:PHE:HB3	2.42	0.54
1:C:565:GLU:O	1:C:681:MET:HA	2.08	0.54
1:E:644:ASN:HD22	1:E:684:VAL:HB	1.72	0.54
1:E:74:ALA:HA	1:E:102:LEU:O	2.07	0.54
1:A:381:TYR:CD1	1:A:478:MET:HE3	2.44	0.54
1:A:388:THR:HG21	1:A:395:TYR:CD1	2.43	0.54
1:A:35:LEU:O	1:A:39:LEU:HD12	2.08	0.54
2:B:528:GLU:HG2	2:B:535:LEU:HG	1.89	0.54
1:C:693:LEU:HB3	1:C:700:ARG:HD2	1.89	0.54
1:E:360:PRO:HB2	1:E:363:ASP:HB2	1.90	0.54
1:E:584:ASN:HD21	1:E:694:HIS:H	1.55	0.54
1:A:579:SER:HB2	1:A:704:GLN:OE1	2.08	0.53
1:E:304:GLU:HG2	1:E:304:GLU:O	2.08	0.53
1:A:365:ASN:O	1:A:369:ILE:HG12	2.08	0.53
1:C:158:ASN:ND2	1:C:159:LYS:HG2	2.24	0.53
1:C:410:LYS:HG3	1:C:430:ALA:HB2	1.90	0.53
1:C:552:VAL:HG13	1:C:553:PRO:CD	2.37	0.53
1:E:142:VAL:O	1:E:145:GLN:HB2	2.08	0.53
1:A:321:LYS:NZ	1:A:325:ARG:HD3	2.23	0.53
1:C:43:ALA:HB1	1:C:78:TYR:O	2.08	0.53
1:E:369:ILE:HD12	1:E:401:PHE:HB3	1.90	0.53
1:A:117:ALA:HA	1:A:481:MET:SD	2.48	0.53
1:A:338:ILE:O	1:A:342:LEU:HB2	2.07	0.53
1:A:500:ASP:HB3	1:A:552:VAL:HG21	1.90	0.53
1:C:200:VAL:O	1:C:200:VAL:CG1	2.56	0.53
1:C:360:PRO:HB2	1:C:363:ASP:HB2	1.90	0.53
1:C:411:VAL:HG12	1:C:412:ARG:N	2.23	0.53
1:C:781:THR:HG22	1:C:785:ARG:HH21	1.73	0.53
1:E:108:HIS:HB2	1:E:111:PHE:CE2	2.44	0.53
1:E:831:GLU:OE1	1:E:831:GLU:N	2.39	0.53
1:A:103:ILE:HD12	1:A:122:THR:HG22	1.90	0.53
1:A:132:ILE:HD12	1:A:162:ARG:CD	2.39	0.53
2:B:467:ARG:HG3	2:B:558:TRP:CD1	2.44	0.53
1:C:211:PHE:O	1:C:219:ALA:HA	2.09	0.53
2:D:531:ILE:HD13	2:D:533:HIS:CE1	2.44	0.53
1:E:39:LEU:HD11	1:E:334:LEU:HD13	1.90	0.53
1:E:707:PRO:O	1:E:711:ARG:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:470:TYR:CD2	3:B:700:TAD:H3D	2.44	0.53
1:E:2:VAL:N	1:E:44:GLY:O	2.42	0.53
1:C:228:ARG:C	1:C:230:ALA:N	2.60	0.53
1:C:772:LEU:HD12	1:C:773:PRO:HD2	1.91	0.53
2:D:503:VAL:HG12	2:D:564:THR:HG22	1.91	0.53
1:E:10:ARG:HG3	1:E:10:ARG:NH1	2.23	0.53
1:E:385:MET:HG2	1:E:465:LYS:HA	1.91	0.53
2:F:426:HIS:NE2	2:F:594:ILE:HB	2.23	0.53
1:A:585:ARG:HB2	1:A:692:THR:OG1	2.08	0.53
1:A:2:VAL:HG22	1:A:3:ALA:N	2.23	0.52
2:D:518:LEU:O	2:D:520:ALA:N	2.41	0.52
1:A:226:ALA:HB2	1:A:241:MET:HB3	1.90	0.52
2:B:495:ASN:OD1	2:B:495:ASN:N	2.41	0.52
1:C:478:MET:O	1:C:479:LYS:C	2.47	0.52
1:E:129:VAL:HG12	1:E:130:ASP:N	2.24	0.52
1:E:739:ALA:HB2	1:E:791:GLN:OE1	2.10	0.52
1:A:478:MET:O	1:A:479:LYS:C	2.47	0.52
1:A:10:ARG:NH2	1:A:447:ASP:OD1	2.42	0.52
1:A:561:VAL:HG21	1:A:775:ASN:CA	2.39	0.52
1:C:126:LEU:HD11	1:C:156:VAL:HG21	1.92	0.52
1:E:200:VAL:O	1:E:200:VAL:HG22	2.10	0.52
1:E:485:VAL:HG22	1:E:485:VAL:O	2.09	0.52
2:F:440:HIS:HB2	2:F:471:ILE:HG22	1.92	0.52
1:C:155:VAL:HG21	1:C:185:VAL:HG11	1.91	0.52
1:E:490:GLN:HB3	1:E:531:ALA:HB2	1.91	0.52
1:E:495:VAL:HG13	1:E:504:LEU:HD22	1.90	0.52
1:A:111:PHE:HB3	1:A:114:GLU:HG2	1.91	0.52
1:A:110:ASP:C	1:A:112:SER:H	2.12	0.52
1:A:485:VAL:HG22	1:A:485:VAL:O	2.10	0.52
1:A:542:LEU:HD13	1:A:556:ILE:HG21	1.91	0.52
2:B:530:LEU:HA	2:B:604:PRO:HB3	1.91	0.52
1:C:160:VAL:HG23	1:C:212:GLY:O	2.09	0.52
1:C:240:MET:O	1:C:244:LEU:HG	2.10	0.52
1:C:522:MET:HA	1:C:527:GLU:O	2.10	0.52
1:C:581:ASN:ND2	1:C:699:DDE:O	2.42	0.52
1:E:152:LYS:CD	1:E:200:VAL:HG23	2.38	0.52
1:E:225:PHE:HZ	1:E:328:LEU:HD11	1.72	0.52
1:E:75:ILE:HG22	1:E:77:LEU:HD12	1.91	0.52
1:A:491:VAL:HG13	1:A:538:LEU:HD21	1.91	0.52
1:A:831:GLU:OE1	1:A:831:GLU:N	2.40	0.52
1:C:155:VAL:HG12	1:C:156:VAL:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:LYS:HB3	1:C:162:ARG:HD2	1.92	0.52
1:C:685:ARG:NE	1:C:687:ASN:HD21	2.07	0.52
1:C:729:PHE:O	1:C:771:TYR:HA	2.09	0.52
1:E:262:THR:CG2	1:E:266:GLY:HA2	2.40	0.52
1:E:749:LYS:O	1:E:750:LYS:HD2	2.09	0.52
1:C:27:HIS:HD2	1:C:29:ASP:H	1.57	0.52
1:A:391:LYS:CG	1:A:392:GLY:H	2.17	0.52
1:C:563:TYR:O	1:C:564:ARG:HD2	2.10	0.52
1:C:578:LYS:HA	1:C:584:ASN:O	2.09	0.52
2:D:488:ASP:OD1	2:D:489:ALA:N	2.43	0.52
2:D:529:ARG:HH22	2:D:603:GLN:NE2	2.08	0.52
2:D:531:ILE:CG2	2:D:533:HIS:H	2.23	0.52
1:E:792:ALA:O	1:E:794:PRO:HD3	2.09	0.52
1:A:149:GLU:HA	1:A:355:GLN:NE2	2.21	0.51
1:A:563:TYR:O	1:A:564:ARG:HD2	2.10	0.51
2:B:503:VAL:HG12	2:B:564:THR:HG22	1.92	0.51
1:C:192:TYR:HA	1:C:763:THR:HG21	1.92	0.51
1:C:221:THR:OG1	1:C:224:GLN:HG3	2.10	0.51
1:C:676:ILE:HD11	1:C:722:PRO:HB3	1.92	0.51
2:D:546:GLU:HG3	2:D:547:GLU:HG3	1.89	0.51
2:F:552:LEU:H	2:F:552:LEU:HD12	1.75	0.51
1:C:226:ALA:HB2	1:C:241:MET:HB3	1.92	0.51
1:C:277:ILE:HD12	1:C:277:ILE:N	2.25	0.51
2:F:426:HIS:CD2	2:F:594:ILE:HB	2.45	0.51
1:A:284:LEU:HD23	1:A:299:LEU:CD2	2.39	0.51
1:E:103:ILE:HD12	1:E:103:ILE:N	2.26	0.51
1:E:284:LEU:HD13	1:E:324:MET:CE	2.40	0.51
1:E:365:ASN:O	1:E:369:ILE:HG12	2.10	0.51
1:C:256:LYS:HE3	1:C:256:LYS:HA	1.91	0.51
1:C:273:PHE:O	1:C:277:ILE:HB	2.11	0.51
1:C:391:LYS:HG3	1:C:392:GLY:N	2.26	0.51
1:C:685:ARG:HG2	1:C:685:ARG:HH11	1.75	0.51
1:C:737:GLU:HG3	1:C:766:PHE:CE1	2.46	0.51
1:E:39:LEU:HD23	1:E:335:LEU:HD23	1.91	0.51
1:E:36:THR:O	1:E:40:VAL:HG23	2.10	0.51
1:E:74:ALA:O	1:E:439:GLY:HA2	2.10	0.51
2:F:537:LEU:C	2:F:538:ARG:HD2	2.31	0.51
1:A:129:VAL:HG13	1:A:134:GLY:C	2.30	0.51
1:A:836:GLN:N	1:A:836:GLN:HE21	1.98	0.51
2:B:457:ALA:HB2	2:B:558:TRP:CG	2.45	0.51
1:E:150:ARG:NH1	1:E:351:TYR:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:PRO:HG3	1:A:394:PHE:HE1	1.73	0.51
1:A:388:THR:HG21	1:A:395:TYR:CG	2.45	0.51
1:C:404:THR:HG22	1:C:449:PRO:CA	2.33	0.51
1:C:759:GLN:CG	1:C:760:ARG:N	2.62	0.51
1:E:414:GLN:HB3	1:E:418:TYR:CD2	2.44	0.51
1:E:685:ARG:HE	1:E:687:ASN:ND2	2.01	0.51
1:E:75:ILE:HG22	1:E:77:LEU:CD1	2.41	0.51
1:A:32:LYS:HZ1	1:A:105:SER:HB2	1.75	0.51
1:A:230:ALA:O	1:A:235:VAL:HG22	2.10	0.51
1:A:510:ARG:HG3	1:A:510:ARG:HH11	1.76	0.51
1:A:571:SER:HB2	1:A:589:LYS:HG3	1.91	0.51
2:B:470:TYR:CE2	3:B:700:TAD:H3D	2.46	0.51
1:C:189:VAL:HG13	1:C:200:VAL:HG12	1.91	0.51
1:C:831:GLU:OE1	1:C:831:GLU:N	2.44	0.51
1:E:731:VAL:HG23	1:E:796:MET:HB3	1.92	0.51
1:A:125:ALA:HB2	1:A:151:ILE:HG21	1.92	0.51
1:A:584:ASN:ND2	1:A:694:HIS:H	2.09	0.51
1:C:109:VAL:CG2	1:C:138:GLN:HG3	2.41	0.51
2:F:467:ARG:NH2	2:F:536:PRO:HG3	2.24	0.51
1:A:124:GLY:HA3	1:A:342:LEU:HD22	1.92	0.51
1:A:164:LEU:HD12	1:A:285:PHE:CE1	2.46	0.51
1:A:454:ILE:HG13	1:A:455:GLY:N	2.25	0.51
1:E:211:PHE:N	1:E:211:PHE:CD2	2.79	0.51
1:E:520:THR:HA	1:E:529:ILE:O	2.10	0.51
1:A:126:LEU:HD11	1:A:156:VAL:HG21	1.92	0.50
1:A:348:ALA:HA	1:A:351:TYR:CZ	2.47	0.50
1:E:77:LEU:CB	1:E:100:ILE:HB	2.40	0.50
1:A:306:VAL:O	1:A:306:VAL:HG23	2.11	0.50
1:C:369:ILE:HD12	1:C:401:PHE:HB3	1.94	0.50
1:E:186:ASN:CB	1:E:201:GLN:HE21	2.25	0.50
1:E:244:LEU:O	1:E:273:PHE:HB2	2.11	0.50
1:E:285:PHE:CD2	1:E:320:LEU:HD11	2.46	0.50
1:E:536:LEU:CG	1:E:540:ILE:HD11	2.36	0.50
1:E:585:ARG:HD2	1:E:692:THR:OG1	2.11	0.50
2:F:464:ALA:O	2:F:467:ARG:HB3	2.12	0.50
1:A:161:ASP:OD1	1:A:213:SER:HB2	2.12	0.50
1:A:369:ILE:HD12	1:A:401:PHE:HB3	1.93	0.50
1:A:784:LEU:HD23	1:A:794:PRO:CG	2.32	0.50
2:B:458:ARG:O	2:B:459:SER:HB2	2.11	0.50
2:D:447:ALA:HA	2:D:499:LEU:HD21	1.94	0.50
1:E:773:PRO:HB2	1:E:776:GLU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:522:GLU:HG2	2:F:523:ALA:N	2.26	0.50
1:C:27:HIS:CD2	1:C:29:ASP:H	2.29	0.50
1:C:32:LYS:NZ	1:C:105:SER:HB2	2.27	0.50
1:C:524:GLU:OE2	2:D:490:ARG:NH2	2.43	0.50
1:E:278:LEU:O	1:E:282:PHE:HB2	2.10	0.50
1:A:16:VAL:CG1	1:A:345:PRO:HB2	2.41	0.50
1:A:380:LEU:HD23	1:A:381:TYR:N	2.27	0.50
1:C:520:THR:HG22	1:C:530:VAL:HG22	1.93	0.50
1:E:478:MET:O	1:E:480:VAL:N	2.45	0.50
2:F:520:ALA:CB	2:F:522:GLU:OE2	2.60	0.50
1:A:392:GLY:HA3	1:A:513:LYS:HD3	1.93	0.50
1:C:306:VAL:HG23	1:C:306:VAL:O	2.11	0.50
1:E:152:LYS:HZ2	1:E:153:PRO:HD2	1.76	0.50
1:A:309:GLY:H	1:A:312:LYS:NZ	2.09	0.50
1:A:677:PHE:N	1:A:677:PHE:CD2	2.80	0.50
1:A:70:ILE:HG22	1:A:388:THR:HG22	1.93	0.50
2:B:450:ILE:HG23	2:B:455:VAL:HG22	1.94	0.50
1:C:244:LEU:HD22	1:C:277:ILE:CD1	2.41	0.50
1:C:284:LEU:HD11	1:C:303:LEU:CD1	2.41	0.50
2:F:445:GLU:OE1	2:F:494:ARG:NH2	2.42	0.50
2:F:429:LEU:HD13	2:F:502:TYR:CD2	2.46	0.50
2:F:518:LEU:O	2:F:519:ALA:C	2.50	0.50
1:A:132:ILE:HD11	1:A:162:ARG:HG2	1.93	0.50
1:C:454:ILE:HG13	1:C:455:GLY:N	2.25	0.50
1:C:432:GLN:HB2	1:C:457:VAL:O	2.12	0.50
2:F:473:GLY:HA3	2:F:597:LEU:HD11	1.92	0.50
1:A:155:VAL:CG1	1:A:156:VAL:N	2.75	0.50
1:A:411:VAL:HG12	1:A:412:ARG:N	2.26	0.50
1:C:388:THR:HG21	1:C:395:TYR:CG	2.47	0.50
1:C:436:LEU:HD23	1:C:454:ILE:CD1	2.42	0.50
1:E:25:ILE:HG22	1:E:139:THR:HG23	1.93	0.50
1:E:581:ASN:O	1:E:582:LYS:HB2	2.12	0.50
1:E:750:LYS:O	1:E:751:ARG:HB2	2.12	0.50
2:F:520:ALA:HB3	2:F:522:GLU:OE2	2.12	0.50
1:A:507:GLY:O	1:A:510:ARG:HB3	2.11	0.49
1:A:675:PRO:HD3	1:A:714:TYR:CD1	2.47	0.49
1:C:750:LYS:O	1:C:751:ARG:HB2	2.12	0.49
1:E:760:ARG:HD3	1:E:763:THR:OG1	2.12	0.49
1:A:727:PRO:HG2	1:A:774:VAL:HB	1.93	0.49
1:A:758:GLU:HG2	1:A:759:GLN:N	2.27	0.49
2:B:465:ILE:HD12	2:B:535:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:GLU:OE1	1:C:183:GLU:HA	2.10	0.49
1:E:611:ASP:OD2	1:E:613:LYS:HB2	2.12	0.49
1:A:24:VAL:HG23	1:A:102:LEU:HD11	1.94	0.49
1:A:628:THR:HG21	2:F:403:ASP:HB3	1.94	0.49
1:C:395:TYR:CE1	1:C:457:VAL:HG13	2.47	0.49
1:C:466:THR:HG22	1:C:467:GLY:N	2.28	0.49
1:C:589:LYS:HD2	1:C:689:LEU:HD11	1.94	0.49
1:C:644:ASN:ND2	1:C:684:VAL:H	2.09	0.49
1:C:749:LYS:O	1:C:750:LYS:HD2	2.12	0.49
2:D:528:GLU:HA	2:D:531:ILE:HG22	1.95	0.49
1:E:132:ILE:HD13	1:E:162:ARG:HD3	1.94	0.49
1:E:388:THR:HG21	1:E:395:TYR:CD1	2.48	0.49
1:E:406:LYS:HB3	1:E:447:ASP:HB3	1.93	0.49
1:E:536:LEU:O	1:E:539:GLU:N	2.45	0.49
1:A:589:LYS:HE3	1:A:689:LEU:CD1	2.41	0.49
1:A:760:ARG:HD3	1:A:763:THR:OG1	2.13	0.49
2:B:403:ASP:HA	1:C:628:THR:HG21	1.93	0.49
2:B:505:ARG:HG2	2:B:508:LEU:HD12	1.95	0.49
1:C:208:THR:HG22	1:C:341:HIS:CG	2.47	0.49
1:C:588:LEU:HD22	1:C:686:VAL:HG13	1.94	0.49
1:C:742:GLY:O	1:C:745:SER:HB3	2.12	0.49
1:C:76:SER:O	1:C:77:LEU:HD12	2.12	0.49
1:E:694:HIS:CE1	1:E:699:DDE:HD2	2.47	0.49
1:A:39:LEU:HB3	1:A:77:LEU:HD21	1.94	0.49
1:A:432:GLN:O	1:A:433:ARG:HD3	2.12	0.49
1:C:354:GLU:OE2	1:C:361:ALA:HB1	2.12	0.49
1:C:433:ARG:HB3	1:C:457:VAL:HB	1.93	0.49
1:C:588:LEU:CD1	1:C:588:LEU:C	2.80	0.49
1:E:353:ALA:HB3	1:E:370:LYS:HG3	1.94	0.49
2:F:423:LEU:HD11	2:F:590:LYS:HD3	1.92	0.49
2:F:552:LEU:CD1	2:F:552:LEU:N	2.75	0.49
1:C:588:LEU:HD22	1:C:686:VAL:CG1	2.42	0.49
2:D:552:LEU:CD1	2:D:552:LEU:N	2.74	0.49
1:A:273:PHE:CD1	1:A:277:ILE:HD12	2.47	0.49
1:A:354:GLU:HG3	1:A:370:LYS:HE2	1.94	0.49
1:C:836:GLN:N	1:C:836:GLN:HE21	1.99	0.49
1:E:9:MET:O	1:E:12:LEU:HB3	2.13	0.49
1:A:563:TYR:O	1:A:564:ARG:CD	2.61	0.49
1:A:742:GLY:O	1:A:746:VAL:HG23	2.13	0.49
2:D:470:TYR:CE2	3:D:701:TAD:H3D	2.47	0.49
2:D:518:LEU:CD2	2:D:518:LEU:H	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:ASP:OD1	1:E:238:ALA:HB3	2.12	0.49
1:E:493:VAL:HG22	1:E:556:ILE:CD1	2.43	0.49
1:E:666:ALA:CB	1:E:709:MET:HB3	2.43	0.49
1:A:77:LEU:HB2	1:A:100:ILE:HB	1.93	0.49
1:E:109:VAL:CG2	1:E:138:GLN:HG3	2.41	0.49
2:F:489:ALA:C	2:F:490:ARG:HG3	2.32	0.49
1:A:228:ARG:HH12	1:A:327:PHE:HE1	1.60	0.48
1:A:464:LEU:CD2	1:A:483:PHE:HE1	2.23	0.48
1:A:490:GLN:HB3	1:A:531:ALA:CB	2.42	0.48
1:A:45:ILE:HB	1:A:76:SER:OG	2.13	0.48
1:E:108:HIS:O	1:E:111:PHE:HD2	1.96	0.48
1:E:68:ILE:HG21	1:E:395:TYR:OH	2.13	0.48
1:E:733:ILE:HG21	1:E:743:ILE:HD11	1.95	0.48
2:F:429:LEU:HD13	2:F:502:TYR:CG	2.48	0.48
1:A:322:VAL:HG22	1:A:325:ARG:NH2	2.24	0.48
1:A:677:PHE:N	1:A:677:PHE:HD2	2.11	0.48
1:A:685:ARG:HE	1:A:687:ASN:HD21	1.60	0.48
1:C:120:ARG:NH1	1:C:479:LYS:HG3	2.28	0.48
1:C:429:LYS:HG3	1:C:462:PHE:CZ	2.48	0.48
2:D:461:ASP:OD1	2:D:463:ASP:HB2	2.13	0.48
2:D:417:TRP:CE2	2:D:568:PRO:HB2	2.48	0.48
1:E:240:MET:O	1:E:244:LEU:HG	2.13	0.48
1:E:399:ARG:HD3	1:E:401:PHE:CZ	2.48	0.48
1:E:538:LEU:O	1:E:542:LEU:HG	2.14	0.48
1:E:588:LEU:CD1	1:E:588:LEU:C	2.80	0.48
1:A:147:LEU:HD11	1:A:189:VAL:HA	1.94	0.48
1:A:72:SER:HA	1:A:439:GLY:O	2.13	0.48
1:C:390:ASP:O	1:C:391:LYS:HB3	2.13	0.48
2:D:551:ARG:HG3	2:D:551:ARG:NH1	2.28	0.48
1:E:179:ALA:O	1:E:183:GLU:HG3	2.11	0.48
1:E:284:LEU:HD13	1:E:324:MET:HE1	1.96	0.48
2:F:419:VAL:HG11	2:F:590:LYS:HB2	1.94	0.48
1:A:223:ARG:NH1	1:A:223:ARG:HG2	2.28	0.48
1:A:501:LEU:C	1:A:501:LEU:HD23	2.33	0.48
1:A:759:GLN:HB2	1:A:766:PHE:CE2	2.48	0.48
2:B:486:GLU:CG	2:B:487:PRO:HD2	2.43	0.48
1:E:23:SER:O	1:E:125:ALA:HA	2.14	0.48
1:E:89:ILE:C	1:E:91:GLN:H	2.16	0.48
1:C:501:LEU:HB3	1:C:502:PRO:HD3	1.94	0.48
1:E:251:ASN:ND2	1:E:269:LEU:HD21	2.28	0.48
1:A:186:ASN:HB3	1:A:201:GLN:NE2	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:THR:HG22	1:A:259:ASN:H	1.78	0.48
1:C:129:VAL:HG13	1:C:134:GLY:C	2.34	0.48
1:C:237:LYS:HA	1:C:240:MET:CB	2.43	0.48
1:C:644:ASN:HD22	1:C:684:VAL:H	1.61	0.48
2:D:561:ALA:O	2:D:564:THR:HG23	2.14	0.48
1:E:174:LEU:O	1:E:177:THR:HB	2.12	0.48
2:F:471:ILE:HG21	2:F:501:VAL:HG21	1.96	0.48
1:A:627:VAL:O	1:A:631:ARG:HG3	2.12	0.48
1:C:129:VAL:HG13	1:C:134:GLY:O	2.13	0.48
1:C:10:ARG:CZ	1:C:449:PRO:HD3	2.44	0.48
1:E:126:LEU:HD11	1:E:156:VAL:HG21	1.96	0.48
1:E:225:PHE:CD2	1:E:277:ILE:HD12	2.49	0.48
1:E:306:VAL:HG23	1:E:306:VAL:O	2.14	0.48
1:E:653:VAL:HG11	1:E:691:VAL:HB	1.96	0.48
1:A:161:ASP:N	1:A:161:ASP:OD1	2.47	0.48
1:C:164:LEU:HD12	1:C:285:PHE:CD1	2.48	0.48
1:C:490:GLN:HB3	1:C:531:ALA:HB2	1.96	0.48
1:C:698:ILE:N	1:C:698:ILE:CD1	2.75	0.48
1:E:225:PHE:CZ	1:E:328:LEU:HD21	2.49	0.48
1:E:348:ALA:O	1:E:352:ARG:HB2	2.14	0.48
1:E:454:ILE:HG13	1:E:455:GLY:N	2.28	0.48
1:E:145:GLN:NE2	1:E:793:PHE:CZ	2.81	0.48
1:A:26:ALA:HB3	1:A:32:LYS:HB2	1.96	0.48
1:A:488:VAL:HG23	1:A:489:VAL:HG22	1.96	0.48
1:C:26:ALA:CB	1:C:128:VAL:HB	2.43	0.48
1:C:581:ASN:O	1:C:582:LYS:CB	2.62	0.48
1:C:591:GLU:O	1:C:685:ARG:HB3	2.13	0.48
1:C:601:ILE:HG12	1:C:606:ILE:HB	1.96	0.48
1:C:694:HIS:CD2	1:C:695:ALA:N	2.82	0.48
1:A:258:THR:CG2	1:A:260:LYS:HG2	2.43	0.48
1:A:659:ILE:HD13	1:A:693:LEU:HD21	1.96	0.48
1:C:644:ASN:HD22	1:C:684:VAL:HB	1.79	0.48
1:C:698:ILE:H	1:C:698:ILE:CD1	2.22	0.48
1:A:103:ILE:HD13	1:A:121:VAL:CG2	2.44	0.47
1:A:262:THR:HA	1:A:267:LYS:O	2.14	0.47
1:C:507:GLY:O	1:C:510:ARG:HB2	2.14	0.47
2:D:422:LEU:HD22	2:D:422:LEU:O	2.14	0.47
1:E:210:ALA:HB2	1:E:221:THR:HG22	1.95	0.47
1:E:324:MET:HE2	1:E:324:MET:HA	1.95	0.47
1:E:754:VAL:HA	1:E:770:ALA:CB	2.42	0.47
1:A:109:VAL:CG2	1:A:138:GLN:CG	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LEU:HD13	1:A:456:LEU:HD11	1.94	0.47
1:A:466:THR:CG2	1:A:467:GLY:N	2.77	0.47
1:E:739:ALA:HB1	1:E:788:THR:HB	1.96	0.47
2:B:508:LEU:N	2:B:509:PRO:CD	2.77	0.47
1:C:331:ALA:O	1:C:335:LEU:HG	2.14	0.47
1:E:225:PHE:CE1	1:E:228:ARG:NH1	2.82	0.47
1:E:281:ILE:HG12	1:E:327:PHE:CE2	2.40	0.47
1:E:510:ARG:NH1	1:E:549:HIS:ND1	2.60	0.47
1:A:411:VAL:HG11	1:A:469:LEU:HB3	1.97	0.47
1:A:512:SER:HA	1:A:518:VAL:CG1	2.44	0.47
1:A:606:ILE:HD12	1:A:619:MET:HG3	1.96	0.47
1:C:820:LEU:HD12	1:C:824:LYS:HD2	1.97	0.47
1:E:46:ILE:H	1:E:46:ILE:HD12	1.77	0.47
1:A:363:ASP:O	1:A:367:ILE:HG12	2.14	0.47
1:E:304:GLU:CG	1:E:304:GLU:O	2.62	0.47
1:E:759:GLN:HB2	1:E:766:PHE:CE2	2.49	0.47
1:A:156:VAL:HG21	1:A:334:LEU:HD22	1.96	0.47
1:A:510:ARG:O	1:A:513:LYS:HB2	2.14	0.47
1:C:148:GLY:HA2	1:C:760:ARG:NH2	2.28	0.47
1:E:606:ILE:HD12	1:E:619:MET:HG2	1.95	0.47
1:E:71:LYS:O	1:E:386:VAL:HG21	2.14	0.47
2:F:401:LEU:O	2:F:421:ARG:NE	2.48	0.47
1:A:336:GLU:HG2	1:A:340:LEU:HD12	1.97	0.47
1:A:719:LEU:HD21	1:A:835:TRP:CD2	2.50	0.47
1:C:327:PHE:CD2	1:C:328:LEU:HG	2.50	0.47
1:A:561:VAL:HG21	1:A:775:ASN:CB	2.45	0.47
1:C:258:THR:HG22	1:C:259:ASN:N	2.30	0.47
1:C:638:PRO:HB3	1:C:672:LYS:HD3	1.97	0.47
1:E:109:VAL:HG23	1:E:138:GLN:CD	2.34	0.47
1:E:162:ARG:O	1:E:166:GLU:HB2	2.15	0.47
1:E:68:ILE:HD12	1:E:390:ASP:CB	2.28	0.47
1:E:86:VAL:HG21	1:E:96:ASN:OD1	2.14	0.47
1:A:103:ILE:CD1	1:A:121:VAL:HG23	2.45	0.47
1:C:228:ARG:O	1:C:230:ALA:N	2.48	0.47
1:E:22:MET:HA	1:E:122:THR:HB	1.97	0.47
1:A:627:VAL:CG1	2:F:405:GLY:HA2	2.44	0.47
1:A:39:LEU:H	1:A:39:LEU:HD12	1.80	0.47
1:A:597:VAL:O	1:A:601:ILE:HG13	2.15	0.47
1:C:103:ILE:HD13	1:C:121:VAL:CG2	2.44	0.47
1:C:606:ILE:HD12	1:C:619:MET:CG	2.45	0.47
2:D:484:ASP:OD2	2:D:494:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:484:ASP:OD2	2:D:494:ARG:N	2.48	0.47
2:D:527:VAL:CG2	2:D:542:ILE:HD13	2.40	0.47
1:E:397:PHE:HD1	1:E:437:MET:HG3	1.79	0.47
1:A:522:MET:CE	1:A:526:GLY:O	2.63	0.47
1:A:736:PRO:O	1:A:737:GLU:C	2.53	0.47
1:A:740:VAL:HG21	1:A:766:PHE:CD1	2.49	0.47
1:A:729:PHE:CZ	1:A:774:VAL:HG22	2.49	0.47
1:E:106:PRO:HG2	1:E:115:VAL:HG22	1.97	0.47
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.50	0.47
1:A:221:THR:OG1	1:A:224:GLN:HG3	2.15	0.46
1:C:495:VAL:HG11	1:C:501:LEU:CD1	2.44	0.46
1:C:634:TRP:O	1:C:635:CYS:HB3	2.15	0.46
1:E:677:PHE:N	1:E:677:PHE:CD2	2.83	0.46
1:E:70:ILE:HG22	1:E:388:THR:HG22	1.95	0.46
1:A:759:GLN:HB2	1:A:766:PHE:CD2	2.50	0.46
1:A:91:GLN:O	1:A:93:THR:HG23	2.15	0.46
2:B:473:GLY:CA	2:B:597:LEU:HD11	2.37	0.46
1:C:647:ILE:HG13	1:C:685:ARG:NE	2.29	0.46
1:E:110:ASP:HB3	1:E:536:LEU:HD22	1.97	0.46
1:E:685:ARG:NE	1:E:687:ASN:HD21	2.02	0.46
1:A:459:ILE:HG22	1:A:459:ILE:O	2.16	0.46
1:A:785:ARG:HG2	1:A:785:ARG:HH11	1.80	0.46
1:C:406:LYS:HB3	1:C:447:ASP:CB	2.46	0.46
1:C:654:GLN:HG2	1:C:655:TYR:CD2	2.51	0.46
1:E:239:LYS:HE2	1:E:243:ARG:CZ	2.45	0.46
1:A:120:ARG:NH1	1:A:479:LYS:HG3	2.31	0.46
1:A:140:GLU:HG3	1:A:188:ILE:HD11	1.98	0.46
1:A:619:MET:O	1:A:625:TRP:HB2	2.15	0.46
1:C:304:GLU:HG2	1:C:304:GLU:O	2.14	0.46
1:C:759:GLN:HG3	1:C:766:PHE:CD2	2.50	0.46
2:D:451:VAL:O	2:D:451:VAL:HG12	2.15	0.46
1:E:588:LEU:HD12	1:E:588:LEU:O	2.14	0.46
1:E:626:ASP:O	1:E:628:THR:N	2.49	0.46
2:F:490:ARG:C	2:F:492:ARG:H	2.16	0.46
1:A:495:VAL:HA	1:A:554:LEU:HD23	1.97	0.46
1:C:167:LEU:N	1:C:167:LEU:HD12	2.29	0.46
1:C:729:PHE:HB2	1:C:772:LEU:O	2.16	0.46
1:E:305:ILE:CD1	1:E:327:PHE:HB2	2.46	0.46
1:E:626:ASP:C	1:E:628:THR:N	2.68	0.46
1:E:740:VAL:HG21	1:E:766:PHE:CD1	2.50	0.46
1:A:26:ALA:CB	1:A:128:VAL:HB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:GLN:CD	1:A:766:PHE:HE2	2.18	0.46
1:C:391:LYS:CD	1:C:392:GLY:N	2.74	0.46
1:C:391:LYS:C	1:C:393:ARG:H	2.19	0.46
1:C:404:THR:CG2	1:C:449:PRO:HA	2.33	0.46
1:E:619:MET:O	1:E:625:TRP:HB2	2.16	0.46
1:A:164:LEU:HD12	1:A:285:PHE:CD1	2.50	0.46
1:A:565:GLU:CD	1:A:676:ILE:HB	2.36	0.46
1:A:581:ASN:O	1:A:582:LYS:HB2	2.16	0.46
1:A:609:ARG:HG2	1:A:609:ARG:H	1.54	0.46
1:E:535:GLU:CD	1:E:778:PHE:HD1	2.19	0.46
2:F:465:ILE:HD12	2:F:535:LEU:HD12	1.98	0.46
1:A:392:GLY:HA3	1:A:513:LYS:CD	2.46	0.46
1:A:581:ASN:OD1	1:A:704:GLN:CD	2.54	0.46
1:C:154:VAL:HG12	1:C:154:VAL:O	2.16	0.46
1:C:70:ILE:O	1:C:440:ARG:HG3	2.15	0.46
1:C:759:GLN:HG3	1:C:766:PHE:HD2	1.81	0.46
1:C:89:ILE:CG2	1:C:91:GLN:HG2	2.45	0.46
1:E:143:LEU:O	1:E:144:ARG:C	2.54	0.46
1:E:172:GLU:OE2	1:E:176:GLN:NE2	2.48	0.46
1:E:307:LEU:HB2	1:E:312:LYS:HD3	1.97	0.46
1:E:711:ARG:HD2	2:F:577:ASN:HD21	1.81	0.46
1:A:348:ALA:O	1:A:352:ARG:HB2	2.16	0.46
1:A:391:LYS:HE2	1:A:393:ARG:CD	2.45	0.46
2:B:471:ILE:HG13	2:B:554:THR:HB	1.98	0.46
1:C:129:VAL:HG12	1:C:130:ASP:N	2.31	0.46
1:C:522:MET:HG2	1:C:528:HIS:CE1	2.51	0.46
1:C:685:ARG:NH1	1:C:685:ARG:HG2	2.31	0.46
1:E:186:ASN:HB2	1:E:201:GLN:HE21	1.81	0.46
1:A:493:VAL:HG11	1:A:554:LEU:HD13	1.98	0.46
1:A:581:ASN:O	1:A:582:LYS:CB	2.64	0.46
1:A:731:VAL:HB	1:A:796:MET:HB3	1.98	0.46
2:B:403:ASP:HB2	1:C:628:THR:OG1	2.16	0.46
2:B:518:LEU:HD13	2:B:518:LEU:N	2.31	0.46
1:C:397:PHE:HD1	1:C:437:MET:HG3	1.81	0.46
1:C:576:LEU:HD13	1:C:587:TYR:CE1	2.51	0.46
1:E:186:ASN:OD1	1:E:186:ASN:C	2.54	0.46
1:A:409:GLN:HG2	1:A:411:VAL:HG23	1.98	0.45
1:A:730:LEU:HD22	1:A:730:LEU:C	2.37	0.45
2:B:522:GLU:CD	2:B:522:GLU:H	2.18	0.45
1:C:296:ILE:N	1:C:297:PRO:HD2	2.32	0.45
1:C:528:HIS:C	1:C:529:ILE:HD13	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:588:LEU:O	1:C:588:LEU:HD12	2.16	0.45
2:D:410:SER:HB3	2:D:413:GLY:O	2.16	0.45
2:D:518:LEU:N	2:D:518:LEU:HD22	2.31	0.45
1:E:129:VAL:HG12	1:E:130:ASP:H	1.82	0.45
1:E:581:ASN:ND2	1:E:704:GLN:OE1	2.50	0.45
2:F:422:LEU:HD13	2:F:594:ILE:HD11	1.98	0.45
1:A:235:VAL:CG2	1:A:240:MET:HB2	2.44	0.45
1:A:371:ASN:O	1:A:372:CYS:C	2.54	0.45
1:C:411:VAL:CG1	1:C:412:ARG:N	2.79	0.45
1:C:117:ALA:HA	1:C:481:MET:SD	2.55	0.45
1:C:484:SER:HB3	1:C:797:VAL:HG23	1.94	0.45
1:E:4:PHE:HA	1:E:8:GLN:OE1	2.16	0.45
2:F:417:TRP:CE2	2:F:568:PRO:HB2	2.50	0.45
1:A:249:PHE:CD2	1:A:249:PHE:N	2.84	0.45
1:A:540:ILE:HG13	1:A:541:CYS:N	2.31	0.45
1:C:381:TYR:O	1:C:398:GLY:HA3	2.17	0.45
1:E:358:GLU:HG2	1:E:479:LYS:HD2	1.98	0.45
1:E:39:LEU:HB3	1:E:77:LEU:HD21	1.99	0.45
1:E:68:ILE:HG23	1:E:390:ASP:HB2	1.98	0.45
1:E:836:GLN:N	1:E:836:GLN:HE21	2.10	0.45
1:A:479:LYS:HA	1:A:479:LYS:HD2	1.82	0.45
1:A:653:VAL:HG11	1:A:691:VAL:HB	1.98	0.45
2:B:482:ALA:O	2:B:496:GLY:N	2.48	0.45
1:A:703:GLY:HA2	2:B:493:ILE:HD12	1.99	0.45
1:C:589:LYS:HG3	1:C:689:LEU:HD11	1.97	0.45
1:C:615:ARG:HG2	1:C:619:MET:CE	2.46	0.45
2:D:429:LEU:HD21	2:D:565:VAL:HG11	1.98	0.45
1:E:167:LEU:N	1:E:167:LEU:HD12	2.31	0.45
2:F:500:ARG:O	2:F:566:VAL:HG13	2.17	0.45
1:A:108:HIS:CD2	1:A:109:VAL:H	2.35	0.45
1:A:675:PRO:HD3	1:A:714:TYR:CE1	2.52	0.45
2:B:490:ARG:HH12	2:B:492:ARG:HG2	1.81	0.45
2:B:538:ARG:HD2	2:B:538:ARG:HA	1.69	0.45
1:C:391:LYS:HD2	1:C:392:GLY:N	2.17	0.45
1:C:655:TYR:O	1:C:656:LEU:C	2.54	0.45
1:E:208:THR:HG22	1:E:341:HIS:CG	2.52	0.45
1:A:219:ALA:HB3	1:A:330:ALA:HA	1.99	0.45
2:B:433:GLY:O	2:B:505:ARG:HB2	2.16	0.45
1:E:181:THR:O	1:E:185:VAL:HG23	2.16	0.45
1:E:189:VAL:O	1:E:193:ALA:HB2	2.16	0.45
1:E:284:LEU:CD1	1:E:324:MET:HE1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:461:GLN:NE2	1:E:462:PHE:CE2	2.84	0.45
1:E:578:LYS:HG2	1:E:840:ASP:OD2	2.16	0.45
2:F:488:ASP:CG	2:F:489:ALA:H	2.19	0.45
1:A:2:VAL:CG2	1:A:3:ALA:N	2.80	0.45
1:C:175:TYR:HD1	1:C:273:PHE:CD2	2.34	0.45
1:C:338:ILE:HG23	1:C:342:LEU:HD12	1.98	0.45
1:E:6:VAL:O	1:E:10:ARG:HB3	2.16	0.45
1:A:357:TYR:C	1:A:359:GLY:H	2.20	0.45
2:B:547:GLU:O	2:B:548:GLU:C	2.55	0.45
1:C:494:GLU:HB3	1:C:555:LYS:HG2	1.99	0.45
2:D:446:ALA:O	2:D:450:ILE:HD12	2.17	0.45
1:E:182:VAL:HG12	1:E:182:VAL:O	2.17	0.45
1:E:120:ARG:CZ	1:E:479:LYS:HB3	2.46	0.45
1:E:536:LEU:O	1:E:540:ILE:HD12	2.17	0.45
1:A:510:ARG:CG	1:A:510:ARG:HH11	2.30	0.45
1:A:710:ARG:CG	1:A:710:ARG:HH11	2.15	0.45
2:B:488:ASP:C	2:B:488:ASP:OD1	2.55	0.45
2:B:558:TRP:O	2:B:562:GLU:HG3	2.17	0.45
1:C:611:ASP:O	1:C:612:PHE:C	2.55	0.45
1:C:89:ILE:HG21	1:C:93:THR:HG21	1.99	0.45
1:E:349:GLN:O	1:E:370:LYS:HA	2.17	0.45
1:A:760:ARG:NH1	1:A:763:THR:HG21	2.32	0.45
1:C:158:ASN:CG	1:C:159:LYS:H	2.20	0.45
1:C:633:ILE:HG12	1:C:647:ILE:CD1	2.46	0.45
1:C:70:ILE:HD13	1:C:442:VAL:HG12	1.98	0.45
1:C:73:THR:HG22	1:C:73:THR:O	2.17	0.45
1:C:85:ASP:OD1	1:C:223:ARG:NH2	2.49	0.45
1:E:411:VAL:HG12	1:E:412:ARG:N	2.31	0.45
1:E:356:LEU:HA	1:E:479:LYS:CG	2.47	0.45
1:A:546:GLU:O	1:A:551:GLY:HA2	2.18	0.44
1:C:2:VAL:HG22	1:C:3:ALA:N	2.32	0.44
1:C:424:ASP:OD1	1:C:425:ASP:N	2.50	0.44
1:C:504:LEU:HD13	1:C:554:LEU:CD1	2.47	0.44
1:A:19:VAL:O	1:A:345:PRO:HD3	2.17	0.44
1:C:304:GLU:CG	1:C:304:GLU:O	2.65	0.44
1:C:388:THR:HG21	1:C:395:TYR:CD1	2.53	0.44
1:E:147:LEU:HB3	1:E:192:TYR:O	2.17	0.44
1:E:501:LEU:HD23	1:E:501:LEU:C	2.38	0.44
1:E:546:GLU:HG2	1:E:546:GLU:O	2.17	0.44
1:E:735:CYS:SG	1:E:739:ALA:HB3	2.56	0.44
1:A:797:VAL:HG22	1:A:798:PHE:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:471:ILE:HG21	2:B:501:VAL:HG21	2.00	0.44
1:C:109:VAL:HG21	1:C:138:GLN:HG3	2.00	0.44
1:C:760:ARG:HD3	1:C:763:THR:HG1	1.82	0.44
1:C:757:GLU:HG3	1:C:768:VAL:HG22	1.99	0.44
1:C:816:GLY:O	1:C:820:LEU:HD23	2.17	0.44
1:E:111:PHE:HZ	1:E:540:ILE:HG12	1.82	0.44
1:E:171:LYS:NZ	1:E:283:ARG:HH21	2.15	0.44
2:F:439:TYR:HA	2:F:499:LEU:O	2.17	0.44
1:A:486:SER:HA	1:A:487:PRO:HD3	1.79	0.44
1:A:500:ASP:O	1:A:503:LYS:N	2.46	0.44
1:A:493:VAL:CG1	1:A:554:LEU:HD13	2.47	0.44
1:A:698:ILE:CD1	1:A:698:ILE:H	2.16	0.44
1:C:666:ALA:HB2	1:C:706:ILE:HA	2.00	0.44
1:E:388:THR:HG21	1:E:395:TYR:CG	2.52	0.44
1:E:433:ARG:HE	1:E:444:PRO:HB3	1.82	0.44
1:E:654:GLN:HG2	1:E:655:TYR:CG	2.52	0.44
1:E:727:PRO:HG2	1:E:774:VAL:HB	1.99	0.44
1:A:129:VAL:HG11	1:A:181:THR:HG23	2.00	0.44
1:A:3:ALA:CA	1:A:46:ILE:HG22	2.46	0.44
1:C:494:GLU:HG2	1:C:495:VAL:H	1.82	0.44
2:D:457:ALA:O	2:D:458:ARG:HG3	2.18	0.44
1:E:507:GLY:CA	1:E:549:HIS:HB3	2.47	0.44
1:A:208:THR:HG22	1:A:341:HIS:CG	2.52	0.44
2:B:498:LEU:HD12	2:B:571:ILE:CG2	2.47	0.44
1:E:522:MET:HA	1:E:527:GLU:O	2.18	0.44
1:E:75:ILE:HD13	1:E:439:GLY:CA	2.47	0.44
1:C:414:GLN:HB3	1:C:418:TYR:CD2	2.53	0.44
1:C:90:LYS:HG3	1:C:90:LYS:O	2.18	0.44
1:E:387:PRO:HG3	1:E:394:PHE:CE1	2.52	0.44
1:E:75:ILE:HD13	1:E:439:GLY:HA3	2.00	0.44
1:E:772:LEU:HD12	1:E:773:PRO:HD2	2.00	0.44
1:A:392:GLY:CA	1:A:513:LYS:HD3	2.47	0.44
1:A:437:MET:O	1:A:439:GLY:N	2.51	0.44
1:A:510:ARG:HD2	1:A:549:HIS:ND1	2.33	0.44
1:A:593:ILE:HG22	1:A:597:VAL:HB	1.99	0.44
1:A:81:MET:O	1:A:96:ASN:HB3	2.18	0.44
1:C:663:VAL:HG13	1:C:709:MET:HG2	1.99	0.44
2:D:473:GLY:HA3	2:D:597:LEU:HD11	2.00	0.44
2:D:530:LEU:HD23	2:D:604:PRO:HD3	2.00	0.44
1:E:239:LYS:O	1:E:239:LYS:HG2	2.17	0.44
1:A:321:LYS:HZ1	1:A:325:ARG:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ILE:CG1	1:A:541:CYS:N	2.80	0.44
1:A:634:TRP:O	1:A:635:CYS:HB3	2.17	0.44
1:C:131:THR:HB	1:C:132:ILE:HD12	2.00	0.44
1:C:150:ARG:HD3	1:C:197:LEU:HD21	1.99	0.44
1:C:490:GLN:HA	1:C:531:ALA:HA	1.98	0.44
1:C:677:PHE:N	1:C:677:PHE:CD2	2.86	0.44
1:E:588:LEU:HD22	1:E:686:VAL:CG1	2.48	0.44
2:F:508:LEU:N	2:F:509:PRO:CD	2.81	0.44
1:A:183:GLU:O	1:A:187:VAL:HG23	2.17	0.43
1:A:19:VAL:HA	1:A:99:LEU:O	2.17	0.43
1:A:124:GLY:CA	1:A:342:LEU:HD22	2.48	0.43
1:A:410:LYS:HG2	1:A:430:ALA:CB	2.42	0.43
1:A:460:ASP:N	1:A:460:ASP:OD1	2.50	0.43
1:A:667:PHE:CZ	1:A:671:THR:HG21	2.52	0.43
1:C:729:PHE:CD2	1:C:774:VAL:HG22	2.53	0.43
1:C:828:MET:CE	2:D:576:ARG:HE	2.30	0.43
1:E:677:PHE:N	1:E:677:PHE:HD2	2.16	0.43
2:F:450:ILE:O	2:F:454:GLY:HA2	2.17	0.43
1:C:70:ILE:HD13	1:C:442:VAL:CG1	2.48	0.43
1:C:546:GLU:OE1	1:C:553:PRO:HD3	2.17	0.43
1:A:186:ASN:HB3	1:A:201:GLN:HG2	2.00	0.43
1:A:633:ILE:HG12	1:A:647:ILE:CD1	2.48	0.43
1:A:833:PRO:HB2	1:A:838:TYR:HE1	1.83	0.43
2:B:404:GLY:H	1:C:628:THR:HG23	1.83	0.43
1:E:736:PRO:HB2	1:E:738:GLN:HG2	2.00	0.43
1:E:759:GLN:HG2	1:E:760:ARG:N	2.32	0.43
2:F:505:ARG:HG2	2:F:508:LEU:HD12	2.01	0.43
2:B:517:THR:HG22	2:B:545:PRO:HB2	2.00	0.43
2:B:583:ASP:HA	2:B:584:PRO:HD2	1.86	0.43
1:C:515:ASP:HA	1:C:516:PRO:HD3	1.87	0.43
1:C:744:TYR:O	1:C:748:ASN:ND2	2.51	0.43
2:D:453:GLY:O	2:D:456:ARG:HD2	2.18	0.43
1:E:132:ILE:CD1	1:E:132:ILE:N	2.80	0.43
1:E:307:LEU:HD13	1:E:312:LYS:HA	2.01	0.43
1:E:394:PHE:CZ	1:E:513:LYS:O	2.71	0.43
1:E:524:GLU:C	1:E:526:GLY:N	2.70	0.43
1:E:564:ARG:HG3	1:E:682:ARG:HB2	1.99	0.43
2:F:451:VAL:HG12	2:F:451:VAL:O	2.18	0.43
1:A:588:LEU:CD1	1:A:588:LEU:C	2.86	0.43
1:A:577:SER:HB2	1:A:712:ALA:HB2	2.01	0.43
1:A:729:PHE:CD2	1:A:774:VAL:HG22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ASP:O	1:C:134:GLY:HA2	2.17	0.43
1:C:225:PHE:CD2	1:C:277:ILE:HG13	2.53	0.43
1:C:46:ILE:HD12	1:C:46:ILE:HA	1.79	0.43
1:C:564:ARG:CG	1:C:682:ARG:HB2	2.48	0.43
2:D:451:VAL:O	2:D:451:VAL:CG1	2.67	0.43
1:E:189:VAL:O	1:E:193:ALA:CB	2.67	0.43
1:E:303:LEU:O	1:E:304:GLU:HB3	2.18	0.43
1:E:536:LEU:O	1:E:539:GLU:HB3	2.18	0.43
2:F:465:ILE:HB	2:F:535:LEU:HB3	2.00	0.43
1:A:198:GLY:O	1:A:200:VAL:HG23	2.19	0.43
1:A:86:VAL:HG21	1:A:96:ASN:OD1	2.18	0.43
1:C:77:LEU:CB	1:C:100:ILE:HB	2.47	0.43
1:C:149:GLU:HA	1:C:355:GLN:HE22	1.83	0.43
2:D:499:LEU:HB3	2:D:566:VAL:CG1	2.49	0.43
1:E:101:ASN:ND2	1:E:453:ILE:HB	2.34	0.43
1:E:171:LYS:NZ	1:E:283:ARG:NH2	2.65	0.43
1:E:220:PHE:HA	1:E:224:GLN:OE1	2.17	0.43
1:E:225:PHE:CE2	1:E:328:LEU:HD11	2.53	0.43
1:E:4:PHE:CE2	1:E:45:ILE:HD12	2.54	0.43
1:E:663:VAL:HG13	1:E:709:MET:HG2	1.99	0.43
1:E:823:ARG:NH1	1:E:828:MET:HB2	2.34	0.43
1:E:89:ILE:HG22	1:E:91:GLN:HB3	2.00	0.43
1:A:222:ILE:HG22	1:A:241:MET:HB2	2.01	0.43
1:A:730:LEU:HB2	1:A:799:ASP:HB2	2.00	0.43
1:C:386:VAL:HA	1:C:387:PRO:HD3	1.91	0.43
1:C:773:PRO:HB2	1:C:776:GLU:HB2	2.00	0.43
1:E:203:TYR:CD2	1:E:206:ARG:HD2	2.53	0.43
1:E:350:ALA:O	1:E:370:LYS:HG2	2.19	0.43
1:A:71:LYS:HB3	1:A:386:VAL:CG2	2.44	0.43
1:A:739:ALA:O	1:A:788:THR:HG22	2.19	0.43
1:C:260:LYS:C	1:C:262:THR:H	2.22	0.43
1:C:555:LYS:O	1:C:555:LYS:HG3	2.19	0.43
1:E:111:PHE:CZ	1:E:540:ILE:HG12	2.53	0.43
1:E:371:ASN:O	1:E:372:CYS:C	2.57	0.43
1:A:106:PRO:HG2	1:A:115:VAL:HG22	2.01	0.43
1:A:433:ARG:CG	1:A:433:ARG:NH1	2.82	0.43
1:A:636:PHE:CE1	1:A:645:LEU:HD21	2.54	0.43
2:B:422:LEU:HD22	2:B:422:LEU:O	2.18	0.43
1:C:155:VAL:CG1	1:C:156:VAL:N	2.82	0.43
1:C:464:LEU:HD11	1:C:516:PRO:HB2	2.00	0.43
1:C:735:CYS:HA	1:C:736:PRO:HD3	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:LEU:C	1:E:145:GLN:N	2.70	0.43
1:E:166:GLU:O	1:E:168:GLN:HG3	2.18	0.43
1:E:209:VAL:HG12	1:E:211:PHE:CE1	2.54	0.43
1:E:569:SER:O	1:E:720:ALA:HB1	2.19	0.43
2:F:420:GLU:H	2:F:420:GLU:CD	2.22	0.43
2:F:458:ARG:O	2:F:459:SER:HB2	2.19	0.43
1:A:21:ASN:ND2	1:A:345:PRO:HG3	2.34	0.43
1:A:408:GLY:O	1:A:409:GLN:C	2.57	0.43
2:B:484:ASP:OD2	2:B:494:ARG:NE	2.48	0.43
1:C:485:VAL:O	1:C:485:VAL:HG12	2.18	0.43
1:C:565:GLU:OE1	1:C:676:ILE:HG12	2.18	0.43
2:D:401:LEU:HD23	2:D:567:ILE:HG22	2.00	0.43
1:E:15:LYS:HG3	1:E:94:ASP:OD2	2.18	0.43
2:F:471:ILE:HG13	2:F:554:THR:HB	2.01	0.43
1:A:546:GLU:HG3	1:A:552:VAL:O	2.18	0.42
1:A:654:GLN:O	1:A:655:TYR:HB2	2.18	0.42
2:B:404:GLY:HA2	1:C:626:ASP:CG	2.40	0.42
2:B:439:TYR:CE2	2:B:475:PRO:HD3	2.54	0.42
1:C:781:THR:CG2	1:C:785:ARG:HH21	2.31	0.42
2:D:471:ILE:HG13	2:D:554:THR:HB	2.01	0.42
2:F:516:LEU:O	2:F:545:PRO:HD2	2.19	0.42
1:A:413:ILE:HD13	1:A:459:ILE:HG23	2.01	0.42
1:A:515:ASP:OD1	1:A:517:CYS:N	2.47	0.42
1:A:581:ASN:HB2	1:A:583:HIS:H	1.83	0.42
1:A:615:ARG:HG2	1:A:619:MET:HE1	2.00	0.42
1:C:387:PRO:HG3	1:C:394:PHE:HE1	1.84	0.42
1:C:74:ALA:O	1:C:439:GLY:HA2	2.19	0.42
2:B:404:GLY:H	1:C:628:THR:CG2	2.32	0.42
1:E:634:TRP:O	1:E:635:CYS:HB3	2.18	0.42
1:E:707:PRO:HB3	2:F:578:VAL:O	2.19	0.42
1:E:733:ILE:HG21	1:E:743:ILE:CD1	2.50	0.42
1:A:435:VAL:HG12	1:A:444:PRO:HA	1.99	0.42
1:A:615:ARG:HG2	1:A:619:MET:CE	2.49	0.42
1:C:25:ILE:HD12	1:C:125:ALA:HB1	1.96	0.42
1:C:735:CYS:SG	1:C:739:ALA:HB3	2.58	0.42
1:C:784:LEU:HD23	1:C:794:PRO:CG	2.34	0.42
1:E:144:ARG:HG2	1:E:192:TYR:CD2	2.54	0.42
1:E:203:TYR:HD2	1:E:206:ARG:HD2	1.85	0.42
1:E:305:ILE:HD13	1:E:327:PHE:HB2	2.01	0.42
1:E:500:ASP:CB	1:E:552:VAL:HG11	2.48	0.42
1:E:677:PHE:CZ	1:E:679:GLU:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LYS:C	1:A:233:PHE:N	2.73	0.42
1:A:809:LEU:O	1:A:811:PRO:HD3	2.20	0.42
1:C:148:GLY:O	1:C:355:GLN:NE2	2.52	0.42
1:C:345:PRO:HB3	1:C:399:ARG:HH21	1.85	0.42
1:C:564:ARG:HG3	1:C:682:ARG:HB2	2.01	0.42
1:E:274:ASN:HA	1:E:278:LEU:HB2	2.01	0.42
1:A:542:LEU:HD13	1:A:556:ILE:HD13	2.01	0.42
2:D:551:ARG:H	2:D:551:ARG:HG2	1.47	0.42
2:D:558:TRP:O	2:D:559:PRO:C	2.57	0.42
1:E:39:LEU:HD11	1:E:334:LEU:HD12	2.00	0.42
1:E:563:TYR:HB2	1:E:679:GLU:HG3	2.01	0.42
1:A:406:LYS:CG	1:A:447:ASP:HB3	2.46	0.42
1:A:46:ILE:HD12	1:A:46:ILE:HA	1.90	0.42
1:A:595:GLU:OE1	1:A:599:LEU:HD13	2.19	0.42
1:C:153:PRO:HD2	1:C:200:VAL:HG13	2.00	0.42
1:C:591:GLU:HG2	1:C:685:ARG:CG	2.50	0.42
1:C:589:LYS:CD	1:C:689:LEU:HD11	2.50	0.42
2:D:461:ASP:C	2:D:463:ASP:H	2.23	0.42
1:E:149:GLU:O	1:E:352:ARG:HD2	2.19	0.42
1:E:626:ASP:C	1:E:628:THR:H	2.23	0.42
1:E:840:ASP:CG	1:E:842:LEU:HD13	2.39	0.42
1:E:17:THR:O	1:E:93:THR:HG22	2.19	0.42
2:F:479:TYR:CG	2:F:582:LEU:HB2	2.53	0.42
1:A:129:VAL:HG12	1:A:130:ASP:N	2.35	0.42
1:A:13:MET:SD	1:A:436:LEU:HD21	2.60	0.42
1:A:655:TYR:CD2	1:A:700:ARG:NH1	2.88	0.42
1:A:792:ALA:O	1:A:794:PRO:HD3	2.19	0.42
1:A:4:PHE:HA	1:A:8:GLN:OE1	2.20	0.42
2:B:454:GLY:O	2:B:456:ARG:HD3	2.18	0.42
1:C:504:LEU:HD13	1:C:554:LEU:HD11	2.01	0.42
1:C:581:ASN:HB3	1:C:583:HIS:HB2	2.00	0.42
2:D:428:GLN:O	2:D:432:ARG:HG2	2.20	0.42
2:D:561:ALA:HA	2:D:564:THR:HG23	2.01	0.42
1:E:289:MET:HE3	1:E:317:LYS:HA	2.01	0.42
1:E:454:ILE:HG13	1:E:455:GLY:H	1.84	0.42
1:A:459:ILE:CD1	1:A:469:LEU:HD21	2.49	0.42
1:A:70:ILE:HD13	1:A:442:VAL:HG12	2.02	0.42
2:B:486:GLU:HG3	2:B:487:PRO:HD2	2.01	0.42
1:C:32:LYS:HZ1	1:C:105:SER:HB2	1.84	0.42
1:C:386:VAL:HG11	1:C:437:MET:CE	2.49	0.42
1:C:406:LYS:HA	1:C:447:ASP:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:554:LEU:HB3	1:C:555:LYS:H	1.62	0.42
1:E:126:LEU:HD11	1:E:156:VAL:CG2	2.50	0.42
1:E:35:LEU:O	1:E:39:LEU:HD12	2.20	0.42
1:E:654:GLN:O	1:E:655:TYR:HB2	2.20	0.42
1:E:78:TYR:CE1	1:E:97:SER:HB3	2.44	0.42
1:C:459:ILE:O	1:C:461:GLN:N	2.53	0.42
1:C:43:ALA:O	1:C:77:LEU:HA	2.19	0.42
1:E:311:GLU:HB3	1:E:322:VAL:HG11	2.02	0.42
1:E:809:LEU:O	1:E:811:PRO:HD3	2.20	0.42
1:A:220:PHE:C	1:A:220:PHE:CD1	2.93	0.42
1:A:254:THR:O	1:A:255:LYS:HB2	2.19	0.42
1:A:750:LYS:HE2	1:A:783:GLU:OE1	2.20	0.42
2:B:505:ARG:NH1	2:B:505:ARG:HG3	2.35	0.42
1:E:325:ARG:HH11	1:E:325:ARG:HG2	1.85	0.42
1:E:731:VAL:HG13	1:E:731:VAL:O	2.20	0.42
2:B:479:TYR:CG	2:B:582:LEU:HB2	2.55	0.41
1:C:111:PHE:HE1	1:C:540:ILE:HD11	1.85	0.41
1:C:466:THR:CG2	1:C:467:GLY:N	2.83	0.41
2:B:417:TRP:CE2	2:B:568:PRO:HB2	2.55	0.41
2:B:484:ASP:CG	2:B:494:ARG:HE	2.23	0.41
1:C:788:THR:O	1:C:790:GLY:N	2.54	0.41
2:F:490:ARG:C	2:F:492:ARG:N	2.73	0.41
2:F:538:ARG:HD2	2:F:538:ARG:HA	1.80	0.41
2:F:455:VAL:HG11	2:F:561:ALA:HB1	2.01	0.41
1:A:654:GLN:NE2	1:A:655:TYR:CE1	2.83	0.41
1:C:158:ASN:CG	1:C:159:LYS:N	2.74	0.41
1:C:237:LYS:O	1:C:241:MET:HG2	2.20	0.41
1:C:365:ASN:O	1:C:369:ILE:HG12	2.21	0.41
1:C:792:ALA:O	1:C:794:PRO:HD3	2.20	0.41
1:E:145:GLN:O	1:E:148:GLY:N	2.53	0.41
1:E:211:PHE:CD2	1:E:220:PHE:CE1	3.08	0.41
1:A:735:CYS:HA	1:A:736:PRO:HD3	1.87	0.41
2:B:420:GLU:CD	2:B:420:GLU:H	2.23	0.41
1:C:277:ILE:HG22	1:C:278:LEU:N	2.35	0.41
1:C:781:THR:HG22	1:C:785:ARG:NH2	2.35	0.41
2:D:531:ILE:HD11	2:D:537:LEU:HA	2.02	0.41
1:E:143:LEU:O	1:E:147:LEU:HG	2.20	0.41
1:E:195:GLU:H	1:E:195:GLU:HG3	1.60	0.41
1:E:225:PHE:CD2	1:E:277:ILE:HG23	2.56	0.41
1:E:694:HIS:CE1	1:E:699:DDE:CD2	3.03	0.41
1:E:89:ILE:C	1:E:91:GLN:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:426:HIS:CG	2:F:594:ILE:HD12	2.55	0.41
1:A:10:ARG:CG	1:A:11:SER:N	2.83	0.41
1:A:484:SER:HB2	1:A:797:VAL:CG2	2.51	0.41
1:C:288:ILE:HG23	1:C:319:LEU:CD2	2.48	0.41
1:E:556:ILE:CG2	1:E:557:SER:N	2.60	0.41
1:E:607:ASN:HD21	1:E:609:ARG:NH1	2.19	0.41
2:F:498:LEU:HD12	2:F:571:ILE:CG2	2.51	0.41
1:C:581:ASN:HB3	1:C:583:HIS:HD2	1.83	0.41
1:C:12:LEU:HG	1:C:99:LEU:HB2	2.02	0.41
2:D:443:PHE:CZ	2:D:446:ALA:HB2	2.55	0.41
1:E:493:VAL:HG22	1:E:556:ILE:HD12	2.03	0.41
1:A:702:GLY:O	1:A:706:ILE:HG13	2.21	0.41
1:C:371:ASN:O	1:C:372:CYS:C	2.58	0.41
1:C:728:VAL:N	1:C:800:HIS:O	2.53	0.41
1:E:145:GLN:O	1:E:146:ALA:C	2.58	0.41
1:E:174:LEU:HD11	1:E:178:PHE:CZ	2.56	0.41
1:A:172:GLU:CD	1:A:271:ARG:HH21	2.24	0.41
1:C:464:LEU:HD11	1:C:516:PRO:CB	2.51	0.41
1:C:504:LEU:O	1:C:506:GLU:N	2.53	0.41
1:C:647:ILE:HG13	1:C:685:ARG:HE	1.85	0.41
1:C:75:ILE:HG22	1:C:77:LEU:CD1	2.51	0.41
2:D:417:TRP:NE1	2:D:568:PRO:HB2	2.36	0.41
1:E:108:HIS:HB2	1:E:111:PHE:HE2	1.86	0.41
1:E:111:PHE:O	1:E:115:VAL:HG23	2.21	0.41
1:E:69:THR:N	1:E:389:SER:OG	2.49	0.41
2:F:537:LEU:HD13	2:F:555:ILE:O	2.21	0.41
1:A:183:GLU:HA	1:A:183:GLU:OE1	2.20	0.41
1:A:626:ASP:C	1:A:628:THR:N	2.74	0.41
2:B:442:THR:OG1	2:B:443:PHE:N	2.54	0.41
1:C:249:PHE:N	1:C:249:PHE:CD2	2.88	0.41
1:C:436:LEU:HD23	1:C:454:ILE:HD11	2.03	0.41
1:E:89:ILE:HG23	1:E:340:LEU:O	2.21	0.41
1:E:4:PHE:CD2	1:E:45:ILE:HD12	2.56	0.41
1:E:658:GLU:OE2	1:E:700:ARG:NH2	2.54	0.41
1:A:391:LYS:HE2	1:A:393:ARG:CG	2.51	0.41
1:A:411:VAL:CG1	1:A:412:ARG:N	2.83	0.41
1:A:89:ILE:CG2	1:A:91:GLN:HG2	2.50	0.41
2:B:474:ASP:O	2:B:475:PRO:C	2.59	0.41
1:C:563:TYR:HB2	1:C:679:GLU:HG3	2.03	0.41
1:C:666:ALA:CB	1:C:709:MET:HB3	2.51	0.41
1:C:677:PHE:N	1:C:677:PHE:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:GLN:O	1:C:93:THR:HG23	2.21	0.41
2:D:419:VAL:O	2:D:423:LEU:HG	2.21	0.41
2:D:508:LEU:HA	2:D:508:LEU:HD23	1.77	0.41
1:E:267:LYS:HA	1:E:268:PRO:HD3	1.89	0.41
1:E:638:PRO:HG2	1:E:680:GLU:OE1	2.21	0.41
1:A:397:PHE:HD1	1:A:437:MET:HG3	1.86	0.41
2:B:512:TYR:O	2:B:542:ILE:HD12	2.21	0.41
1:C:615:ARG:HG2	1:C:619:MET:HE1	2.03	0.41
1:C:685:ARG:HE	1:C:687:ASN:ND2	2.17	0.41
1:E:262:THR:HG21	1:E:266:GLY:HA2	2.01	0.41
1:E:314:LEU:O	1:E:319:LEU:HB2	2.20	0.41
1:E:711:ARG:HD2	2:F:577:ASN:ND2	2.36	0.41
1:A:77:LEU:CB	1:A:100:ILE:HB	2.50	0.40
1:A:211:PHE:CD2	1:A:220:PHE:CE1	3.09	0.40
1:A:16:VAL:HG21	1:A:450:ALA:O	2.21	0.40
1:C:261:ASP:O	1:C:269:LEU:N	2.54	0.40
1:E:144:ARG:O	1:E:147:LEU:HB2	2.22	0.40
1:E:511:LEU:HG	1:E:518:VAL:HG11	2.03	0.40
1:E:69:THR:O	1:E:389:SER:N	2.53	0.40
1:A:23:SER:HB3	1:A:122:THR:HG21	2.04	0.40
1:C:256:LYS:HA	1:C:256:LYS:NZ	2.36	0.40
1:C:594:ASP:HB3	1:C:596:GLU:OE1	2.22	0.40
2:D:583:ASP:HA	2:D:584:PRO:HD2	1.95	0.40
1:E:386:VAL:HA	1:E:387:PRO:HD3	1.83	0.40
2:F:409:PHE:HB3	2:F:444:LEU:HD22	2.02	0.40
1:A:129:VAL:CG2	1:A:135:VAL:HG22	2.52	0.40
1:A:327:PHE:CD2	1:A:328:LEU:HG	2.57	0.40
1:A:463:LEU:HD22	1:A:467:GLY:HA3	2.03	0.40
1:A:736:PRO:C	1:A:738:GLN:N	2.75	0.40
1:A:527:GLU:HG3	2:B:412:ARG:NH1	2.35	0.40
2:B:461:ASP:O	2:B:464:ALA:HB3	2.22	0.40
1:C:9:MET:O	1:C:13:MET:HG3	2.21	0.40
1:C:71:LYS:HB3	1:C:386:VAL:HG23	2.03	0.40
1:C:734:GLN:HE21	1:C:734:GLN:CA	2.32	0.40
1:C:729:PHE:CE2	1:C:774:VAL:HG22	2.56	0.40
1:C:82:SER:O	1:C:86:VAL:HG23	2.22	0.40
2:D:531:ILE:HG21	2:D:531:ILE:HD13	1.79	0.40
1:E:222:ILE:CD1	1:E:245:TRP:HB2	2.50	0.40
1:A:635:CYS:SG	1:A:664:VAL:HG13	2.61	0.40
1:A:760:ARG:HB3	1:A:763:THR:OG1	2.21	0.40
1:C:167:LEU:HD12	1:C:167:LEU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:HIS:HB2	1:C:218:TRP:HD1	1.86	0.40
1:C:495:VAL:HG11	1:C:501:LEU:HD12	2.02	0.40
1:C:647:ILE:HB	1:C:687:ASN:ND2	2.36	0.40
1:C:773:PRO:O	1:C:776:GLU:N	2.45	0.40
1:E:828:MET:CE	2:F:576:ARG:HD3	2.51	0.40
1:A:109:VAL:HG23	1:A:138:GLN:CD	2.41	0.40
1:A:200:VAL:O	1:A:200:VAL:CG1	2.69	0.40
1:A:362:ASP:O	1:A:363:ASP:C	2.60	0.40
1:A:411:VAL:HG13	1:A:470:THR:O	2.22	0.40
1:A:585:ARG:HD2	1:A:692:THR:OG1	2.19	0.40
1:E:144:ARG:HG2	1:E:192:TYR:CG	2.57	0.40
1:E:732:GLU:OE1	1:E:769:LYS:HE2	2.22	0.40
2:F:484:ASP:OD2	2:F:494:ARG:HG2	2.21	0.40
2:F:455:VAL:HA	3:F:702:TAD:N1A	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:ASP:OD2	2:F:563:ARG:NH2[2_556]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	818/842 (97%)	736 (90%)	69 (8%)	13 (2%)	11	37
1	C	818/842 (97%)	727 (89%)	78 (10%)	13 (2%)	11	37
1	E	818/842 (97%)	719 (88%)	89 (11%)	10 (1%)	15	46
2	B	205/207 (99%)	188 (92%)	14 (7%)	3 (2%)	12	39
2	D	205/207 (99%)	185 (90%)	15 (7%)	5 (2%)	7	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	205/207 (99%)	181 (88%)	18 (9%)	6 (3%)	5	21
All	All	3069/3147 (98%)	2736 (89%)	283 (9%)	50 (2%)	11	37

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	518	LEU
2	D	519	ALA
1	A	112	SER
1	A	479	LYS
1	A	498	ALA
1	A	582	LYS
1	A	737	GLU
1	C	112	SER
1	C	309	GLY
1	C	460	ASP
2	D	405	GLY
2	D	491	GLY
1	E	112	SER
1	E	479	LYS
1	E	743	ILE
2	F	519	ALA
2	F	520	ALA
1	A	111	PHE
1	A	761	PRO
1	C	111	PHE
1	C	229	TYR
1	C	261	ASP
1	C	479	LYS
2	D	459	SER
1	E	446	ASP
1	A	237	LYS
1	A	261	ASP
1	A	363	ASP
1	A	438	MET
1	E	428	ILE
1	E	460	ASP
1	E	525	SER
2	B	459	SER
1	C	232	LYS
1	C	743	ILE
1	E	556	ILE

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Mol	Chain	Res	Type
1	E	761	PRO
2	F	493	ILE
1	A	806	SER
2	B	404	GLY
2	B	523	ALA
1	C	737	GLU
1	E	558	PRO
2	F	489	ALA
1	C	505	VAL
2	F	404	GLY
2	F	584	PRO
1	A	196	VAL
1	C	329	PRO
1	C	428	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	699/714 (98%)	668 (96%)	31 (4%)	33	67
1	C	699/714 (98%)	661 (95%)	38 (5%)	26	59
1	E	699/714 (98%)	666 (95%)	33 (5%)	30	65
2	B	161/162 (99%)	148 (92%)	13 (8%)	14	38
2	D	161/162 (99%)	149 (92%)	12 (8%)	16	42
2	F	161/162 (99%)	148 (92%)	13 (8%)	14	38
All	All	2580/2628 (98%)	2440 (95%)	140 (5%)	26	59

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	36	THR
1	A	81	MET
1	A	94	ASP

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Mol	Chain	Res	Type
1	A	113	SER
1	A	154	VAL
1	A	236	ASP
1	A	261	ASP
1	A	275	MET
1	A	304	GLU
1	A	347	THR
1	A	352	ARG
1	A	362	ASP
1	A	452	ASN
1	A	460	ASP
1	A	489	VAL
1	A	544	ASP
1	A	577	SER
1	A	595	GLU
1	A	597	VAL
1	A	599	LEU
1	A	609	ARG
1	A	677	PHE
1	A	698	ILE
1	A	710	ARG
1	A	718	LEU
1	A	730	LEU
1	A	734	GLN
1	A	738	GLN
1	A	749	LYS
1	A	836	GLN
2	B	411	THR
2	B	422	LEU
2	B	456	ARG
2	B	467	ARG
2	B	490	ARG
2	B	494	ARG
2	B	513	ARG
2	B	518	LEU
2	B	540	ASP
2	B	547	GLU
2	B	552	LEU
2	B	560	LEU
2	B	602	SER
1	C	23	SER
1	C	33	SER

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Mol	Chain	Res	Type
1	C	36	THR
1	C	81	MET
1	C	83	ASP
1	C	94	ASP
1	C	113	SER
1	C	130	ASP
1	C	154	VAL
1	C	256	LYS
1	C	260	LYS
1	C	261	ASP
1	C	304	GLU
1	C	347	THR
1	C	352	ARG
1	C	460	ASP
1	C	461	GLN
1	C	489	VAL
1	C	500	ASP
1	C	524	GLU
1	C	543	GLN
1	C	544	ASP
1	C	546	GLU
1	C	548	ASP
1	C	577	SER
1	C	597	VAL
1	C	599	LEU
1	C	651	LYS
1	C	677	PHE
1	C	698	ILE
1	C	710	ARG
1	C	718	LEU
1	C	730	LEU
1	C	734	GLN
1	C	738	GLN
1	C	767	THR
1	C	820	LEU
1	C	836	GLN
2	D	403	ASP
2	D	411	THR
2	D	422	LEU
2	D	494	ARG
2	D	505	ARG
2	D	513	ARG

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Mol	Chain	Res	Type
2	D	547	GLU
2	D	551	ARG
2	D	560	LEU
2	D	577	ASN
2	D	602	SER
2	D	603	GLN
1	E	22	MET
1	E	36	THR
1	E	94	ASP
1	E	186	ASN
1	E	194	ASP
1	E	211	PHE
1	E	216	HIS
1	E	263	ASP
1	E	282	PHE
1	E	304	GLU
1	E	313	ASP
1	E	347	THR
1	E	352	ARG
1	E	422	LYS
1	E	460	ASP
1	E	494	GLU
1	E	497	ASN
1	E	544	ASP
1	E	577	SER
1	E	597	VAL
1	E	599	LEU
1	E	627	VAL
1	E	677	PHE
1	E	698	ILE
1	E	710	ARG
1	E	718	LEU
1	E	730	LEU
1	E	734	GLN
1	E	761	PRO
1	E	767	THR
1	E	800	HIS
1	E	836	GLN
1	E	837	GLU
2	F	403	ASP
2	F	411	THR
2	F	422	LEU

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Mol	Chain	Res	Type
2	F	458	ARG
2	F	467	ARG
2	F	494	ARG
2	F	513	ARG
2	F	518	LEU
2	F	531	ILE
2	F	547	GLU
2	F	560	LEU
2	F	563	ARG
2	F	577	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	91	GLN
1	A	108	HIS
1	A	201	GLN
1	A	355	GLN
1	A	371	ASN
1	A	414	GLN
1	A	497	ASN
1	A	537	HIS
1	A	584	ASN
1	A	644	ASN
1	A	687	ASN
1	A	694	HIS
1	A	734	GLN
1	A	738	GLN
1	A	748	ASN
1	A	836	GLN
2	B	424	GLN
2	B	448	GLN
1	C	21	ASN
1	C	27	HIS
1	C	91	GLN
1	C	108	HIS
1	C	138	GLN
1	C	168	GLN
1	C	176	GLN
1	C	201	GLN
1	C	371	ASN

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Mol	Chain	Res	Type
1	C	452	ASN
1	C	537	HIS
1	C	549	HIS
1	C	581	ASN
1	C	583	HIS
1	C	584	ASN
1	C	644	ASN
1	C	687	ASN
1	C	694	HIS
1	C	734	GLN
1	C	738	GLN
1	C	748	ASN
1	C	753	GLN
1	C	800	HIS
1	C	836	GLN
2	D	428	GLN
2	D	448	GLN
2	D	577	ASN
2	D	603	GLN
1	E	27	HIS
1	E	91	GLN
1	E	101	ASN
1	E	138	GLN
1	E	201	GLN
1	E	371	ASN
1	E	414	GLN
1	E	452	ASN
1	E	497	ASN
1	E	537	HIS
1	E	547	HIS
1	E	581	ASN
1	E	583	HIS
1	E	584	ASN
1	E	644	ASN
1	E	687	ASN
1	E	694	HIS
1	E	734	GLN
1	E	738	GLN
1	E	748	ASN
1	E	753	GLN
1	E	800	HIS
1	E	836	GLN

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Mol	Chain	Res	Type
2	F	428	GLN
2	F	448	GLN
2	F	577	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	DDE	A	699	1	6,10,21	0.92	0	5,12,30	1.34	1 (20%)
1	DDE	C	699	1	15,20,21	1.17	1 (6%)	15,28,30	1.80	4 (26%)
1	DDE	E	699	1	15,20,21	1.27	1 (6%)	15,28,30	1.78	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DDE	A	699	1	-	0/4/6/23	0/1/1/1
1	DDE	C	699	1	-	0/19/21/23	0/1/1/1
1	DDE	E	699	1	-	0/19/21/23	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	699	DDE	CAT-CE1	3.62	1.54	1.50
1	E	699	DDE	CAT-CE1	3.72	1.54	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	699	DDE	OAG-CBI-CBW	-3.94	115.78	120.64
1	C	699	DDE	OAG-CBI-CBW	-3.91	115.83	120.64
1	C	699	DDE	CAU-CBW-CBI	-3.10	105.01	111.12
1	E	699	DDE	CAU-CBW-CBI	-3.07	105.08	111.12
1	C	699	DDE	O-C-CA	-2.03	119.41	125.02
1	A	699	DDE	CD2-NE2-CE1	2.09	109.04	105.78
1	E	699	DDE	OAG-CBI-NAD	3.12	127.84	123.06
1	C	699	DDE	OAG-CBI-NAD	3.21	127.97	123.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	699	DDE	1	0
1	C	699	DDE	5	0
1	E	699	DDE	6	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TAD	B	700	-	39,47,47	1.25	4 (10%)	39,72,72	2.48	9 (23%)
3	TAD	D	701	-	39,47,47	1.26	4 (10%)	39,72,72	2.43	9 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TAD	F	702	-	39,47,47	1.28	4 (10%)	39,72,72	2.46	10 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TAD	B	700	-	-	0/18/62/62	0/5/5/5
3	TAD	D	701	-	-	0/18/62/62	0/5/5/5
3	TAD	F	702	-	-	0/18/62/62	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	TAD	PN-O2N	-3.33	1.48	1.56
3	D	701	TAD	PN-O2N	-3.30	1.48	1.56
3	F	702	TAD	PN-O2N	-3.29	1.48	1.56
3	B	700	TAD	PA-O2A	-3.29	1.48	1.56
3	F	702	TAD	PA-O2A	-3.25	1.48	1.56
3	D	701	TAD	PA-O2A	-3.24	1.48	1.56
3	B	700	TAD	PA-O5B	3.09	1.60	1.57
3	D	701	TAD	PA-O5B	3.12	1.60	1.57
3	F	702	TAD	PA-O5B	3.22	1.61	1.57
3	B	700	TAD	PN-O5D	3.51	1.61	1.57
3	D	701	TAD	PN-O5D	3.55	1.61	1.57
3	F	702	TAD	PN-O5D	3.71	1.61	1.57

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	TAD	N3A-C2A-N1A	-9.99	120.16	128.86
3	D	701	TAD	N3A-C2A-N1A	-9.63	120.47	128.86
3	F	702	TAD	N3A-C2A-N1A	-9.60	120.49	128.86
3	F	702	TAD	C4D-O4D-C1D	-5.99	102.54	109.48
3	B	700	TAD	C4D-O4D-C1D	-5.96	102.57	109.48
3	D	701	TAD	C4D-O4D-C1D	-5.85	102.70	109.48
3	F	702	TAD	C4B-O4B-C1B	-5.66	103.75	109.77
3	B	700	TAD	C4B-O4B-C1B	-5.45	103.97	109.77
3	D	701	TAD	C4B-O4B-C1B	-5.26	104.17	109.77
3	D	701	TAD	C4N-C5N-S1N	-4.82	105.87	111.79
3	B	700	TAD	C4N-C5N-S1N	-4.82	105.88	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	702	TAD	C4N-C5N-S1N	-4.73	105.98	111.79
3	F	702	TAD	O4B-C4B-C5B	-2.34	101.50	109.40
3	B	700	TAD	O4B-C4B-C5B	-2.28	101.72	109.40
3	D	701	TAD	O4B-C4B-C5B	-2.24	101.85	109.40
3	F	702	TAD	C4A-C5A-N7A	-2.08	107.41	109.41
3	D	701	TAD	C2A-N1A-C6A	2.01	122.29	118.77
3	F	702	TAD	O6N-C6N-C4N	2.03	121.38	119.65
3	F	702	TAD	C2A-N1A-C6A	2.05	122.36	118.77
3	D	701	TAD	O6N-C6N-C4N	2.11	121.44	119.65
3	B	700	TAD	O6N-C6N-C4N	2.12	121.45	119.65
3	B	700	TAD	C2A-N1A-C6A	2.20	122.62	118.77
3	D	701	TAD	O2N-PN-O1N	2.33	117.89	110.09
3	F	702	TAD	O2N-PN-O1N	2.41	118.16	110.09
3	B	700	TAD	O2N-PN-O1N	2.42	118.21	110.09
3	F	702	TAD	O2A-PA-O1A	2.61	118.83	110.09
3	B	700	TAD	O2A-PA-O1A	2.67	119.02	110.09
3	D	701	TAD	O2A-PA-O1A	2.69	119.08	110.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	700	TAD	2	0
3	D	701	TAD	2	0
3	F	702	TAD	3	0

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, 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	822/842 (97%)	0.07	22 (2%) 55 50	8, 46, 77, 106	0
1	C	822/842 (97%)	0.44	86 (10%) 7 5	6, 56, 106, 121	0
1	E	822/842 (97%)	1.27	244 (29%) 1 0	6, 83, 108, 127	0
2	B	207/207 (100%)	-0.43	1 (0%) 90 90	2, 16, 53, 71	0
2	D	207/207 (100%)	-0.39	2 (0%) 82 81	3, 17, 53, 67	0
2	F	207/207 (100%)	-0.34	2 (0%) 82 81	3, 20, 53, 68	0
All	All	3087/3147 (98%)	0.40	357 (11%) 5 4	2, 50, 102, 127	0

All (357) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	554	LEU	8.2
1	E	258	THR	7.9
1	E	256	LYS	7.2
1	E	254	THR	6.9
1	E	97	SER	6.6
1	E	257	TRP	6.6
1	E	67	GLY	6.6
1	E	216	HIS	6.4
1	C	499	ASN	6.3
1	E	80	GLU	6.2
1	E	308	LYS	5.9
1	E	90	LYS	5.8
1	E	48	ALA	5.7
1	E	298	VAL	5.7
1	E	179	ALA	5.7
1	C	313	ASP	5.5
1	E	89	ILE	5.5
1	E	195	GLU	5.4
1	E	296	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
1	E	737	GLU	5.2
1	E	259	ASN	5.2
1	E	310	ASP	5.2
1	C	513	LYS	5.2
1	E	132	ILE	5.1
1	E	269	LEU	5.1
1	E	240	MET	5.1
1	C	306	VAL	5.1
1	E	194	ASP	5.1
1	E	231	LYS	5.1
1	C	495	VAL	5.0
1	E	795	GLN	5.0
1	E	243	ARG	5.0
1	E	134	GLY	5.0
1	C	550	ALA	5.0
1	E	78	TYR	4.9
1	E	239	LYS	4.9
1	E	260	LYS	4.9
1	E	196	VAL	4.8
1	E	343	PRO	4.8
1	E	93	THR	4.8
1	E	299	LEU	4.7
1	E	359	GLY	4.7
1	E	193	ALA	4.7
1	E	781	THR	4.6
1	C	553	PRO	4.6
1	E	197	LEU	4.6
1	E	47	SER	4.6
1	E	91	GLN	4.5
1	E	167	LEU	4.5
1	E	96	ASN	4.5
1	E	307	LEU	4.5
1	C	307	LEU	4.4
1	E	367	ILE	4.4
1	E	369	ILE	4.3
1	E	317	LYS	4.3
1	E	361	ALA	4.3
1	E	312	LYS	4.3
1	E	3	ALA	4.3
1	C	547	HIS	4.3
1	E	30	HIS	4.3
1	E	306	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	494	GLU	4.3
1	E	510	ARG	4.2
1	C	251	ASN	4.2
1	C	235	VAL	4.2
1	E	137	VAL	4.2
1	C	528	HIS	4.2
1	E	398	GLY	4.2
1	E	138	GLN	4.2
1	C	233	PHE	4.2
1	C	291	PHE	4.1
1	A	67	GLY	4.1
1	E	321	LYS	4.1
1	C	314	LEU	4.1
1	E	770	ALA	4.1
1	E	441	PHE	4.1
1	E	215	LEU	4.1
1	E	262	THR	4.1
1	E	232	LYS	4.1
1	E	94	ASP	4.1
1	C	496	LYS	4.1
1	E	553	PRO	4.0
1	E	166	GLU	4.0
1	E	28	VAL	4.0
1	E	742	GLY	4.0
1	E	354	GLU	3.9
1	C	232	LYS	3.9
1	E	99	LEU	3.9
1	E	108	HIS	3.9
1	E	255	LYS	3.9
1	E	136	CYS	3.9
1	E	320	LEU	3.9
1	E	33	SER	3.8
1	E	392	GLY	3.8
1	E	233	PHE	3.8
1	E	200	VAL	3.8
1	E	242	ASP	3.8
1	E	245	TRP	3.8
1	E	311	GLU	3.8
1	C	234	GLY	3.7
1	C	502	PRO	3.7
1	A	361	ALA	3.7
1	E	740	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	762	GLY	3.7
1	C	744	TYR	3.7
1	E	68	ILE	3.7
1	E	358	GLU	3.7
1	E	280	PRO	3.7
1	C	544	ASP	3.6
1	E	766	PHE	3.6
1	E	46	ILE	3.6
1	E	794	PRO	3.6
1	E	110	ASP	3.6
1	C	501	LEU	3.6
1	E	290	ASN	3.6
1	E	360	PRO	3.6
1	C	504	LEU	3.5
1	E	246	GLY	3.5
1	E	221	THR	3.5
1	E	761	PRO	3.5
1	E	314	LEU	3.5
1	E	356	LEU	3.5
1	E	353	ALA	3.4
1	E	287	ALA	3.4
1	E	784	LEU	3.4
1	C	296	ILE	3.4
1	E	347	THR	3.4
1	E	366	CYS	3.4
1	E	550	ALA	3.4
1	A	392	GLY	3.4
1	E	292	LYS	3.4
1	E	495	VAL	3.4
1	E	348	ALA	3.4
1	A	398	GLY	3.3
1	E	98	PHE	3.3
1	E	322	VAL	3.3
1	E	759	GLN	3.3
1	C	310	ASP	3.3
1	C	270	GLU	3.3
1	C	47	SER	3.3
1	E	95	GLY	3.3
1	E	86	VAL	3.3
2	F	520	ALA	3.3
1	E	189	VAL	3.2
1	E	555	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	311	GLU	3.2
1	C	509	LYS	3.2
1	E	5	THR	3.2
1	C	167	LEU	3.2
1	C	549	HIS	3.2
1	E	339	VAL	3.2
1	E	452	ASN	3.2
1	C	522	MET	3.1
1	C	4	PHE	3.1
1	E	297	PRO	3.1
1	A	5	THR	3.1
1	C	293	LYS	3.1
1	E	440	ARG	3.1
1	E	294	ASP	3.1
1	E	453	ILE	3.1
1	E	318	ALA	3.1
1	E	301	GLU	3.1
1	E	264	ALA	3.1
1	E	349	GLN	3.1
1	E	175	TYR	3.1
1	E	744	TYR	3.1
1	E	316	GLY	3.1
1	C	510	ARG	3.1
1	C	67	GLY	3.1
1	C	3	ALA	3.0
1	C	325	ARG	3.0
1	E	763	THR	3.0
2	F	519	ALA	3.0
1	E	362	ASP	3.0
2	D	489	ALA	3.0
1	E	29	ASP	3.0
1	E	45	ILE	3.0
1	E	83	ASP	3.0
1	E	286	THR	3.0
1	E	207	GLY	2.9
2	B	489	ALA	2.9
1	E	747	LEU	2.9
1	E	180	ARG	2.9
1	E	476	HIS	2.9
1	E	234	GLY	2.9
1	E	131	THR	2.9
1	E	34	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	790	GLY	2.9
1	E	309	GLY	2.9
1	E	265	GLU	2.9
1	E	741	GLY	2.9
1	C	508	LEU	2.9
1	E	424	ASP	2.8
1	E	2	VAL	2.8
1	E	365	ASN	2.8
1	C	740	VAL	2.8
1	E	789	GLY	2.8
1	E	177	THR	2.8
1	A	357	TYR	2.8
1	C	312	LYS	2.8
1	E	220	PHE	2.8
1	C	546	GLU	2.8
1	E	757	GLU	2.8
1	C	236	ASP	2.7
1	E	745	SER	2.7
1	E	333	ALA	2.7
2	D	519	ALA	2.7
1	E	777	SER	2.7
1	E	304	GLU	2.7
1	C	46	ILE	2.7
1	E	6	VAL	2.7
1	E	302	LYS	2.7
1	E	230	ALA	2.7
1	E	419	VAL	2.7
1	C	498	ALA	2.7
1	E	107	GLY	2.7
1	E	126	LEU	2.7
1	E	501	LEU	2.7
1	E	163	ALA	2.7
1	E	235	VAL	2.7
1	E	162	ARG	2.7
1	C	301	GLU	2.6
1	C	316	GLY	2.6
1	E	421	GLY	2.6
1	E	303	LEU	2.6
1	E	442	VAL	2.6
1	E	357	TYR	2.6
1	E	551	GLY	2.6
1	C	421	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	7	ASP	2.6
1	E	323	VAL	2.6
1	E	241	MET	2.6
1	E	313	ASP	2.6
1	C	493	VAL	2.6
1	C	323	VAL	2.6
1	E	760	ARG	2.5
1	E	472	SER	2.5
1	E	20	ARG	2.5
1	E	289	MET	2.5
1	E	187	VAL	2.5
1	A	46	ILE	2.5
1	E	188	ILE	2.5
1	E	217	GLY	2.5
1	E	253	LYS	2.5
1	E	494	GLU	2.5
1	C	2	VAL	2.5
1	E	263	ASP	2.5
1	A	359	GLY	2.5
1	E	82	SER	2.5
1	C	761	PRO	2.5
1	E	743	ILE	2.5
1	E	496	LYS	2.5
1	C	168	GLN	2.5
1	E	44	GLY	2.5
1	C	28	VAL	2.5
1	E	88	GLU	2.5
1	E	780	PHE	2.5
1	E	525	SER	2.4
1	E	371	ASN	2.4
1	E	471	THR	2.4
1	A	308	LYS	2.4
1	E	295	GLU	2.4
1	A	233	PHE	2.4
1	E	105	SER	2.4
1	C	315	GLU	2.4
1	E	276	PHE	2.4
1	C	252	PRO	2.4
1	E	479	LYS	2.4
1	E	399	ARG	2.4
1	E	389	SER	2.4
1	C	529	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	124	GLY	2.3
1	E	541	CYS	2.3
1	E	756	SER	2.3
1	C	305	ILE	2.3
1	E	796	MET	2.3
1	C	551	GLY	2.3
1	E	395	TYR	2.3
1	E	211	PHE	2.3
1	E	748	ASN	2.3
1	E	201	GLN	2.3
1	E	250	PHE	2.3
1	E	474	THR	2.3
1	E	504	LEU	2.3
1	E	73	THR	2.3
1	A	47	SER	2.3
1	C	523	SER	2.3
1	A	360	PRO	2.3
1	E	764	PRO	2.3
1	A	389	SER	2.3
1	C	88	GLU	2.3
1	E	261	ASP	2.3
1	C	267	LYS	2.3
1	E	4	PHE	2.3
1	E	758	GLU	2.3
1	E	735	CYS	2.2
1	E	548	ASP	2.2
1	E	376	ALA	2.2
1	E	355	GLN	2.2
1	E	334	LEU	2.2
1	E	145	GLN	2.2
1	C	265	GLU	2.2
1	E	526	GLY	2.2
1	A	513	LYS	2.2
1	C	552	VAL	2.2
1	A	452	ASN	2.2
1	E	325	ARG	2.2
1	E	508	LEU	2.2
1	C	5	THR	2.2
1	C	8	GLN	2.2
1	C	69	THR	2.2
1	E	549	HIS	2.2
1	C	321	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	239	LYS	2.1
1	C	6	VAL	2.1
1	E	284	LEU	2.1
1	E	423	LYS	2.1
1	E	337	MET	2.1
1	E	319	LEU	2.1
1	A	365	ASN	2.1
1	C	514	SER	2.1
1	E	341	HIS	2.1
1	E	203	TYR	2.1
1	E	335	LEU	2.1
1	C	29	ASP	2.1
1	C	294	ASP	2.1
1	E	279	ASP	2.1
1	A	454	ILE	2.1
1	C	288	ILE	2.1
1	C	268	PRO	2.1
1	C	7	ASP	2.1
1	E	288	ILE	2.1
1	E	444	PRO	2.1
1	A	307	LEU	2.1
1	E	111	PHE	2.1
1	A	48	ALA	2.1
1	E	492	ALA	2.1
1	C	261	ASP	2.1
1	C	210	ALA	2.1
1	C	86	VAL	2.1
1	A	475	ALA	2.1
1	A	10	ARG	2.1
1	C	262	THR	2.0
1	E	192	TYR	2.0
1	C	525	SER	2.0
1	E	383	SER	2.0
1	C	503	LYS	2.0
1	A	196	VAL	2.0
1	C	249	PHE	2.0
1	E	143	LEU	2.0
1	E	547	HIS	2.0
1	E	159	LYS	2.0
1	E	336	GLU	2.0
1	E	244	LEU	2.0
1	E	135	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	231	LYS	2.0
1	C	427	PHE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	DDE	E	699	20/21	0.91	0.22	-	27,53,81,82	0
1	DDE	C	699	20/21	0.93	0.21	-	27,53,81,82	0
1	DDE	A	699	10/21	0.94	0.13	-	40,48,58,58	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	TAD	D	701	43/43	0.90	0.19	0.42	20,31,44,46	0
3	TAD	F	702	43/43	0.91	0.18	0.22	27,37,49,51	0
3	TAD	B	700	43/43	0.91	0.18	0.22	23,32,44,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.