



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:06 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

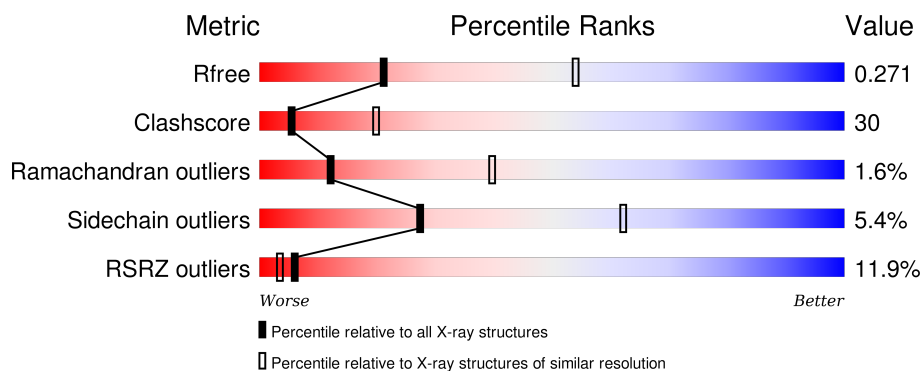
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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  $\geq 3$ , 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	
1	C	842	
1	E	842	
2	B	207	
2	D	207	

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Mol	Chain	Length	Quality of chain
2	F	207	<div><div><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			

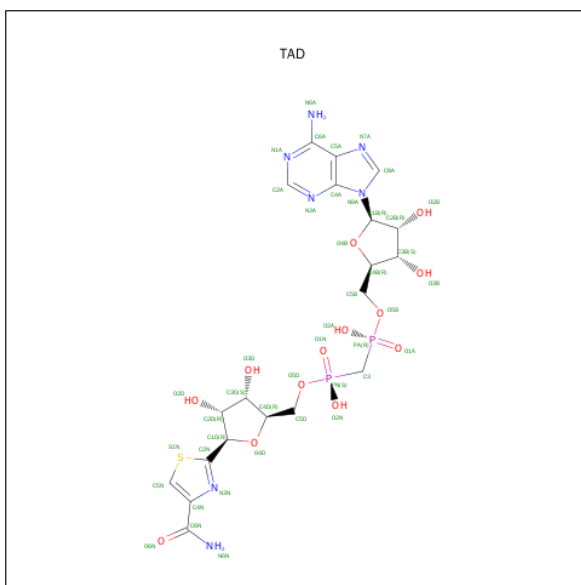
There are 3 discrepancies between the modelled and reference sequences:

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: C<sub>20</sub>H<sub>27</sub>N<sub>7</sub>O<sub>13</sub>P<sub>2</sub>S).

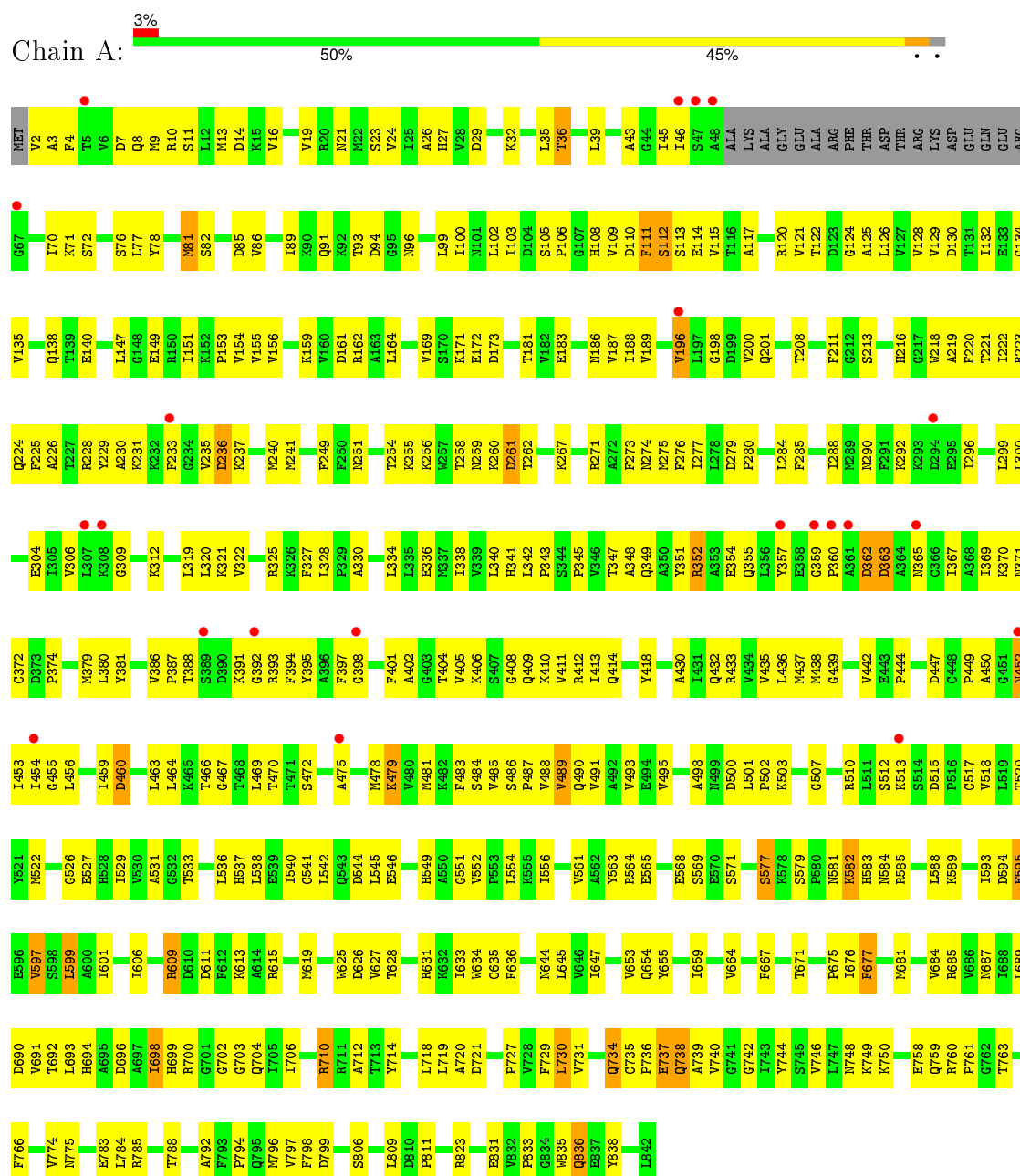


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total 43	C 20	N 7	O 13	P 2	S 1	0	0
3	D	1	Total 43	C 20	N 7	O 13	P 2	S 1	0	0
3	F	1	Total 43	C 20	N 7	O 13	P 2	S 1	0	0

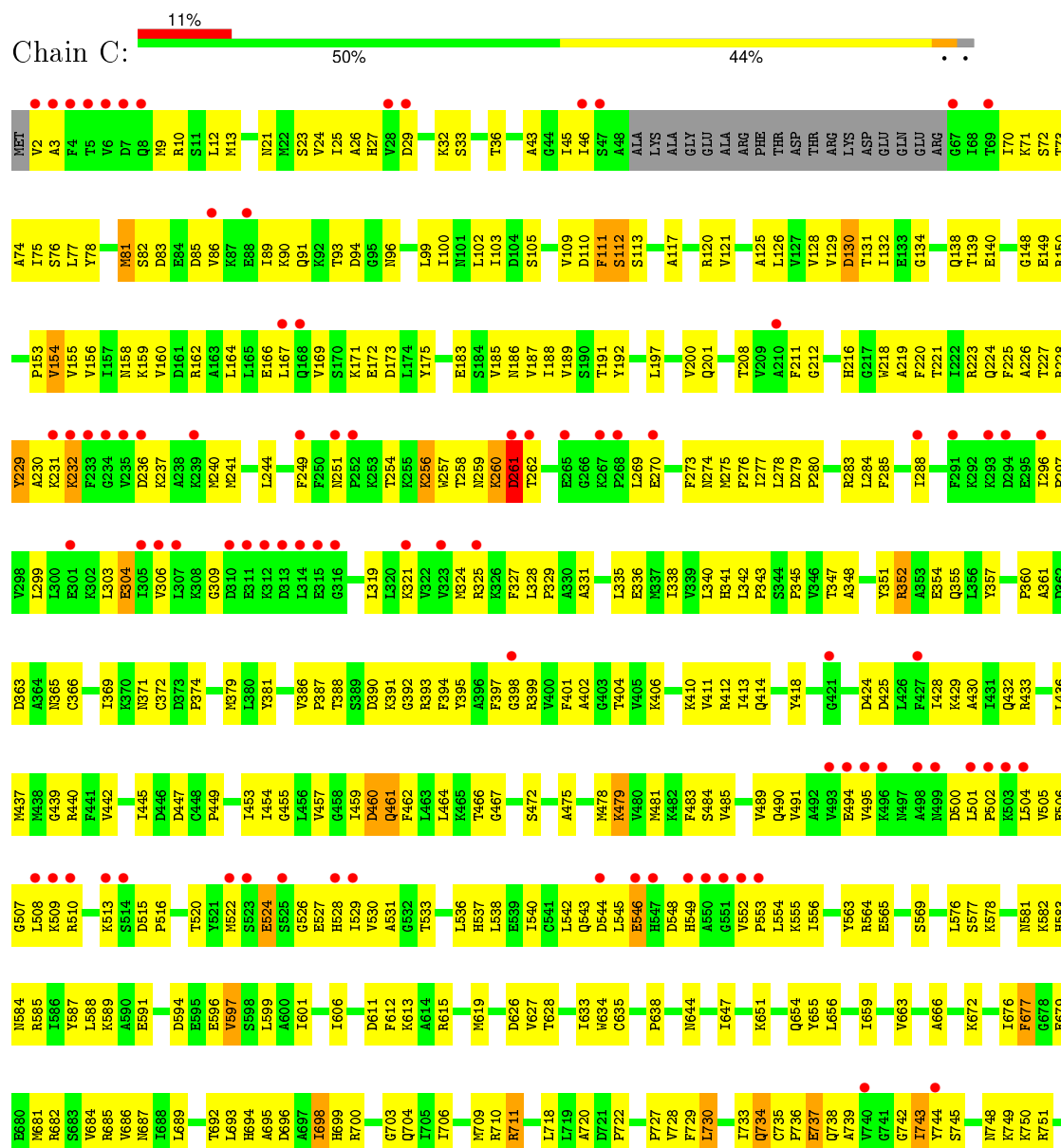
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

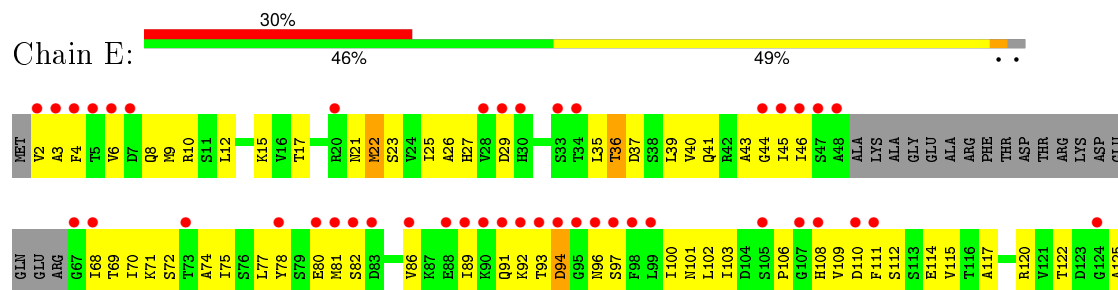
#### • Molecule 1: Elongation factor 2

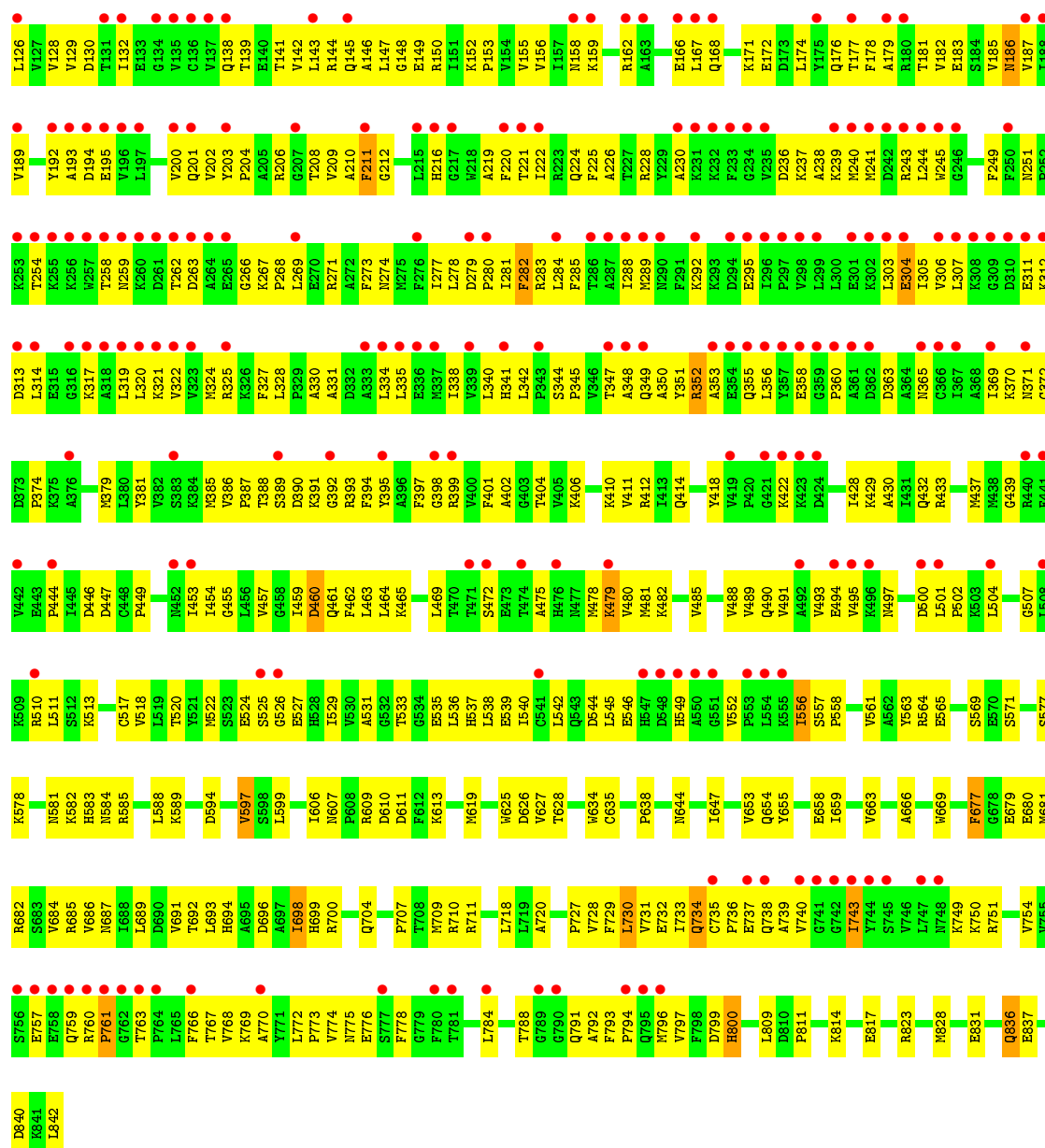


- Molecule 1: Elongation factor 2

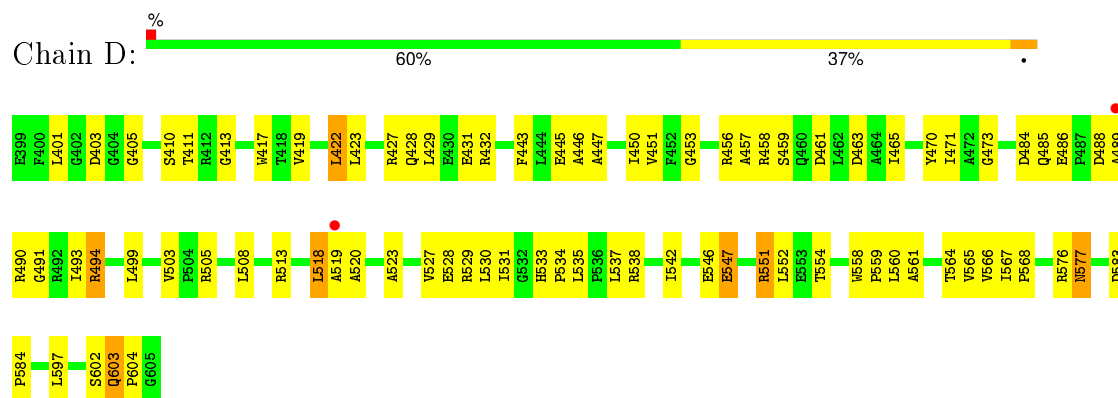


- Molecule 1: Elongation factor 2

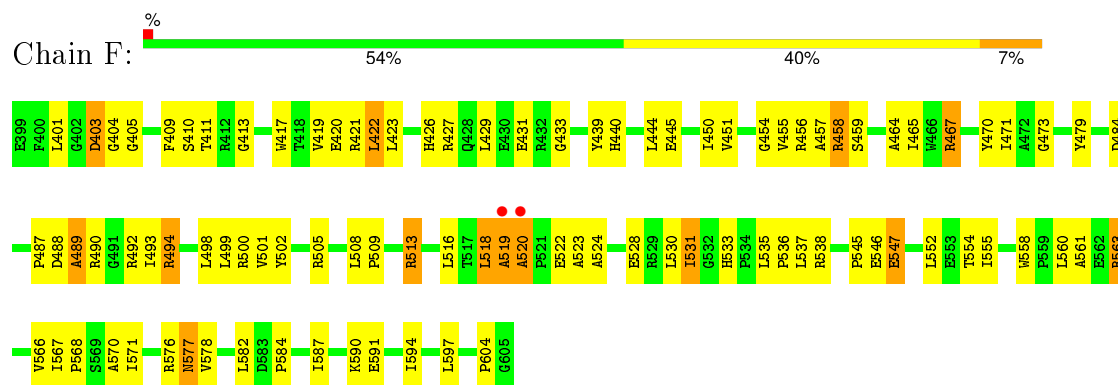








• Molecule 2: exotoxin A



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	41.3	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 91815 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	24125	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:C:836:GLN:HE21	1:C:836:GLN:H	1.21	0.88
1:A:836:GLN:HE21	1:A:836:GLN:H	1.18	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:694:HIS:CD2	1:A:696:ASP:H	1.91	0.85
1:A:391:LYS:HG2	1:A:392:GLY:H	1.41	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:552:LEU:HD12	2:B:552:LEU:N	1.93	0.84
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.59	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
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
2:B:455:VAL:O	2:B:456:ARG:HD2	1.79	0.83
1:E:699:DDE:HAC2	1:E:699:DDE:NAD	1.94	0.82
1:E:147:LEU:CD1	1:E:192:TYR:HB2	2.10	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:E:694:HIS:O	1:E:700:ARG:HD3	1.79	0.81
1:E:155:VAL:HG21	1:E:202:VAL:HG21	1.60	0.81
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.61	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:HG3	2:F:547:GLU:HG3	1.64	0.78
2:F:546:GLU:CG	2:F:547:GLU:HG3	2.13	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:E:647:ILE:HB	1:E:687:ASN:HD22	1.50	0.77
1:C:703:GLY:HA2	2:D:493:ILE:HD13	1.66	0.77
2:F:488:ASP:HB3	2:F:492:ARG:HB2	1.67	0.77
1:A:836:GLN:NE2	1:A:836:GLN:H	1.82	0.77
1:A:464:LEU:HD23	1:A:483:PHE:CE1	2.20	0.77
1:A:464:LEU:HD23	1:A:483:PHE:HE1	1.50	0.77
1:E:288:ILE:HG23	1:E:319:LEU:HD23	1.67	0.77
1:E:71:LYS:HB3	1:E:386:VAL:HG23	1.67	0.77
2:D:527:VAL:HG22	2:D:542:ILE:CD1	2.14	0.77
1:A:410:LYS:HG2	1:A:430:ALA:HB2	1.67	0.77
1:E:581:ASN:ND2	1:E:704:GLN:HG3	1.98	0.76
1:E:281:ILE:HG12	1:E:327:PHE:HE2	1.50	0.76
2:D:432:ARG:NE	2:D:432:ARG:HA	2.00	0.76
1:C:277:ILE:O	1:C:280:PRO:HD2	1.86	0.76
1:A:149:GLU:HA	1:A:355:GLN:HE22	1.48	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:710:ARG:NH1	1:A:710:ARG:HG3	1.99	0.76
1:A:35:LEU:HD22	1:A:334:LEU:HD11	1.68	0.76
1:A:32:LYS:NZ	1:A:105:SER:HB2	2.01	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:91:GLN:HE22	1:E:344:SER:N	1.85	0.74
1:E:836:GLN:NE2	1:E:836:GLN:H	1.84	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:E:381:TYR:OH	1:E:481:MET:HG3	1.88	0.74
1:A:322:VAL:HG22	1:A:325:ARG:HH21	1.53	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
1:E:379:MET:HB2	1:E:402:ALA:HB3	1.70	0.73
2:B:524:ALA:O	2:B:528:GLU:HG3	1.88	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
2:F:433:GLY:O	2:F:505:ARG:HB2	1.89	0.72
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.71	0.72
1:E:594:ASP:HB2	1:E:597:VAL:HG23	1.72	0.72
1:C:545:LEU:HD12	1:C:549:HIS:CD2	2.24	0.72
2:B:410:SER:HB3	2:B:413:GLY:O	1.89	0.71
1:E:757:GLU:HG3	1:E:768:VAL:HG22	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:HG2	1:A:447:ASP:HB3	1.72	0.71
1:C:533:THR:H	1:C:537:HIS:CD2	2.08	0.71
1:E:464:LEU:HD21	1:E:485:VAL:HB	1.72	0.71
1:E:404:THR:HG22	1:E:449:PRO:HA	1.71	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: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:452:ASN:N	1:A:452:ASN:HD22	1.88	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:C:192:TYR:HA	1:C:763:THR:CG2	2.20	0.70
1:A:510:ARG:HG2	1:A:549:HIS:ND1	2.06	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:E:27:HIS:CD2	1:E:29:ASP:H	2.04	0.69
1:C:584:ASN:HD22	1:C:693:LEU:HA	1.56	0.69
1:C:410:LYS:HA	1:C:430:ALA:HA	1.74	0.69
1:C:743:ILE:HD13	1:C:784:LEU:HD11	1.72	0.69
1:C:374:PRO:O	1:C:404:THR:HG23	1.93	0.69
1:C:140:GLU:HG3	1:C:188:ILE:HD13	1.74	0.69
2:B:513:ARG:HH11	2:B:513:ARG:HB2	1.57	0.69
1:E:186:ASN:HB2	1:E:201:GLN:HG2	1.72	0.69
1:E:155:VAL:HG23	1:E:202:VAL:HG11	1.74	0.69
1:C:321:LYS:O	1:C:325:ARG:HG3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:734:GLN:N	1:E:734:GLN:HE21	1.90	0.69
2:D:427:ARG:O	2:D:431:GLU:HG3	1.93	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:E:693:LEU:HB3	1:E:700:ARG:HD2	1.76	0.68
1:E:220:PHE:HB3	1:E:328:LEU:HD13	1.74	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:A:140:GLU:HG3	1:A:188:ILE:CD1	2.23	0.67
1:A:130:ASP:OD1	1:A:159:LYS:HD2	1.94	0.67
1:E:391:LYS:HG3	1:E:392:GLY:N	2.08	0.67
1:C:584:ASN:HD21	1:C:694:HIS:H	1.42	0.67
1:A:533:THR:N	1:A:537:HIS:HD2	1.91	0.67
1:C:584:ASN:ND2	1:C:694:HIS:H	1.93	0.67
1:C:21:ASN:ND2	1:C:345:PRO:HG3	2.09	0.67
1:C:237:LYS:HA	1:C:240:MET:HB3	1.76	0.67
1:E:43:ALA:O	1:E:77:LEU:HA	1.95	0.67
1:E:158:ASN:ND2	1:E:159:LYS:HG3	2.09	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: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:C:172:GLU:HA	1:C:274:ASN:HD21	1.59	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:E:698:ILE:N	1:E:698:ILE:HD13	2.10	0.66
1:C:495:VAL:HG21	1:C:501:LEU:HD12	1.78	0.66
1:E:152:LYS:HD2	1:E:200:VAL:HG23	1.77	0.66
1:C:820:LEU:O	1:C:824:LYS:HG3	1.93	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: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:698:ILE:N	1:C:698:ILE:HD13	2.11	0.66
1:C:285:PHE:HE2	1:C:324:MET:SD	2.19	0.66
1:C:730:LEU:HB2	1:C:799:ASP:HB2	1.75	0.66
1:C:734:GLN:HE21	1:C:734:GLN:N	1.92	0.66
1:C:103:ILE:HD11	1:C:453:ILE:HG12	1.77	0.66
1:E:411:VAL:HG11	1:E:469:LEU:HB3	1.78	0.66
2:D:552:LEU:HD12	2:D:552:LEU:N	2.09	0.66
2:B:405:GLY:CA	1:C:627:VAL:HG12	2.25	0.66
1:A:545:LEU:HD12	1:A:549:HIS:HB2	1.77	0.66
1:E:45:ILE:HD11	1:E:78:TYR:HB2	1.77	0.66
1:E:321:LYS:O	1:E:325:ARG:HG3	1.96	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:E:225:PHE:CZ	1:E:328:LEU:HD11	2.30	0.66
1:A:729:PHE:CE2	1:A:774:VAL:HG22	2.31	0.66
1:E:391:LYS:HB3	1:E:393:ARG:HG2	1.78	0.65
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: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:E:10:ARG:HG3	1:E:10:ARG:HH11	1.61	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
2:B:405:GLY:HA2	1:C:627:VAL:CG1	2.26	0.65
1:A:126:LEU:HD11	1:A:156:VAL:CG2	2.26	0.65
1:E:141:THR:HA	1:E:144:ARG:NH2	2.11	0.65
1:C:588:LEU:C	1:C:588:LEU:HD12	2.16	0.65
1:A:698:ILE:N	1:A:698:ILE:HD13	2.11	0.65
2:B:457:ALA:HB2	2:B:558:TRP:CE3	2.31	0.65
1:A:348:ALA:HA	1:A:351:TYR:CE2	2.32	0.65
1:A:153:PRO:HD2	1:A:200:VAL:CG1	2.27	0.65
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.78	0.65
1:A:500:ASP:HB2	1:A:552:VAL:HG11	1.79	0.65
1:C:132:ILE:N	1:C:132:ILE:HD12	2.11	0.65
1:A:406:LYS:HG2	1:A:447:ASP:CB	2.26	0.65
1:A:381:TYR:HB2	1:A:478:MET:HE3	1.78	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:C:10:ARG:HD3	1:C:445:ILE:HD11	1.78	0.64
1:C:227:THR:O	1:C:230:ALA:HB3	1.97	0.64
1:A:7:ASP:O	1:A:10:ARG:HG2	1.97	0.64
1:E:589:LYS:HE3	1:E:689:LEU:HD11	1.79	0.64
1:C:191:THR:O	1:C:763:THR:HG22	1.96	0.64
1:A:132:ILE:HD12	1:A:162:ARG:NE	2.13	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:A:220:PHE:HB3	1:A:328:LEU:HD13	1.78	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:E:71:LYS:HE3	1:E:387:PRO:CD	2.20	0.64
1:E:381:TYR:O	1:E:398:GLY:HA3	1.98	0.64
1:A:500:ASP:CB	1:A:552:VAL:HG11	2.27	0.64
2:D:551:ARG:HH11	2:D:551:ARG:HG2	1.60	0.63
1:A:501:LEU:HB3	1:A:502:PRO:HD3	1.79	0.63
1:A:226:ALA:CB	1:A:241:MET:HB3	2.26	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
1:E:814:LYS:HA	1:E:817:GLU:OE2	1.99	0.63
1:E:459:ILE:HG21	1:E:463:LEU:HD12	1.81	0.63
1:E:132:ILE:N	1:E:132:ILE:HD12	2.13	0.63
2:D:457:ALA:HB2	2:D:558:TRP:CE3	2.34	0.63
1:E:584:ASN:ND2	1:E:694:HIS:H	1.97	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:A:387:PRO:HG3	1:A:394:PHE:CE1	2.34	0.62
1:A:391:LYS:HB3	1:A:393:ARG:HG2	1.80	0.62
1:E:739:ALA:O	1:E:788:THR:HG22	2.00	0.62
1:C:45:ILE:HD11	1:C:78:TYR:CB	2.29	0.62
1:E:581:ASN:HB3	1:E:583:HIS:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:457:ALA:HB2	2:D:558:TRP: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
2:D:527:VAL:HG13	2:D:542:ILE:HD12	1.81	0.62
1:C:464:LEU:HD23	1:C:483:PHE:HE1	1.61	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:E:71:LYS:HB3	1:E:386:VAL:CG2	2.30	0.61
1:C:536:LEU:HD12	1:C:537:HIS:N	2.15	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:E:644:ASN:ND2	1:E:684:VAL:H	1.98	0.61
1:A:588:LEU:HD12	1:A:588:LEU:C	2.20	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: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: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
2:F:505:ARG:NH1	2:F:505:ARG:HG3	2.15	0.61
1:E:500:ASP:HB2	1:E:552:VAL:HG11	1.81	0.61
1:C:26:ALA:HB2	1:C:128:VAL:HB	1.83	0.61
2:D:445:GLU:OE1	2:D:494:ARG:NH2	2.34	0.61
1:A:561:VAL:HG21	1:A:775:ASN:HA	1.83	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:C:611:ASP:OD2	1:C:613:LYS:HB2	2.00	0.61
1:A:309:GLY:H	1:A:312:LYS:HZ3	1.46	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:536:LEU:HG	1:E:540:ILE:HD12	1.81	0.60
1:E:39:LEU:HD11	1:E:334:LEU:CD1	2.32	0.60
2:F:456:ARG:O	2:F:458:ARG:HD3	2.01	0.60
1:A:200:VAL:HG12	1:A:200:VAL:O	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:C:491:VAL:HG13	1:C:538:LEU:HD21	1.83	0.60
1:A:381:TYR:O	1:A:398:GLY:HA3	2.01	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:A:744:TYR:O	1:A:748:ASN:ND2	2.35	0.60
1:E:114:GLU:O	1:E:117:ALA:HB3	2.01	0.60
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.83	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:345:PRO:O	1:A:349:GLN:HG3	2.00	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:A:229:TYR:CE2	1:A:276:PHE:HB3	2.37	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
2:B:423:LEU:HD11	2:B:590:LYS:HD3	1.83	0.59
1:A:106:PRO:HG3	1:A:114:GLU:HG3	1.84	0.59
1:C:784:LEU:CD2	1:C:794:PRO:HG3	2.30	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:A:9:MET:O	1:A:13:MET:HG3	2.02	0.59
2:D:531:ILE:CD1	2:D:537:LEU:HD23	2.32	0.59
1:A:472:SER:HB3	1:A:475:ALA:HB2	1.84	0.59
1:E:472:SER:HB3	1:E:475:ALA:HB2	1.84	0.59
1:E:279:ASP:HB3	1:E:280:PRO:HD3	1.85	0.59
1:C:26:ALA:HB3	1:C:32:LYS:HB2	1.84	0.59
1:C:581:ASN:HB3	1:C:583:HIS:CD2	2.38	0.59
1:C:545:LEU:HA	1:C:549:HIS:HD2	1.68	0.59
1:C:103:ILE:HD13	1:C:121:VAL:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:ASP:OD2	1:A:613:LYS:HB2	2.02	0.59
1:A:581:ASN:ND2	1:A:699:DDE:O	2.35	0.59
1:E:221:THR:OG1	1:E:224:GLN:HG3	2.03	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: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:25:ILE:HG22	1:C:139:THR:HG23	1.85	0.58
1:C:799:ASP:OD1	1:C:800:HIS:HD2	1.87	0.58
1:C:110:ASP:C	1:C:112:SER:H	2.07	0.58
1:C:685:ARG:HE	1:C:687:ASN:HD21	1.51	0.58
1:E:659:ILE:HD13	1:E:693:LEU:HD21	1.85	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
2:D:518:LEU:H	2:D:518:LEU:HD22	1.67	0.58
1:C:45:ILE:HB	1:C:76:SER:HB2	1.84	0.58
1:C:110:ASP:OD1	1:C:781:THR:HG21	2.04	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:A:464:LEU:CD2	1:A:485:VAL:HB	2.20	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
1:A:171:LYS:HE2	1:A:279:ASP:OD1	2.03	0.58
2:F:570:ALA:HB3	2:F:591:GLU:OE1	2.04	0.58
1:E:522:MET:CB	2:F:490:ARG:HH22	2.14	0.58
1:C:10:ARG:NH2	1:C:449:PRO:HD3	2.19	0.58
1:C:283:ARG:HB3	1:C:299:LEU:HD21	1.86	0.58
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:HD2	1:A:29:ASP:H	1.50	0.57
2:F:488:ASP:HB3	2:F:492:ARG:HB3	1.83	0.57
1:E:120:ARG:HE	1:E:356:LEU:HD22	1.69	0.57
1:A:27:HIS:CD2	1:A:29:ASP:H	2.21	0.57
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.85	0.57
1:E:581:ASN:ND2	1:E:704:GLN:CG	2.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ALA:HB2	1:A:128:VAL:HB	1.86	0.57
1:C:251:ASN:HB3	1:C:254:THR:OG1	2.04	0.57
1:C:581:ASN:O	1:C:582:LYS:HB2	2.04	0.57
1:A:584:ASN:HD21	1:A:700:ARG:HG2	1.70	0.57
1:C:391:LYS:CG	1:C:392:GLY:N	2.68	0.57
1:C:387:PRO:HG3	1:C:394:PHE:CE1	2.38	0.57
1:E:3:ALA:HA	1:E:46:ILE:O	2.04	0.57
1:A:36:THR:HG22	1:A:102:LEU:HD21	1.87	0.57
1:E:699:DDE:CAC	1:E:699:DDE:NAD	2.60	0.57
1:E:374:PRO:O	1:E:404:THR:HG23	2.04	0.57
1:A:290:ASN:HB3	1:A:292:LYS:HE2	1.86	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:C:727:PRO:HG2	1:C:774:VAL:HB	1.85	0.57
1:C:406:LYS:HB3	1:C:447:ASP:HB3	1.85	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:644:ASN:HD22	1:E:684:VAL:H	1.52	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:A:288:ILE:HG23	1:A:319:LEU:HD23	1.85	0.57
1:E:251:ASN:HB3	1:E:254:THR:OG1	2.05	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:C:89:ILE:HG22	1:C:91:GLN:HG2	1.87	0.57
1:A:374:PRO:O	1:A:404:THR:HG23	2.04	0.57
1:A:459:ILE:HG21	1:A:463:LEU:HD12	1.87	0.57
1:E:728:VAL:HB	1:E:800:HIS:HD2	1.67	0.57
1:E:37:ASP:O	1:E:41:GLN:HG3	2.05	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
2:D:465:ILE:HD12	2:D:535:LEU:HD12	1.87	0.56
1:A:594:ASP:HB2	1:A:597:VAL:HG23	1.87	0.56
1:E:338:ILE:HG23	1:E:342:LEU:HD12	1.86	0.56
1:A:3:ALA:HA	1:A:46:ILE:O	2.03	0.56
1:E:226:ALA:O	1:E:230:ALA:HB2	2.05	0.56
1:A:490:GLN:HB3	1:A:531:ALA:HB2	1.86	0.56
1:E:391:LYS:CG	1:E:392:GLY:H	2.13	0.56
1:C:733:ILE:HG21	1:C:743:ILE:CD1	2.36	0.56
1:E:222:ILE:HD13	1:E:245:TRP:HB2	1.87	0.56
1:C:698:ILE:H	1:C:698:ILE:HD13	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:ALA:HB3	1:E:330:ALA:HA	1.86	0.56
1:A:82:SER:HB2	1:A:85:ASP:OD2	2.04	0.56
1:A:485:VAL:O	1:A:487:PRO:HD3	2.06	0.56
2:F:487:PRO:HA	2:F:492:ARG:O	2.06	0.56
1:A:225:PHE:CE2	1:A:277:ILE:HG23	2.40	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:A:258:THR:HG22	1:A:259:ASN:N	2.20	0.56
1:E:17:THR:HB	1:E:92:LYS:O	2.05	0.56
1:E:607:ASN:HB3	1:E:610:ASP:OD2	2.05	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: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: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: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:565:GLU:O	1:A:681:MET:HA	2.06	0.56
1:A:454:ILE:HG13	1:A:455:GLY:H	1.71	0.56
2:F:546:GLU:HG2	2:F:547:GLU:HG3	1.87	0.56
1:C:501:LEU:C	1:C:501:LEU:HD23	2.26	0.56
1:E:120:ARG:HE	1:E:356:LEU:CD2	2.18	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:C:24:VAL:HG23	1:C:102:LEU:HD11	1.86	0.56
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
1:A:223:ARG:HH11	1:A:223:ARG:HG2	1.70	0.55
1:E:204:PRO:HG3	1:E:209:VAL:HG11	1.88	0.55
2:D:551:ARG:CG	2:D:551:ARG:NH1	2.61	0.55
1:A:196:VAL:HG12	1:A:196:VAL:O	2.06	0.55
1:C:140:GLU:HG3	1:C:188:ILE:HD11	1.84	0.55
1:A:493:VAL:HG12	1:A:554:LEU:HD22	1.89	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:C:216:HIS:HB2	1:C:218:TRP:CD1	2.41	0.55
1:A:216:HIS:HB2	1:A:218:TRP:CD1	2.42	0.55
1:C:585:ARG:HD2	1:C:692:THR:OG1	2.07	0.55
1:C:273:PHE:HA	1:C:277:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:TYR:OH	1:A:481:MET:HG3	2.06	0.55
2:F:519:ALA:O	2:F:520:ALA:HB2	2.06	0.55
1:C:169:VAL:CG2	1:C:173:ASP:HB2	2.37	0.55
2:B:537:LEU:O	2:B:538:ARG:HD3	2.06	0.55
1:A:405:VAL:HA	1:A:409:GLN:OE1	2.07	0.55
2:D:537:LEU:O	2:D:538:ARG:HD2	2.06	0.55
2:F:524:ALA:O	2:F:528:GLU:HG3	2.07	0.55
1:E:292:LYS:HD3	1:E:295:GLU:OE2	2.06	0.55
1:A:536:LEU:O	1:A:540:ILE:HG23	2.07	0.55
1:E:491:VAL:HG21	1:E:542:LEU:HD21	1.89	0.55
1:C:256:LYS:HA	1:C:256:LYS:CE	2.38	0.54
1:C:200:VAL:O	1:C:200:VAL:HG13	2.07	0.54
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: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: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:E:429:LYS:HG3	1:E:462:PHE:CZ	2.42	0.54
1:C:760:ARG:HD3	1:C:763:THR:OG1	2.07	0.54
1:C:542:LEU:CD1	1:C:556:ILE:HD11	2.28	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:E:46:ILE:N	1:E:46:ILE:HD12	2.22	0.54
1:A:338:ILE:HG23	1:A:342:LEU:HD12	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:736:PRO:HB2	1:A:738:GLN:HG3	1.89	0.54
1:A:285:PHE:CE2	1:A:320:LEU:HD11	2.42	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
1:C:711:ARG:HD2	2:D:577:ASN:HD21	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: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
2:D:470:TYR:CD2	3:D:701:TAD:H3D	2.42	0.54
1:E:561:VAL:HG21	1:E:775:ASN:CB	2.38	0.54
1:C:126:LEU:HD11	1:C:156:VAL:CG2	2.38	0.54
1:A:43:ALA:HB1	1:A:78:TYR:O	2.08	0.54
1:C:357:TYR:CD2	1:C:366:CYS:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:490:ARG:NH1	2:B:492:ARG:HG2	2.22	0.54
1:A:466:THR:HG22	1:A:467:GLY:N	2.23	0.54
1:C:348:ALA:O	1:C:352:ARG:HB2	2.08	0.54
1:E:74:ALA:HA	1:E:102:LEU:O	2.07	0.54
1:E:644:ASN:HD22	1:E:684:VAL:HB	1.72	0.54
1:C:229:TYR:CZ	1:C:276:PHE:HB3	2.42	0.54
1:A:89:ILE:HG22	1:A:91:GLN:HG2	1.88	0.54
1:C:565:GLU:O	1:C:681:MET:HA	2.08	0.54
1:E:584:ASN:HD21	1:E:694:HIS:H	1.55	0.54
1:C:693:LEU:HB3	1:C:700:ARG:HD2	1.89	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:A:381:TYR:CD1	1:A:478:MET:HE3	2.44	0.54
1:E:360:PRO:HB2	1:E:363:ASP:HB2	1.90	0.54
1:A:388:THR:HG21	1:A:395:TYR:CD1	2.43	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:E:142:VAL:O	1:E:145:GLN:HB2	2.08	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:C:158:ASN:ND2	1:C:159:LYS:HG2	2.24	0.53
1:A:365:ASN:O	1:A:369:ILE:HG12	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:E:108:HIS:HB2	1:E:111:PHE:CE2	2.44	0.53
1:C:200:VAL:O	1:C:200:VAL:CG1	2.56	0.53
1:A:500:ASP:HB3	1:A:552:VAL:HG21	1.90	0.53
1:C:781:THR:HG22	1:C:785:ARG:HH21	1.73	0.53
1:C:411:VAL:HG12	1:C:412:ARG:N	2.23	0.53
1:C:360:PRO:HB2	1:C:363:ASP:HB2	1.90	0.53
1:E:831:GLU:OE1	1:E:831:GLU:N	2.39	0.53
2:B:467:ARG:HG3	2:B:558:TRP:CD1	2.44	0.53
1:A:132:ILE:HD12	1:A:162:ARG:CD	2.39	0.53
1:A:103:ILE:HD12	1:A:122:THR:HG22	1.90	0.53
1:E:39:LEU:HD11	1:E:334:LEU:HD13	1.90	0.53
2:D:531:ILE:HD13	2:D:533:HIS:CE1	2.44	0.53
1:C:211:PHE:O	1:C:219:ALA:HA	2.09	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)
1:E:2:VAL:N	1:E:44:GLY:O	2.42	0.53
2:B:470:TYR:CD2	3:B:700:TAD:H3D	2.44	0.53
1:C:228:ARG:C	1:C:230:ALA:N	2.60	0.53
1:E:385:MET:HG2	1:E:465:LYS:HA	1.91	0.53
1:E:10:ARG:HG3	1:E:10:ARG:NH1	2.23	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
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
2:D:518:LEU:O	2:D:520:ALA:N	2.41	0.52
1:A:2:VAL:HG22	1:A:3:ALA:N	2.23	0.52
1:E:739:ALA:HB2	1:E:791:GLN:OE1	2.10	0.52
1:A:226:ALA:HB2	1:A:241:MET:HB3	1.90	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
2:B:495:ASN:OD1	2:B:495:ASN:N	2.41	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:E:485:VAL:HG22	1:E:485:VAL:O	2.09	0.52
1:E:200:VAL:O	1:E:200:VAL:HG22	2.10	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
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:495:VAL:HG13	1:E:504:LEU:HD22	1.90	0.52
1:E:490:GLN:HB3	1:E:531:ALA:HB2	1.91	0.52
1:C:581:ASN:ND2	1:C:699:DDE:O	2.42	0.52
1:A:485:VAL:HG22	1:A:485:VAL:O	2.10	0.52
1:E:225:PHE:HZ	1:E:328:LEU:HD11	1.72	0.52
1:C:240:MET:O	1:C:244:LEU:HG	2.10	0.52
1:E:75:ILE:HG22	1:E:77:LEU:HD12	1.91	0.52
1:E:152:LYS:CD	1:E:200:VAL:HG23	2.38	0.52
1:A:111:PHE:HB3	1:A:114:GLU:HG2	1.91	0.52
2:B:530:LEU:HA	2:B:604:PRO:HB3	1.91	0.52
1:C:522:MET:HA	1:C:527:GLU:O	2.10	0.52
1:C:160:VAL:HG23	1:C:212:GLY:O	2.09	0.52
1:A:542:LEU:HD13	1:A:556:ILE:HG21	1.91	0.52
1:A:110:ASP:C	1:A:112:SER:H	2.12	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:VAL:HG12	1:C:156:VAL:N	2.25	0.52
1:A:491:VAL:HG13	1:A:538:LEU:HD21	1.91	0.52
1:E:749:LYS:O	1:E:750:LYS:HD2	2.09	0.52
1:A:831:GLU:OE1	1:A:831:GLU:N	2.40	0.52
1:E:262:THR:CG2	1:E:266:GLY:HA2	2.40	0.52
1:C:27:HIS:HD2	1:C:29:ASP:H	1.57	0.52
1:C:578:LYS:HA	1:C:584:ASN:O	2.09	0.52
1:A:391:LYS:CG	1:A:392:GLY:H	2.17	0.52
1:E:792:ALA:O	1:E:794:PRO:HD3	2.09	0.52
2:D:531:ILE:CG2	2:D:533:HIS:H	2.23	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
1:C:563:TYR:O	1:C:564:ARG:HD2	2.10	0.52
1:C:192:TYR:HA	1:C:763:THR:HG21	1.92	0.51
1:A:149:GLU:HA	1:A:355:GLN:NE2	2.21	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: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
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: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:E:365:ASN:O	1:E:369:ILE:HG12	2.10	0.51
1:E:284:LEU:HD13	1:E:324:MET:CE	2.40	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:C:737:GLU:HG3	1:C:766:PHE:CE1	2.46	0.51
1:C:391:LYS:HG3	1:C:392:GLY:N	2.26	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:E:39:LEU:HD23	1:E:335:LEU:HD23	1.91	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:C:685:ARG:HG2	1:C:685:ARG:HH11	1.75	0.51
1:E:36:THR:O	1:E:40:VAL:HG23	2.10	0.51
2:B:457:ALA:HB2	2:B:558:TRP:CG	2.45	0.51
1:A:836:GLN:HE21	1:A:836:GLN:N	1.98	0.51
1:E:150:ARG:NH1	1:E:351:TYR:O	2.43	0.51
1:A:129:VAL:HG13	1:A:134:GLY:C	2.30	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:C:759:GLN:CG	1:C:760:ARG:N	2.62	0.51
1:C:404:THR:HG22	1:C:449:PRO:CA	2.33	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:388:THR:HG21	1:A:395:TYR:CG	2.45	0.51
1:E:414:GLN:HB3	1:E:418:TYR:CD2	2.44	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
1:A:32:LYS:HZ1	1:A:105:SER:HB2	1.75	0.51
1:C:189:VAL:HG13	1:C:200:VAL:HG12	1.91	0.51
1:A:230:ALA:O	1:A:235:VAL:HG22	2.10	0.51
2:B:470:TYR:CE2	3:B:700:TAD:H3D	2.46	0.51
1:E:731:VAL:HG23	1:E:796:MET:HB3	1.92	0.51
1:C:831:GLU:OE1	1:C:831:GLU:N	2.44	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
1:A:125:ALA:HB2	1:A:151:ILE:HG21	1.92	0.51
2:F:467:ARG:NH2	2:F:536:PRO:HG3	2.24	0.51
1:E:211:PHE:N	1:E:211:PHE:CD2	2.79	0.51
1:A:454:ILE:HG13	1:A:455:GLY:N	2.25	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:E:520:THR:HA	1:E:529:ILE:O	2.10	0.51
1:E:77:LEU:CB	1:E:100:ILE:HB	2.40	0.50
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:536:LEU:CG	1:E:540:ILE:HD11	2.36	0.50
1:E:244:LEU:O	1:E:273:PHE:HB2	2.11	0.50
1:E:186:ASN:CB	1:E:201:GLN:HE21	2.25	0.50
1:E:285:PHE:CD2	1:E:320:LEU:HD11	2.46	0.50
2:F:464:ALA:O	2:F:467:ARG:HB3	2.12	0.50
1:E:585:ARG:HD2	1:E:692:THR:OG1	2.11	0.50
1:C:369:ILE:HD12	1:C:401:PHE:HB3	1.94	0.50
1:A:306:VAL:O	1:A:306:VAL:HG23	2.11	0.50
1:A:784:LEU:HD23	1:A:794:PRO:CG	2.32	0.50
2:F:522:GLU:HG2	2:F:523:ALA:N	2.26	0.50
1:A:369:ILE:HD12	1:A:401:PHE:HB3	1.93	0.50
1:A:161:ASP:OD1	1:A:213:SER:HB2	2.12	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:B:458:ARG:O	2:B:459:SER:HB2	2.11	0.50
1:E:278:LEU:O	1:E:282:PHE:HB2	2.10	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:C:27:HIS:CD2	1:C:29:ASP:H	2.29	0.50
1:E:478:MET:O	1:E:480:VAL:N	2.45	0.50
1:A:380:LEU:HD23	1:A:381:TYR:N	2.27	0.50
1:A:16:VAL:CG1	1:A:345:PRO:HB2	2.41	0.50
2:F:520:ALA:CB	2:F:522:GLU:OE2	2.60	0.50
1:C:520:THR:HG22	1:C:530:VAL:HG22	1.93	0.50
1:A:392:GLY:HA3	1:A:513:LYS:HD3	1.93	0.50
1:E:152:LYS:HZ2	1:E:153:PRO:HD2	1.76	0.50
1:C:306:VAL:O	1:C:306:VAL:HG23	2.11	0.50
1:C:244:LEU:HD22	1:C:277:ILE:CD1	2.41	0.50
2:B:450:ILE:HG23	2:B:455:VAL:HG22	1.94	0.50
1:A:309:GLY:H	1:A:312:LYS:NZ	2.09	0.50
2:F:518:LEU:O	2:F:519:ALA:C	2.50	0.50
1:A:70:ILE:HG22	1:A:388:THR:HG22	1.93	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
1:A:677:PHE:N	1:A:677:PHE:CD2	2.80	0.50
2:F:429:LEU:HD13	2:F:502:TYR:CD2	2.46	0.50
1:C:454:ILE:HG13	1:C:455:GLY:N	2.25	0.50
1:A:132:ILE:HD11	1:A:162:ARG:HG2	1.93	0.50
2:F:473:GLY:HA3	2:F:597:LEU:HD11	1.92	0.50
1:C:432:GLN:HB2	1:C:457:VAL:O	2.12	0.50
1:E:581:ASN:O	1:E:582:LYS:HB2	2.12	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:436:LEU:HD23	1:C:454:ILE:CD1	2.42	0.50
2:F:520:ALA:HB3	2:F:522:GLU:OE2	2.12	0.50
1:E:750:LYS:O	1:E:751:ARG:HB2	2.12	0.50
1:C:388:THR:HG21	1:C:395:TYR:CG	2.47	0.50
1:E:25:ILE:HG22	1:E:139:THR:HG23	1.93	0.50
1:A:507:GLY:O	1:A:510:ARG:HB3	2.11	0.49
1:E:760:ARG:HD3	1:E:763:THR:OG1	2.12	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
2:B:465:ILE:HD12	2:B:535:LEU:HD12	1.94	0.49
1:A:727:PRO:HG2	1:A:774:VAL:HB	1.93	0.49
1:C:183:GLU:OE1	1:C:183:GLU:HA	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:611:ASP:OD2	1:E:613:LYS:HB2	2.12	0.49
1:A:758:GLU:HG2	1:A:759:GLN:N	2.27	0.49
1:E:388:THR:HG21	1:E:395:TYR:CD1	2.48	0.49
1:E:536:LEU:O	1:E:539:GLU:N	2.45	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:A:24:VAL:HG23	1:A:102:LEU:HD11	1.94	0.49
1:C:395:TYR:CE1	1:C:457:VAL:HG13	2.47	0.49
1:C:749:LYS:O	1:C:750:LYS:HD2	2.12	0.49
1:C:466:THR:HG22	1:C:467:GLY:N	2.28	0.49
1:C:644:ASN:ND2	1:C:684:VAL:H	2.09	0.49
1:C:589:LYS:HD2	1:C:689:LEU:HD11	1.94	0.49
1:A:628:THR:HG21	2:F:403:ASP:HB3	1.94	0.49
1:E:406:LYS:HB3	1:E:447:ASP:HB3	1.93	0.49
1:E:694:HIS:CE1	1:E:699:DDE:HD2	2.47	0.49
1:A:589:LYS:HE3	1:A:689:LEU:CD1	2.41	0.49
1:C:76:SER:O	1:C:77:LEU:HD12	2.12	0.49
1:C:588:LEU:HD22	1:C:686:VAL:HG13	1.94	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:A:760:ARG:HD3	1:A:763:THR:OG1	2.13	0.49
1:C:742:GLY:O	1:C:745:SER:HB3	2.12	0.49
1:A:432:GLN:O	1:A:433:ARG:HD3	2.12	0.49
1:A:39:LEU:HB3	1:A:77:LEU:HD21	1.94	0.49
2:F:552:LEU:CD1	2:F:552:LEU:N	2.75	0.49
1:C:588:LEU:CD1	1:C:588:LEU:C	2.80	0.49
1:C:433:ARG:HB3	1:C:457:VAL:HB	1.93	0.49
2:F:423:LEU:HD11	2:F:590:LYS:HD3	1.92	0.49
1:C:354:GLU:OE2	1:C:361:ALA:HB1	2.12	0.49
1:E:353:ALA:HB3	1:E:370:LYS:HG3	1.94	0.49
2:D:552:LEU:CD1	2:D:552:LEU:N	2.74	0.49
1:C:588:LEU:HD22	1:C:686:VAL:CG1	2.42	0.49
1:C:836:GLN:N	1:C:836:GLN:HE21	1.99	0.49
1:A:273:PHE:CD1	1:A:277:ILE:HD12	2.47	0.49
1:E:9:MET:O	1:E:12:LEU:HB3	2.13	0.49
1:A:354:GLU:HG3	1:A:370:LYS:HE2	1.94	0.49
1:E:493:VAL:HG22	1:E:556:ILE:CD1	2.43	0.49
2:D:518:LEU:CD2	2:D:518:LEU:H	2.25	0.49
2:D:470:TYR:CE2	3:D:701:TAD:H3D	2.47	0.49
1:A:563:TYR:O	1:A:564:ARG:CD	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:666:ALA:CB	1:E:709:MET:HB3	2.43	0.49
1:A:742:GLY:O	1:A:746:VAL:HG23	2.13	0.49
1:E:236:ASP:OD1	1:E:238:ALA:HB3	2.12	0.49
2:F:489:ALA:C	2:F:490:ARG:HG3	2.32	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
1:A:464:LEU:CD2	1:A:483:PHE:HE1	2.23	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
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:A:228:ARG:HH12	1:A:327:PHE:HE1	1.60	0.48
1:A:490:GLN:HB3	1:A:531:ALA:CB	2.42	0.48
2:F:429:LEU:HD13	2:F:502:TYR:CG	2.48	0.48
1:E:240:MET:O	1:E:244:LEU:HG	2.13	0.48
1:A:322:VAL:HG22	1:A:325:ARG:NH2	2.24	0.48
1:E:588:LEU:CD1	1:E:588:LEU:C	2.80	0.48
1:A:685:ARG:HE	1:A:687:ASN:HD21	1.60	0.48
1:E:538:LEU:O	1:E:542:LEU:HG	2.14	0.48
1:E:399:ARG:HD3	1:E:401:PHE:CZ	2.48	0.48
1:C:120:ARG:NH1	1:C:479:LYS:HG3	2.28	0.48
1:A:677:PHE:N	1:A:677:PHE:HD2	2.11	0.48
1:C:429:LYS:HG3	1:C:462:PHE:CZ	2.48	0.48
2:D:417:TRP:CE2	2:D:568:PRO:HB2	2.48	0.48
2:D:461:ASP:OD1	2:D:463:ASP:HB2	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: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:E:89:ILE:C	1:E:91:GLN:H	2.16	0.48
1:A:501:LEU:C	1:A:501:LEU:HD23	2.33	0.48
1:A:223:ARG:NH1	1:A:223:ARG:HG2	2.28	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: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:C:237:LYS:HA	1:C:240:MET:CB	2.43	0.48
1:A:258:THR:HG22	1:A:259:ASN:H	1.78	0.48
2:D:561:ALA:O	2:D:564:THR:HG23	2.14	0.48
2:F:471:ILE:HG21	2:F:501:VAL:HG21	1.96	0.48
1:C:644:ASN:HD22	1:C:684:VAL:H	1.61	0.48
1:C:129:VAL:HG13	1:C:134:GLY:C	2.34	0.48
1:E:174:LEU:O	1:E:177:THR:HB	2.12	0.48
1:C:10:ARG:CZ	1:C:449:PRO:HD3	2.44	0.48
1:E:225:PHE:CD2	1:E:277:ILE:HD12	2.49	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:E:126:LEU:HD11	1:E:156:VAL:HG21	1.96	0.48
1:E:653:VAL:HG11	1:E:691:VAL:HB	1.96	0.48
1:E:306:VAL:HG23	1:E:306:VAL:O	2.14	0.48
1:E:145:GLN:NE2	1:E:793:PHE:CZ	2.81	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:C:698:ILE:N	1:C:698:ILE:CD1	2.75	0.48
1:C:164:LEU:HD12	1:C:285:PHE:CD1	2.48	0.48
1:A:161:ASP:N	1:A:161:ASP:OD1	2.47	0.48
1:E:454:ILE:HG13	1:E:455:GLY:N	2.28	0.48
1:C:490:GLN:HB3	1:C:531:ALA:HB2	1.96	0.48
1:C:581:ASN:O	1:C:582:LYS:CB	2.62	0.48
1:A:488:VAL:HG23	1:A:489:VAL:HG22	1.96	0.48
1:C:694:HIS:CD2	1:C:695:ALA:N	2.82	0.48
1:A:26:ALA:HB3	1:A:32:LYS:HB2	1.96	0.48
1:C:26:ALA:CB	1:C:128:VAL:HB	2.43	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:A:659:ILE:HD13	1:A:693:LEU:HD21	1.96	0.48
1:C:698:ILE:H	1:C:698:ILE:CD1	2.22	0.48
1:A:258:THR:CG2	1:A:260:LYS:HG2	2.43	0.48
1:C:644:ASN:HD22	1:C:684:VAL:HB	1.79	0.48
1:E:210:ALA:HB2	1:E:221:THR:HG22	1.95	0.47
1:C:507:GLY:O	1:C:510:ARG:HB2	2.14	0.47
1:A:103:ILE:HD13	1:A:121:VAL:CG2	2.44	0.47
1:E:754:VAL:HA	1:E:770:ALA:CB	2.42	0.47
1:E:324:MET:HE2	1:E:324:MET:HA	1.95	0.47
1:A:262:THR:HA	1:A:267:LYS:O	2.14	0.47
2:D:422:LEU:HD22	2:D:422:LEU:O	2.14	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: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
1:A:380:LEU:HD13	1:A:456:LEU:HD11	1.94	0.47
1:E:510:ARG:NH1	1:E:549:HIS:ND1	2.60	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
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:A:411:VAL:HG11	1:A:469:LEU:HB3	1.97	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: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:E:759:GLN:HB2	1:E:766:PHE:CE2	2.49	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:71:LYS:O	1:E:386:VAL:HG21	2.14	0.47
1:C:148:GLY:HA2	1:C:760:ARG:NH2	2.28	0.47
1:A:510:ARG:O	1:A:513:LYS:HB2	2.14	0.47
1:A:156:VAL:HG21	1:A:334:LEU:HD22	1.96	0.47
2:F:401:LEU:O	2:F:421:ARG:NE	2.48	0.47
1:E:606:ILE:HD12	1:E:619:MET:HG2	1.95	0.47
1:E:68:ILE:HD12	1:E:390:ASP:CB	2.28	0.47
1:E:109:VAL:HG23	1:E:138:GLN:CD	2.34	0.47
1:C:327:PHE:CD2	1:C:328:LEU:HG	2.50	0.47
1:E:86:VAL:HG21	1:E:96:ASN:OD1	2.14	0.47
1:E:162:ARG:O	1:E:166:GLU:HB2	2.15	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: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:638:PRO:HB3	1:C:672:LYS:HD3	1.97	0.47
1:C:228:ARG:O	1:C:230:ALA:N	2.48	0.47
1:A:627:VAL:CG1	2:F:405:GLY:HA2	2.44	0.47
1:A:103:ILE:CD1	1:A:121:VAL:HG23	2.45	0.47
1:E:22:MET:HA	1:E:122:THR:HB	1.97	0.47
2:D:527:VAL:CG2	2:D:542:ILE:HD13	2.40	0.47
1:A:39:LEU:H	1:A:39:LEU:HD12	1.80	0.47
1:C:103:ILE:HD13	1:C:121:VAL:CG2	2.44	0.47
2:D:484:ASP:OD2	2:D:494:ARG:HG2	2.14	0.47
2:D:484:ASP:OD2	2:D:494:ARG:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:VAL:O	1:A:601:ILE:HG13	2.15	0.47
1:C:606:ILE:HD12	1:C:619:MET:CG	2.45	0.47
1:E:397:PHE:HD1	1:E:437:MET:HG3	1.79	0.47
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.50	0.47
1:E:106:PRO:HG2	1:E:115:VAL:HG22	1.97	0.47
1:A:729:PHE:CZ	1:A:774:VAL:HG22	2.49	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:522:MET:CE	1:A:526:GLY:O	2.63	0.47
1:E:70:ILE:HG22	1:E:388:THR:HG22	1.95	0.46
1:C:495:VAL:HG11	1:C:501:LEU:CD1	2.44	0.46
1:A:221:THR:OG1	1:A:224:GLN:HG3	2.15	0.46
1:E:677:PHE:N	1:E:677:PHE:CD2	2.83	0.46
1:C:634:TRP:O	1:C:635:CYS:HB3	2.15	0.46
2:B:473:GLY:CA	2:B:597:LEU:HD11	2.37	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:C:647:ILE:HG13	1:C:685:ARG:NE	2.29	0.46
1:A:91:GLN:O	1:A:93:THR:HG23	2.15	0.46
1:A:759:GLN:HB2	1:A:766:PHE:CD2	2.50	0.46
1:A:459:ILE:HG22	1:A:459:ILE:O	2.16	0.46
1:C:406:LYS:HB3	1:C:447:ASP:CB	2.46	0.46
1:E:239:LYS:HE2	1:E:243:ARG:CZ	2.45	0.46
1:A:785:ARG:HG2	1:A:785:ARG:HH11	1.80	0.46
1:C:654:GLN:HG2	1:C:655:TYR:CD2	2.51	0.46
1:C:759:GLN:HG3	1:C:766:PHE:CD2	2.50	0.46
2:F:490:ARG:C	2:F:492:ARG:H	2.16	0.46
1:A:140:GLU:HG3	1:A:188:ILE:HD11	1.98	0.46
1:E:588:LEU:HD12	1:E:588:LEU:O	2.14	0.46
1:A:120:ARG:NH1	1:A:479:LYS:HG3	2.31	0.46
1:A:619:MET:O	1:A:625:TRP:HB2	2.15	0.46
2:D:451:VAL:O	2:D:451:VAL:HG12	2.15	0.46
1:C:304:GLU:HG2	1:C:304:GLU:O	2.14	0.46
1:E:626:ASP:O	1:E:628:THR:N	2.49	0.46
1:E:305:ILE:CD1	1:E:327:PHE:HB2	2.46	0.46
1:E:740:VAL:HG21	1:E:766:PHE:CD1	2.50	0.46
1:C:729:PHE:HB2	1:C:772:LEU:O	2.16	0.46
1:A:495:VAL:HA	1:A:554:LEU:HD23	1.97	0.46
1:E:626:ASP:C	1:E:628:THR:N	2.68	0.46
1:C:167:LEU:N	1:C:167:LEU:HD12	2.29	0.46
1:C:404:THR:CG2	1:C:449:PRO:HA	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:LYS:C	1:C:393:ARG:H	2.19	0.46
1:C:391:LYS:CD	1:C:392:GLY:N	2.74	0.46
1:A:26:ALA:CB	1:A:128:VAL:HB	2.45	0.46
1:A:759:GLN:CD	1:A:766:PHE:HE2	2.18	0.46
1:E:619:MET:O	1:E:625:TRP:HB2	2.16	0.46
1:A:581:ASN:O	1:A:582:LYS:HB2	2.16	0.46
1:A:565:GLU:CD	1:A:676:ILE:HB	2.36	0.46
1:A:164:LEU:HD12	1:A:285:PHE:CD1	2.50	0.46
2:F:465:ILE:HD12	2:F:535:LEU:HD12	1.98	0.46
1:E:535:GLU:CD	1:E:778:PHE:HD1	2.19	0.46
1:A:609:ARG:HG2	1:A:609:ARG:H	1.54	0.46
1:C:759:GLN:HG3	1:C:766:PHE:HD2	1.81	0.46
1:E:143:LEU:O	1:E:144:ARG:C	2.54	0.46
1:A:392:GLY:HA3	1:A:513:LYS:CD	2.46	0.46
1:E:172:GLU:OE2	1:E:176:GLN:NE2	2.48	0.46
1:A:581:ASN:OD1	1:A:704:GLN:CD	2.54	0.46
1:C:89:ILE:CG2	1:C:91:GLN:HG2	2.45	0.46
1:E:711:ARG:HD2	2:F:577:ASN:HD21	1.81	0.46
1:C:70:ILE:O	1:C:440:ARG:HG3	2.15	0.46
1:E:307:LEU:HB2	1:E:312:LYS:HD3	1.97	0.46
1:C:154:VAL:O	1:C:154:VAL:HG12	2.16	0.46
1:A:391:LYS:HE2	1:A:393:ARG:CD	2.45	0.46
1:E:186:ASN:HB2	1:E:201:GLN:HE21	1.81	0.46
2:B:471:ILE:HG13	2:B:554:THR:HB	1.98	0.46
1:A:348:ALA:O	1:A:352:ARG:HB2	2.16	0.46
1:C:685:ARG:NH1	1:C:685:ARG:HG2	2.31	0.46
1:C:522:MET:HG2	1:C:528:HIS:CE1	2.51	0.46
1:C:129:VAL:HG12	1:C:130:ASP:N	2.31	0.46
1:E:186:ASN:OD1	1:E:186:ASN:C	2.54	0.46
1:A:581:ASN:O	1:A:582:LYS:CB	2.64	0.46
1:C:397:PHE:HD1	1:C:437:MET:HG3	1.81	0.46
1:A:493:VAL:HG11	1:A:554:LEU:HD13	1.98	0.46
2:B:403:ASP:HB2	1:C:628:THR:OG1	2.16	0.46
1:C:576:LEU:HD13	1:C:587:TYR:CE1	2.51	0.46
1:A:731:VAL:HB	1:A:796:MET:HB3	1.98	0.46
2:B:518:LEU:HD13	2:B:518:LEU:N	2.31	0.46
1:E:581:ASN:ND2	1:E:704:GLN:OE1	2.50	0.45
1:A:409:GLN:HG2	1:A:411:VAL:HG23	1.98	0.45
2:D:518:LEU:N	2:D:518:LEU:HD22	2.31	0.45
2:B:522:GLU:CD	2:B:522:GLU:H	2.18	0.45
1:C:588:LEU:O	1:C:588:LEU:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:HIS:C	1:C:529:ILE:HD13	2.37	0.45
2:F:422:LEU:HD13	2:F:594:ILE:HD11	1.98	0.45
1:E:129:VAL:HG12	1:E:130:ASP:H	1.82	0.45
1:A:730:LEU:HD22	1:A:730:LEU:C	2.37	0.45
2:D:410:SER:HB3	2:D:413:GLY:O	2.16	0.45
1:C:296:ILE:N	1:C:297:PRO:HD2	2.32	0.45
1:E:4:PHE:HA	1:E:8:GLN:OE1	2.16	0.45
1:C:484:SER:HB3	1:C:797:VAL:HG23	1.94	0.45
1:A:235:VAL:CG2	1:A:240:MET:HB2	2.44	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
2:F:417:TRP:CE2	2:F:568:PRO:HB2	2.50	0.45
1:A:371:ASN:O	1:A:372:CYS:C	2.54	0.45
1:E:68:ILE:HG23	1:E:390:ASP:HB2	1.98	0.45
1:E:39:LEU:HB3	1:E:77:LEU:HD21	1.99	0.45
1:E:836:GLN:N	1:E:836:GLN:HE21	2.10	0.45
1:E:358:GLU:HG2	1:E:479:LYS:HD2	1.98	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:A:249:PHE:CD2	1:A:249:PHE:N	2.84	0.45
1:A:479:LYS:HA	1:A:479:LYS:HD2	1.82	0.45
1:E:167:LEU:HD12	1:E:167:LEU:N	2.31	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
1:A:703:GLY:HA2	2:B:493:ILE:HD12	1.99	0.45
1:A:653:VAL:HG11	1:A:691:VAL:HB	1.98	0.45
2:D:429:LEU:HD21	2:D:565:VAL:HG11	1.98	0.45
2:B:482:ALA:O	2:B:496:GLY:N	2.48	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:C:391:LYS:HD2	1:C:392:GLY:N	2.17	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:A:675:PRO:HD3	1:A:714:TYR:CE1	2.52	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
2:F:488:ASP:CG	2:F:489:ALA:H	2.19	0.45
1:E:578:LYS:HG2	1:E:840:ASP:OD2	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:461:GLN:NE2	1:E:462:PHE:CE2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:LEU:CD1	1:E:324:MET:HE1	2.46	0.45
2:B:433:GLY:O	2:B:505:ARG:HB2	2.16	0.45
1:A:219:ALA:HB3	1:A:330:ALA:HA	1.99	0.45
1:C:175:TYR:HD1	1:C:273:PHE:CD2	2.34	0.45
1:E:6:VAL:O	1:E:10:ARG:HB3	2.16	0.45
1:A:2:VAL:CG2	1:A:3:ALA:N	2.80	0.45
1:C:338:ILE:HG23	1:C:342:LEU:HD12	1.98	0.45
2:B:547:GLU:O	2:B:548:GLU:C	2.55	0.45
1:E:536:LEU:O	1:E:540:ILE:HD12	2.17	0.45
1:C:494:GLU:HB3	1:C:555:LYS:HG2	1.99	0.45
1:E:120:ARG:CZ	1:E:479:LYS:HB3	2.46	0.45
1:A:357:TYR:C	1:A:359:GLY:H	2.20	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
2:B:558:TRP:O	2:B:562:GLU:HG3	2.17	0.45
1:A:710:ARG:CG	1:A:710:ARG:HH11	2.15	0.45
1:A:510:ARG:CG	1:A:510:ARG:HH11	2.30	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
2:B:488:ASP:C	2:B:488:ASP:OD1	2.55	0.45
1:E:356:LEU:HA	1:E:479:LYS:CG	2.47	0.45
1:E:411:VAL:HG12	1:E:412:ARG:N	2.31	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:A:760:ARG:NH1	1:A:763:THR:HG21	2.32	0.45
1:C:70:ILE:HD13	1:C:442:VAL:HG12	1.98	0.45
1:C:85:ASP:OD1	1:C:223:ARG:NH2	2.49	0.45
1:C:73:THR:HG22	1:C:73:THR:O	2.17	0.45
1:C:504:LEU:HD13	1:C:554:LEU:CD1	2.47	0.44
1:A:546:GLU:O	1:A:551:GLY:HA2	2.18	0.44
1:C:424:ASP:OD1	1:C:425:ASP:N	2.50	0.44
1:C:2:VAL:HG22	1:C:3:ALA:N	2.32	0.44
1:E:147:LEU:HB3	1:E:192:TYR:O	2.17	0.44
1:E:735:CYS:SG	1:E:739:ALA:HB3	2.56	0.44
1:A:19:VAL:O	1:A:345:PRO:HD3	2.17	0.44
1:E:501:LEU:HD23	1:E:501:LEU:C	2.38	0.44
1:C:388:THR:HG21	1:C:395:TYR:CD1	2.53	0.44
1:C:304:GLU:CG	1:C:304:GLU:O	2.65	0.44
1:E:546:GLU:HG2	1:E:546:GLU:O	2.17	0.44
1:C:760:ARG:HD3	1:C:763:THR:HG1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:PHE:HZ	1:E:540:ILE:HG12	1.82	0.44
2:B:471:ILE:HG21	2:B:501:VAL:HG21	2.00	0.44
1:C:816:GLY:O	1:C:820:LEU:HD23	2.17	0.44
1:E:171:LYS:NZ	1:E:283:ARG:HH21	2.15	0.44
1:C:109:VAL:HG21	1:C:138:GLN:HG3	2.00	0.44
1:C:757:GLU:HG3	1:C:768:VAL:HG22	1.99	0.44
1:A:797:VAL:HG22	1:A:798:PHE:N	2.31	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:E:388:THR:HG21	1:E:395:TYR:CG	2.52	0.44
1:A:698:ILE:CD1	1:A:698:ILE:H	2.16	0.44
1:A:500:ASP:O	1:A:503:LYS:N	2.46	0.44
1:E:727:PRO:HG2	1:E:774:VAL:HB	1.99	0.44
1:A:493:VAL:CG1	1:A:554:LEU:HD13	2.47	0.44
1:E:654:GLN:HG2	1:E:655:TYR:CG	2.52	0.44
1:E:433:ARG:HE	1:E:444:PRO:HB3	1.82	0.44
1:C:666:ALA:HB2	1:C:706:ILE:HA	2.00	0.44
1:E:507:GLY:CA	1:E:549:HIS:HB3	2.47	0.44
1:C:494:GLU:HG2	1:C:495:VAL:H	1.82	0.44
1:A:129:VAL:HG11	1:A:181:THR:HG23	2.00	0.44
2:D:457:ALA:O	2:D:458:ARG:HG3	2.18	0.44
1:A:3:ALA:CA	1:A:46:ILE:HG22	2.46	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: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: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: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:A:510:ARG:HD2	1:A:549:HIS:ND1	2.33	0.44
1:A:392:GLY:CA	1:A:513:LYS:HD3	2.47	0.44
2:D:530:LEU:HD23	2:D:604:PRO:HD3	2.00	0.44
1:A:593:ILE:HG22	1:A:597:VAL:HB	1.99	0.44
1:A:437:MET:O	1:A:439:GLY:N	2.51	0.44
1:E:239:LYS:O	1:E:239:LYS:HG2	2.17	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
1:A:81:MET:O	1:A:96:ASN:HB3	2.18	0.44
1:C:131:THR:HB	1:C:132:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LYS:HZ1	1:A:325:ARG:HD3	1.82	0.44
2:F:508:LEU:N	2:F:509:PRO:CD	2.81	0.44
1:E:588:LEU:HD22	1:E:686:VAL:CG1	2.48	0.44
1:A:540:ILE:CG1	1:A:541:CYS:N	2.80	0.44
1:C:490:GLN:HA	1:C:531:ALA:HA	1.98	0.44
1:A:634:TRP:O	1:A:635:CYS:HB3	2.17	0.44
1:C:150:ARG:HD3	1:C:197:LEU:HD21	1.99	0.44
1:C:677:PHE:N	1:C:677:PHE:CD2	2.86	0.44
1:A:410:LYS:HG2	1:A:430:ALA:CB	2.42	0.43
1:A:19:VAL:HA	1:A:99:LEU:O	2.17	0.43
1:C:729:PHE:CD2	1:C:774:VAL:HG22	2.53	0.43
1:A:124:GLY:CA	1:A:342:LEU:HD22	2.48	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:A:183:GLU:O	1:A:187:VAL:HG23	2.17	0.43
1:C:828:MET:CE	2:D:576:ARG:HE	2.30	0.43
1:A:667:PHE:CZ	1:A:671:THR:HG21	2.52	0.43
1:A:460:ASP:N	1:A:460:ASP:OD1	2.50	0.43
1:C:546:GLU:OE1	1:C:553:PRO:HD3	2.17	0.43
1:C:70:ILE:HD13	1:C:442:VAL:CG1	2.48	0.43
1:A:186:ASN:HB3	1:A:201:GLN:HG2	2.00	0.43
2:F:505:ARG:HG2	2:F:508:LEU:HD12	2.01	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
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:394:PHE:CZ	1:E:513:LYS:O	2.71	0.43
1:C:515:ASP:HA	1:C:516:PRO:HD3	1.87	0.43
1:E:132:ILE:CD1	1:E:132:ILE:N	2.80	0.43
1:E:524:GLU:C	1:E:526:GLY:N	2.70	0.43
1:E:307:LEU:HD13	1:E:312:LYS:HA	2.01	0.43
1:E:564:ARG:HG3	1:E:682:ARG:HB2	1.99	0.43
2:B:517:THR:HG22	2:B:545:PRO:HB2	2.00	0.43
2:D:453:GLY:O	2:D:456:ARG:HD2	2.18	0.43
1:C:744:TYR:O	1:C:748:ASN:ND2	2.51	0.43
2:F:451:VAL:HG12	2:F:451:VAL:O	2.18	0.43
2:B:583:ASP:HA	2:B:584:PRO:HD2	1.86	0.43
1:C:225:PHE:CD2	1:C:277:ILE:HG13	2.53	0.43
1:E:536:LEU:O	1:E:539:GLU:HB3	2.18	0.43
1:E:189:VAL:O	1:E:193:ALA:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:PHE:CD2	1:A:774:VAL:HG22	2.53	0.43
1:A:588:LEU:CD1	1:A:588:LEU:C	2.86	0.43
1:E:303:LEU:O	1:E:304:GLU:HB3	2.18	0.43
1:C:564:ARG:CG	1:C:682:ARG:HB2	2.48	0.43
1:C:130:ASP:O	1:C:134:GLY:HA2	2.17	0.43
2:D:451:VAL:O	2:D:451:VAL:CG1	2.67	0.43
2:F:465:ILE:HB	2:F:535:LEU:HB3	2.00	0.43
1:A:577:SER:HB2	1:A:712:ALA:HB2	2.01	0.43
1:C:46:ILE:HD12	1:C:46:ILE:HA	1.79	0.43
1:C:149:GLU:HA	1:C:355:GLN:HE22	1.83	0.43
1:E:89:ILE:HG22	1:E:91:GLN:HB3	2.00	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:C:77:LEU:CB	1:C:100:ILE:HB	2.47	0.43
1:A:198:GLY:O	1:A:200:VAL:HG23	2.19	0.43
1:E:171:LYS:NZ	1:E:283:ARG:NH2	2.65	0.43
2:D:499:LEU:HB3	2:D:566:VAL:CG1	2.49	0.43
1:E:663:VAL:HG13	1:E:709:MET:HG2	1.99	0.43
1:A:86:VAL:HG21	1:A:96:ASN:OD1	2.18	0.43
1:E:101:ASN:ND2	1:E:453:ILE:HB	2.34	0.43
1:E:823:ARG:NH1	1:E:828:MET:HB2	2.34	0.43
1:A:222:ILE:HG22	1:A:241:MET:HB2	2.01	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:350:ALA:O	1:E:370:LYS:HG2	2.19	0.43
1:A:730:LEU:HB2	1:A:799:ASP:HB2	2.00	0.43
1:E:203:TYR:CD2	1:E:206:ARG:HD2	2.53	0.43
1:E:111:PHE:CZ	1:E:540:ILE:HG12	2.53	0.43
1:C:555:LYS:O	1:C:555:LYS:HG3	2.19	0.43
1:A:71:LYS:HB3	1:A:386:VAL:CG2	2.44	0.43
1:C:260:LYS:C	1:C:262:THR:H	2.22	0.43
1:E:371:ASN:O	1:E:372:CYS:C	2.57	0.43
1:A:739:ALA:O	1:A:788:THR:HG22	2.19	0.43
1:E:143:LEU:C	1:E:145:GLN:N	2.70	0.43
1:E:209:VAL:HG12	1:E:211:PHE:CE1	2.54	0.43
1:A:433:ARG:CG	1:A:433:ARG:NH1	2.82	0.43
1:C:464:LEU:HD11	1:C:516:PRO:HB2	2.00	0.43
1:E:166:GLU:O	1:E:168:GLN:HG3	2.18	0.43
2:F:458:ARG:O	2:F:459:SER:HB2	2.19	0.43
1:A:106:PRO:HG2	1:A:115:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:VAL:CG1	1:C:156:VAL:N	2.82	0.43
1:E:569:SER:O	1:E:720:ALA:HB1	2.19	0.43
1:A:636:PHE:CE1	1:A:645:LEU:HD21	2.54	0.43
2:F:420:GLU:H	2:F:420:GLU:CD	2.22	0.43
2:B:422:LEU:HD22	2:B:422:LEU:O	2.18	0.43
1:C:735:CYS:HA	1:C:736:PRO:HD3	1.90	0.43
1:A:408:GLY:O	1:A:409:GLN:C	2.57	0.43
1:A:21:ASN:ND2	1:A:345:PRO:HG3	2.34	0.43
1:C:565:GLU:OE1	1:C:676:ILE:HG12	2.18	0.43
2:F:471:ILE:HG13	2:F:554:THR:HB	2.01	0.43
2:D:401:LEU:HD23	2:D:567:ILE:HG22	2.00	0.43
2:B:484:ASP:OD2	2:B:494:ARG:NE	2.48	0.43
1:E:15:LYS:HG3	1:E:94:ASP:OD2	2.18	0.43
1:C:485:VAL:O	1:C:485:VAL:HG12	2.18	0.43
1:A:654:GLN:O	1:A:655:TYR:HB2	2.18	0.42
1:A:546:GLU:HG3	1:A:552:VAL:O	2.18	0.42
1:C:781:THR:CG2	1:C:785:ARG:HH21	2.31	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
2:F:516:LEU:O	2:F:545:PRO:HD2	2.19	0.42
2:D:471:ILE:HG13	2:D:554:THR:HB	2.01	0.42
1:E:733:ILE:HG21	1:E:743:ILE:CD1	2.50	0.42
1:A:413:ILE:HD13	1:A:459:ILE:HG23	2.01	0.42
1:C:74:ALA:O	1:C:439:GLY:HA2	2.19	0.42
1:A:581:ASN:HB2	1:A:583:HIS:H	1.83	0.42
1:C:387:PRO:HG3	1:C:394:PHE:HE1	1.84	0.42
1:E:707:PRO:HB3	2:F:578:VAL:O	2.19	0.42
2:B:404:GLY:H	1:C:628:THR:CG2	2.32	0.42
1:A:615:ARG:HG2	1:A:619:MET:HE1	2.00	0.42
1:E:634:TRP:O	1:E:635:CYS:HB3	2.18	0.42
1:A:515:ASP:OD1	1:A:517:CYS:N	2.47	0.42
1:E:144:ARG:HG2	1:E:192:TYR:CD2	2.54	0.42
1:C:784:LEU:HD23	1:C:794:PRO:CG	2.34	0.42
1:C:25:ILE:HD12	1:C:125:ALA:HB1	1.96	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:A:615:ARG:HG2	1:A:619:MET:CE	2.49	0.42
1:E:677:PHE:CZ	1:E:679:GLU:HG3	2.54	0.42
1:E:203:TYR:HD2	1:E:206:ARG:HD2	1.85	0.42
1:C:735:CYS:SG	1:C:739:ALA:HB3	2.58	0.42
1:A:435:VAL:HG12	1:A:444:PRO:HA	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:274:ASN:HA	1:E:278:LEU:HB2	2.01	0.42
1:C:564:ARG:HG3	1:C:682:ARG:HB2	2.01	0.42
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:E:39:LEU:HD11	1:E:334:LEU:HD12	2.00	0.42
2:D:551:ARG:HG2	2:D:551:ARG:H	1.47	0.42
2:D:558:TRP:O	2:D:559:PRO:C	2.57	0.42
1:A:542:LEU:HD13	1:A:556:ILE:HD13	2.01	0.42
1:E:563:TYR:HB2	1:E:679:GLU:HG3	2.01	0.42
1:E:840:ASP:CG	1:E:842:LEU:HD13	2.39	0.42
1:A:406:LYS:CG	1:A:447:ASP:HB3	2.46	0.42
1:C:153:PRO:HD2	1:C:200:VAL:HG13	2.00	0.42
1:E:149:GLU:O	1:E:352:ARG:HD2	2.19	0.42
2:F:479:TYR:CG	2:F:582:LEU:HB2	2.53	0.42
1:A:46:ILE:HD12	1:A:46:ILE:HA	1.90	0.42
1:C:591:GLU:HG2	1:C:685:ARG:CG	2.50	0.42
1:E:17:THR:O	1:E:93:THR:HG22	2.19	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:626:ASP:C	1:E:628:THR:H	2.23	0.42
1:A:595:GLU:OE1	1:A:599:LEU:HD13	2.19	0.42
1:C:581:ASN:HB3	1:C:583:HIS:HB2	2.00	0.42
1:A:792:ALA:O	1:A:794:PRO:HD3	2.19	0.42
1:A:655:TYR:CD2	1:A:700:ARG:NH1	2.88	0.42
2:B:454:GLY:O	2:B:456:ARG:HD3	2.18	0.42
2:D:428:GLN:O	2:D:432:ARG:HG2	2.20	0.42
1:C:504:LEU:HD13	1:C:554:LEU:HD11	2.01	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
2:D:561:ALA:HA	2:D:564:THR:HG23	2.01	0.42
1:E:454:ILE:HG13	1:E:455:GLY:H	1.84	0.42
1:E:289:MET:HE3	1:E:317:LYS:HA	2.01	0.42
1:A:4:PHE:HA	1:A:8:GLN:OE1	2.20	0.42
1:E:78:TYR:CE1	1:E:97:SER:HB3	2.44	0.42
1:E:35:LEU:O	1:E:39:LEU:HD12	2.20	0.42
1:C:554:LEU:HB3	1:C:555:LYS:H	1.62	0.42
1:A:459:ILE:CD1	1:A:469:LEU:HD21	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:LYS:HA	1:C:447:ASP:HA	2.01	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:E:126:LEU:HD11	1:E:156:VAL:CG2	2.50	0.42
1:E:654:GLN:O	1:E:655:TYR:HB2	2.20	0.42
1:C:43:ALA:O	1:C:77:LEU:HA	2.19	0.42
1:C:459:ILE:O	1:C:461:GLN:N	2.53	0.42
1:E:809:LEU:O	1:E:811:PRO:HD3	2.20	0.42
1:E:311:GLU:HB3	1:E:322:VAL:HG11	2.02	0.42
1:A:254:THR:O	1:A:255:LYS:HB2	2.19	0.42
1:E:325:ARG:HH11	1:E:325:ARG:HG2	1.85	0.42
1:A:220:PHE:C	1:A:220:PHE:CD1	2.93	0.42
1:E:731:VAL:HG13	1:E:731:VAL:O	2.20	0.42
2:B:505:ARG:NH1	2:B:505:ARG:HG3	2.35	0.42
1:A:750:LYS:HE2	1:A:783:GLU:OE1	2.20	0.42
1:C:466:THR:CG2	1:C:467:GLY:N	2.83	0.41
1:C:111:PHE:HE1	1:C:540:ILE:HD11	1.85	0.41
2:B:479:TYR:CG	2:B:582:LEU:HB2	2.55	0.41
2:F:490:ARG:C	2:F:492:ARG:N	2.73	0.41
2:F:455:VAL:HG11	2:F:561:ALA:HB1	2.01	0.41
2:F:538:ARG:HD2	2:F:538:ARG:HA	1.80	0.41
2:B:484:ASP:CG	2:B:494:ARG:HE	2.23	0.41
2:B:417:TRP:CE2	2:B:568:PRO:HB2	2.55	0.41
1:C:788:THR:O	1:C:790:GLY:N	2.54	0.41
1:E:145:GLN:O	1:E:148:GLY:N	2.53	0.41
1:A:654:GLN:NE2	1:A:655:TYR:CE1	2.83	0.41
1:C:792:ALA:O	1:C:794:PRO:HD3	2.20	0.41
1:E:211:PHE:CD2	1:E:220:PHE:CE1	3.08	0.41
1:C:237:LYS:O	1:C:241:MET:HG2	2.20	0.41
1:C:158:ASN:CG	1:C:159:LYS:N	2.74	0.41
1:C:365:ASN:O	1:C:369:ILE:HG12	2.21	0.41
1:E:694:HIS:CE1	1:E:699:DDE:CD2	3.03	0.41
1:E:143:LEU:O	1:E:147:LEU:HG	2.20	0.41
1:E:89:ILE:C	1:E:91:GLN:N	2.73	0.41
1:E:225:PHE:CD2	1:E:277:ILE:HG23	2.56	0.41
1:C:277:ILE:HG22	1:C:278:LEU:N	2.35	0.41
2:D:531:ILE:HD11	2:D:537:LEU:HA	2.02	0.41
1:A:735:CYS:HA	1:A:736:PRO:HD3	1.87	0.41
1:C:781:THR:HG22	1:C:785:ARG:NH2	2.35	0.41
2:F:426:HIS:CG	2:F:594:ILE:HD12	2.55	0.41
1:E:195:GLU:H	1:E:195:GLU:HG3	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:420:GLU:CD	2:B:420:GLU:H	2.23	0.41
1:E:556:ILE:CG2	1:E:557:SER:N	2.60	0.41
1:A:10:ARG:CG	1:A:11:SER:N	2.83	0.41
1:C:288:ILE:HG23	1:C:319:LEU:CD2	2.48	0.41
1:E:607:ASN:HD21	1:E:609:ARG:NH1	2.19	0.41
1:A:484:SER:HB2	1:A:797:VAL:CG2	2.51	0.41
2:F:498:LEU:HD12	2:F:571:ILE:CG2	2.51	0.41
1:E:493:VAL:HG22	1:E:556:ILE:HD12	2.03	0.41
1:C:581:ASN:HB3	1:C:583:HIS:HD2	1.83	0.41
2:D:443:PHE:CZ	2:D:446:ALA:HB2	2.55	0.41
1:C:12:LEU:HG	1:C:99:LEU:HB2	2.02	0.41
1:E:145:GLN:O	1:E:146:ALA:C	2.58	0.41
1:C:728:VAL:N	1:C:800:HIS:O	2.53	0.41
1:E:174:LEU:HD11	1:E:178:PHE:CZ	2.56	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: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: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
2:F:537:LEU:HD13	2:F:555:ILE:O	2.21	0.41
1:C:75:ILE:HG22	1:C:77:LEU:CD1	2.51	0.41
1:A:172:GLU:CD	1:A:271:ARG:HH21	2.24	0.41
1:C:647:ILE:HG13	1:C:685:ARG:HE	1.85	0.41
2:D:417:TRP:NE1	2:D:568:PRO:HB2	2.36	0.41
1:E:69:THR:N	1:E:389:SER:OG	2.49	0.41
1:E:658:GLU:OE2	1:E:700:ARG:NH2	2.54	0.41
1:E:89:ILE:HG23	1:E:340:LEU:O	2.21	0.41
1:A:391:LYS:HE2	1:A:393:ARG:CG	2.51	0.41
1:E:4:PHE:CD2	1:E:45:ILE:HD12	2.56	0.41
1:A:411:VAL:CG1	1:A:412:ARG:N	2.83	0.41
1:C:436:LEU:HD23	1:C:454:ILE:HD11	2.03	0.41
1:A:89:ILE:CG2	1:A:91:GLN:HG2	2.50	0.41
1:C:91:GLN:O	1:C:93:THR:HG23	2.21	0.41
1:C:563:TYR:HB2	1:C:679:GLU:HG3	2.03	0.41
1:A:626:ASP:C	1:A:628:THR:N	2.74	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
1:A:183:GLU:HA	1:A:183:GLU:OE1	2.20	0.41
2:B:474:ASP:O	2:B:475:PRO:C	2.59	0.41
2:B:442:THR:OG1	2:B:443:PHE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:PHE:N	1:C:249:PHE:CD2	2.88	0.41
1:E:638:PRO:HG2	1:E:680:GLU:OE1	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:314:LEU:O	1:E:319:LEU:HB2	2.20	0.41
1:C:685:ARG:HE	1:C:687:ASN:ND2	2.17	0.41
1:E:711:ARG:HD2	2:F:577:ASN:ND2	2.36	0.41
1:E:262:THR:HG21	1:E:266:GLY:HA2	2.01	0.41
1:A:397:PHE:HD1	1:A:437:MET:HG3	1.86	0.41
1:C:615:ARG:HG2	1:C:619:MET:HE1	2.03	0.41
2:B:512:TYR:O	2:B:542:ILE:HD12	2.21	0.41
1:E:144:ARG:O	1:E:147:LEU:HB2	2.22	0.40
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:E:69:THR:O	1:E:389:SER:N	2.53	0.40
1:C:261:ASP:O	1:C:269:LEU:N	2.54	0.40
1:E:511:LEU:HG	1:E:518:VAL:HG11	2.03	0.40
1:E:386:VAL:HA	1:E:387:PRO:HD3	1.83	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
1:A:23:SER:HB3	1:A:122:THR:HG21	2.04	0.40
2:F:409:PHE:HB3	2:F:444:LEU:HD22	2.02	0.40
2:D:583:ASP:HA	2:D:584:PRO:HD2	1.95	0.40
1:E:222:ILE:CD1	1:E:245:TRP:HB2	2.50	0.40
1:A:463:LEU:HD22	1:A:467:GLY:HA3	2.03	0.40
2:D:531:ILE:HG21	2:D:531:ILE:HD13	1.79	0.40
1:A:129:VAL:CG2	1:A:135:VAL:HG22	2.52	0.40
1:C:734:GLN:HE21	1:C:734:GLN:CA	2.32	0.40
1:A:327:PHE:CD2	1:A:328:LEU:HG	2.57	0.40
1:A:736:PRO:C	1:A:738:GLN:N	2.75	0.40
1:C:71:LYS:HB3	1:C:386:VAL:HG23	2.03	0.40
1:C:729:PHE:CE2	1:C:774:VAL:HG22	2.56	0.40
1:A:527:GLU:HG3	2:B:412:ARG:NH1	2.35	0.40
1:C:82:SER:O	1:C:86:VAL:HG23	2.22	0.40
1:C:9:MET:O	1:C:13:MET:HG3	2.21	0.40
2:B:461:ASP:O	2:B:464:ALA:HB3	2.22	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

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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: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
1:A:635:CYS:SG	1:A:664:VAL:HG13	2.61	0.40
1:E:828:MET:CE	2:F:576:ARG:HD3	2.51	0.40
1:E:144:ARG:HG2	1:E:192:TYR:CG	2.57	0.40
1:A:109:VAL:HG23	1:A:138:GLN:CD	2.41	0.40
2:F:455:VAL:HA	3:F:702:TAD:N1A	2.36	0.40
1:A:411:VAL:HG13	1:A:470:THR:O	2.22	0.40
1:A:200:VAL:CG1	1:A:200:VAL:O	2.69	0.40
1:A:362:ASP:O	1:A:363:ASP:C	2.60	0.40
1:A:585:ARG:HD2	1:A:692:THR:OG1	2.19	0.40
2:F:484:ASP:OD2	2:F:494:ARG:HG2	2.21	0.40
1:E:732:GLU:OE1	1:E:769:LYS:HE2	2.22	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%)	12	40
1	C	818/842 (97%)	727 (89%)	78 (10%)	13 (2%)	12	40
1	E	818/842 (97%)	719 (88%)	89 (11%)	10 (1%)	16	48
2	B	205/207 (99%)	188 (92%)	14 (7%)	3 (2%)	13	42
2	D	205/207 (99%)	185 (90%)	15 (7%)	5 (2%)	7	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	205/207 (99%)	181 (88%)	18 (9%)	6 (3%)	6	23
All	All	3069/3147 (98%)	2736 (89%)	283 (9%)	50 (2%)	12	40

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%)	35	70
1	C	699/714 (98%)	661 (95%)	38 (5%)	27	62
1	E	699/714 (98%)	666 (95%)	33 (5%)	32	68
2	B	161/162 (99%)	148 (92%)	13 (8%)	15	39
2	D	161/162 (99%)	149 (92%)	12 (8%)	17	44
2	F	161/162 (99%)	148 (92%)	13 (8%)	15	39
All	All	2580/2628 (98%)	2440 (95%)	140 (5%)	27	62

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	5,10,21	0.60	0	3,12,30	1.71	1 (33%)
1	DDE	C	699	1	13,20,21	0.77	0	16,28,30	3.01	6 (37%)
1	DDE	E	699	1	13,20,21	0.75	0	16,28,30	3.00	6 (37%)

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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	699	DDE	OAG-CBI-CBW	-4.13	115.78	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	699	DDE	OAG-CBI-CBW	-4.09	115.83	120.72
1	C	699	DDE	CAU-CBW-CBI	-3.02	105.01	110.92
1	E	699	DDE	CAU-CBW-CBI	-2.98	105.08	110.92
1	C	699	DDE	O-C-CA	-2.33	119.41	125.49
1	E	699	DDE	O-C-CA	-2.16	119.87	125.49
1	A	699	DDE	CD2-NE2-CE1	2.11	109.04	105.71
1	E	699	DDE	OAG-CBI-NAD	3.21	127.84	123.08
1	C	699	DDE	OAG-CBI-NAD	3.30	127.97	123.08
1	C	699	DDE	CAU-CAT-CE1	5.19	140.59	112.58
1	E	699	DDE	CAU-CAT-CE1	5.29	141.09	112.58
1	E	699	DDE	CAT-CAU-CBW	8.31	144.75	112.43
1	C	699	DDE	CAT-CAU-CBW	8.31	144.76	112.43

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	-	37,47,47	1.28	4 (10%)	42,72,72	2.63	10 (23%)
3	TAD	D	701	-	37,47,47	1.29	4 (10%)	42,72,72	2.57	9 (21%)
3	TAD	F	702	-	37,47,47	1.31	4 (10%)	42,72,72	2.60	11 (26%)

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	-3.32	1.48	1.56
3	D	701	TAD	PN-O2N	-3.29	1.48	1.56
3	F	702	TAD	PN-O2N	-3.28	1.48	1.56
3	B	700	TAD	PA-O2A	-3.28	1.48	1.56
3	F	702	TAD	PA-O2A	-3.24	1.48	1.56
3	D	701	TAD	PA-O2A	-3.23	1.48	1.56
3	B	700	TAD	PA-O5B	3.09	1.60	1.57
3	D	701	TAD	PA-O5B	3.13	1.60	1.57
3	F	702	TAD	PA-O5B	3.23	1.61	1.57
3	B	700	TAD	PN-O5D	3.51	1.61	1.57
3	D	701	TAD	PN-O5D	3.56	1.61	1.57
3	F	702	TAD	PN-O5D	3.72	1.61	1.57

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	TAD	N3A-C2A-N1A	-11.41	120.16	128.89
3	D	701	TAD	N3A-C2A-N1A	-11.00	120.47	128.89
3	F	702	TAD	N3A-C2A-N1A	-10.97	120.49	128.89
3	F	702	TAD	C4D-O4D-C1D	-6.89	102.54	109.58
3	B	700	TAD	C4D-O4D-C1D	-6.85	102.57	109.58
3	D	701	TAD	C4D-O4D-C1D	-6.72	102.70	109.58
3	F	702	TAD	C4B-O4B-C1B	-5.44	103.75	109.72
3	B	700	TAD	C4B-O4B-C1B	-5.23	103.97	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	701	TAD	C4B-O4B-C1B	-5.05	104.17	109.72
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
3	F	702	TAD	C4N-C5N-S1N	-4.73	105.98	111.79
3	D	701	TAD	O5B-PA-O1A	-2.65	106.94	113.98
3	B	700	TAD	O5B-PA-O1A	-2.60	107.07	113.98
3	F	702	TAD	O5B-PA-O1A	-2.54	107.22	113.98
3	F	702	TAD	C4A-C5A-N7A	-2.25	107.41	109.48
3	F	702	TAD	O4B-C4B-C5B	-2.19	101.50	109.32
3	D	701	TAD	C4A-C5A-N7A	-2.15	107.50	109.48
3	B	700	TAD	O4B-C4B-C5B	-2.13	101.72	109.32
3	D	701	TAD	O4B-C4B-C5B	-2.09	101.85	109.32
3	B	700	TAD	C4A-C5A-N7A	-2.08	107.56	109.48
3	F	702	TAD	O5D-PN-O1N	-2.01	108.63	113.98
3	F	702	TAD	C2A-N1A-C6A	2.01	122.36	118.77
3	B	700	TAD	C2A-N1A-C6A	2.16	122.62	118.77
3	D	701	TAD	O2N-PN-O1N	2.47	117.89	110.12
3	F	702	TAD	O2N-PN-O1N	2.56	118.16	110.12
3	B	700	TAD	O2N-PN-O1N	2.57	118.21	110.12
3	F	702	TAD	O2A-PA-O1A	2.77	118.83	110.12
3	B	700	TAD	O2A-PA-O1A	2.83	119.02	110.12
3	D	701	TAD	O2A-PA-O1A	2.85	119.08	110.12

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	822/842 (97%)	0.08	22 (2%) 58 52	8, 46, 77, 106	0
1	C	822/842 (97%)	0.45	89 (10%) 8 4	6, 56, 106, 121	0
1	E	822/842 (97%)	1.30	252 (30%) 1 0	6, 83, 108, 127	0
2	B	207/207 (100%)	-0.42	1 (0%) 91 90	2, 16, 53, 71	0
2	D	207/207 (100%)	-0.38	2 (0%) 84 82	3, 17, 53, 67	0
2	F	207/207 (100%)	-0.33	2 (0%) 84 82	3, 20, 53, 68	0
All	All	3087/3147 (98%)	0.41	368 (11%) 6 3	2, 50, 102, 127	0

All (368) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	554	LEU	8.3
1	E	258	THR	8.1
1	E	256	LYS	7.3
1	E	254	THR	7.1
1	E	257	TRP	6.8
1	E	97	SER	6.7
1	E	67	GLY	6.6
1	E	216	HIS	6.5
1	C	499	ASN	6.5
1	E	80	GLU	6.4
1	E	308	LYS	6.0
1	E	90	LYS	5.9
1	E	298	VAL	5.7
1	C	313	ASP	5.7
1	E	48	ALA	5.7
1	E	179	ALA	5.6
1	E	89	ILE	5.6
1	E	195	GLU	5.5
1	E	259	ASN	5.4

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Mol	Chain	Res	Type	RSRZ
1	E	737	GLU	5.4
1	E	310	ASP	5.3
1	E	296	ILE	5.3
1	C	513	LYS	5.3
1	E	240	MET	5.3
1	E	194	ASP	5.2
1	E	132	ILE	5.2
1	E	269	LEU	5.2
1	E	231	LYS	5.2
1	E	795	GLN	5.1
1	C	306	VAL	5.1
1	C	495	VAL	5.1
1	E	78	TYR	5.1
1	E	134	GLY	5.0
1	E	343	PRO	5.0
1	E	239	LYS	5.0
1	E	260	LYS	5.0
1	C	550	ALA	4.9
1	E	93	THR	4.9
1	E	196	VAL	4.9
1	E	299	LEU	4.8
1	E	243	ARG	4.8
1	C	553	PRO	4.7
1	E	359	GLY	4.7
1	E	781	THR	4.7
1	E	47	SER	4.7
1	E	197	LEU	4.7
1	E	91	GLN	4.7
1	E	96	ASN	4.7
1	E	193	ALA	4.6
1	E	167	LEU	4.6
1	E	307	LEU	4.6
1	C	307	LEU	4.5
1	E	367	ILE	4.5
1	E	317	LYS	4.4
1	E	369	ILE	4.4
1	E	312	LYS	4.4
1	C	251	ASN	4.4
1	C	494	GLU	4.4
1	C	547	HIS	4.3
1	E	30	HIS	4.3
1	E	138	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	306	VAL	4.3
1	C	528	HIS	4.3
1	E	361	ALA	4.3
1	C	235	VAL	4.3
1	E	137	VAL	4.3
1	E	3	ALA	4.3
1	E	398	GLY	4.2
1	C	233	PHE	4.2
1	E	321	LYS	4.2
1	C	291	PHE	4.2
1	C	314	LEU	4.2
1	E	94	ASP	4.2
1	E	262	THR	4.2
1	E	441	PHE	4.2
1	A	67	GLY	4.2
1	E	553	PRO	4.2
1	E	232	LYS	4.2
1	C	496	LYS	4.2
1	E	215	LEU	4.2
1	E	166	GLU	4.1
1	E	770	ALA	4.1
1	E	510	ARG	4.1
1	E	28	VAL	4.0
1	E	354	GLU	4.0
1	E	742	GLY	4.0
1	C	232	LYS	4.0
1	E	136	CYS	4.0
1	E	108	HIS	3.9
1	E	99	LEU	3.9
1	E	255	LYS	3.9
1	E	33	SER	3.9
1	E	320	LEU	3.9
1	E	242	ASP	3.9
1	E	392	GLY	3.9
1	E	233	PHE	3.9
1	E	245	TRP	3.9
1	C	502	PRO	3.9
1	E	311	GLU	3.8
1	E	200	VAL	3.8
1	C	744	TYR	3.8
1	C	234	GLY	3.8
1	E	280	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	544	ASP	3.8
1	E	358	GLU	3.8
1	E	68	ILE	3.8
1	E	762	GLY	3.8
1	E	794	PRO	3.8
1	E	110	ASP	3.7
1	E	740	VAL	3.7
1	A	361	ALA	3.7
1	E	766	PHE	3.7
1	E	290	ASN	3.7
1	E	360	PRO	3.7
1	E	46	ILE	3.7
1	C	501	LEU	3.7
1	E	761	PRO	3.6
1	E	221	THR	3.6
1	C	504	LEU	3.6
1	E	246	GLY	3.6
1	E	366	CYS	3.5
1	E	314	LEU	3.5
1	E	356	LEU	3.5
1	E	347	THR	3.5
1	E	784	LEU	3.5
1	C	296	ILE	3.5
1	E	292	LYS	3.5
1	E	759	GLN	3.4
1	C	310	ASP	3.4
1	A	392	GLY	3.4
1	E	353	ALA	3.4
1	C	270	GLU	3.4
1	E	98	PHE	3.4
1	E	495	VAL	3.4
1	E	287	ALA	3.4
1	A	398	GLY	3.4
1	C	47	SER	3.4
1	E	322	VAL	3.4
1	E	550	ALA	3.4
1	E	348	ALA	3.3
1	E	95	GLY	3.3
1	E	86	VAL	3.3
1	C	311	GLU	3.3
1	E	555	LYS	3.3
1	E	452	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	189	VAL	3.3
1	C	509	LYS	3.3
1	E	5	THR	3.3
2	F	520	ALA	3.2
1	C	522	MET	3.2
1	E	297	PRO	3.2
1	C	167	LEU	3.2
1	E	294	ASP	3.2
1	C	549	HIS	3.2
1	A	5	THR	3.2
1	E	339	VAL	3.2
1	E	349	GLN	3.2
1	C	293	LYS	3.2
1	C	4	PHE	3.2
1	E	301	GLU	3.2
1	E	453	ILE	3.1
1	E	175	TYR	3.1
1	E	744	TYR	3.1
1	E	362	ASP	3.1
1	E	763	THR	3.1
1	E	316	GLY	3.1
1	E	29	ASP	3.1
1	C	67	GLY	3.1
1	E	83	ASP	3.1
1	E	318	ALA	3.1
1	E	286	THR	3.1
1	E	264	ALA	3.0
1	E	45	ILE	3.0
1	C	3	ALA	3.0
1	E	131	THR	3.0
1	E	440	ARG	3.0
2	F	519	ALA	3.0
1	E	207	GLY	3.0
1	E	747	LEU	3.0
1	E	34	THR	3.0
2	D	489	ALA	3.0
1	E	476	HIS	3.0
1	E	234	GLY	2.9
1	C	510	ARG	2.9
1	E	265	GLU	2.9
1	E	424	ASP	2.9
1	E	790	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	489	ALA	2.9
1	E	365	ASN	2.9
1	E	309	GLY	2.9
1	C	325	ARG	2.9
1	C	508	LEU	2.9
1	E	741	GLY	2.9
1	E	177	THR	2.9
1	C	546	GLU	2.8
1	E	2	VAL	2.8
1	E	757	GLU	2.8
1	A	357	TYR	2.8
1	C	236	ASP	2.8
1	C	312	LYS	2.8
1	E	220	PHE	2.8
1	E	789	GLY	2.8
1	E	180	ARG	2.8
1	E	745	SER	2.8
1	C	740	VAL	2.8
1	E	304	GLU	2.8
1	E	777	SER	2.8
1	E	302	LYS	2.8
1	C	46	ILE	2.7
1	C	301	GLU	2.7
1	E	6	VAL	2.7
1	E	419	VAL	2.7
1	E	107	GLY	2.7
1	E	126	LEU	2.7
1	E	501	LEU	2.7
1	E	333	ALA	2.7
2	D	519	ALA	2.7
1	E	7	ASP	2.7
1	E	357	TYR	2.7
1	E	313	ASP	2.7
1	E	230	ALA	2.7
1	C	316	GLY	2.7
1	E	235	VAL	2.7
1	E	421	GLY	2.7
1	E	303	LEU	2.7
1	C	498	ALA	2.7
1	E	241	MET	2.7
1	E	551	GLY	2.7
1	E	442	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	163	ALA	2.6
1	C	421	GLY	2.6
1	E	472	SER	2.6
1	E	323	VAL	2.6
1	E	289	MET	2.6
1	E	263	ASP	2.6
1	C	761	PRO	2.6
1	E	494	GLU	2.6
1	C	493	VAL	2.6
1	C	168	GLN	2.6
1	E	253	LYS	2.6
1	C	323	VAL	2.6
1	E	82	SER	2.6
1	A	46	ILE	2.6
1	E	188	ILE	2.6
1	E	217	GLY	2.6
1	E	496	LYS	2.6
1	E	187	VAL	2.6
1	E	162	ARG	2.5
1	E	371	ASN	2.5
1	E	88	GLU	2.5
1	E	743	ILE	2.5
1	C	2	VAL	2.5
1	A	359	GLY	2.5
1	E	44	GLY	2.5
1	E	471	THR	2.5
1	E	525	SER	2.5
1	E	780	PHE	2.5
1	E	295	GLU	2.5
1	C	28	VAL	2.5
1	A	308	LYS	2.5
1	C	315	GLU	2.5
1	E	105	SER	2.5
1	C	252	PRO	2.5
1	A	233	PHE	2.5
1	E	760	ARG	2.4
1	E	276	PHE	2.4
1	E	20	ARG	2.4
1	E	541	CYS	2.4
1	E	479	LYS	2.4
1	E	389	SER	2.4
1	E	756	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	796	MET	2.4
1	E	748	ASN	2.4
1	E	201	GLN	2.4
1	C	529	ILE	2.4
1	E	124	GLY	2.4
1	E	395	TYR	2.4
1	C	305	ILE	2.4
1	E	474	THR	2.4
1	C	551	GLY	2.4
1	A	360	PRO	2.4
1	E	211	PHE	2.4
1	E	764	PRO	2.4
1	E	735	CYS	2.4
1	E	73	THR	2.4
1	E	261	ASP	2.4
1	A	47	SER	2.3
1	C	523	SER	2.3
1	E	548	ASP	2.3
1	C	88	GLU	2.3
1	E	250	PHE	2.3
1	A	389	SER	2.3
1	E	758	GLU	2.3
1	C	267	LYS	2.3
1	E	504	LEU	2.3
1	E	355	GLN	2.3
1	E	4	PHE	2.3
1	E	145	GLN	2.3
1	E	399	ARG	2.3
1	A	452	ASN	2.3
1	C	265	GLU	2.3
1	A	513	LYS	2.3
1	C	8	GLN	2.3
1	C	5	THR	2.2
1	C	69	THR	2.2
1	E	334	LEU	2.2
1	E	526	GLY	2.2
1	C	321	LYS	2.2
1	E	508	LEU	2.2
1	A	365	ASN	2.2
1	E	549	HIS	2.2
1	C	552	VAL	2.2
1	C	29	ASP	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	239	LYS	2.2
1	C	294	ASP	2.2
1	E	279	ASP	2.2
1	E	376	ALA	2.2
1	E	337	MET	2.2
1	E	423	LYS	2.2
1	C	7	ASP	2.2
1	C	268	PRO	2.2
1	C	514	SER	2.2
1	E	444	PRO	2.2
1	E	203	TYR	2.2
1	E	284	LEU	2.2
1	C	261	ASP	2.2
1	C	6	VAL	2.2
1	E	319	LEU	2.2
1	E	341	HIS	2.2
1	E	335	LEU	2.1
1	A	454	ILE	2.1
1	C	288	ILE	2.1
1	E	111	PHE	2.1
1	E	288	ILE	2.1
1	A	307	LEU	2.1
1	C	262	THR	2.1
1	E	325	ARG	2.1
1	E	192	TYR	2.1
1	C	525	SER	2.1
1	E	383	SER	2.1
1	E	336	GLU	2.1
1	C	503	LYS	2.1
1	A	294	ASP	2.1
1	C	86	VAL	2.1
1	E	159	LYS	2.1
1	E	500	ASP	2.1
1	A	48	ALA	2.1
1	E	492	ALA	2.1
1	C	249	PHE	2.1
1	E	547	HIS	2.1
1	C	231	LYS	2.1
1	E	168	GLN	2.1
1	E	143	LEU	2.1
1	C	210	ALA	2.1
1	E	81	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	196	VAL	2.0
1	E	244	LEU	2.0
1	A	475	ALA	2.0
1	C	427	PHE	2.0
1	E	92	LYS	2.0
1	C	794	PRO	2.0
1	E	422	LYS	2.0
1	E	222	ILE	2.0
1	C	765	LEU	2.0
1	E	135	VAL	2.0
1	E	158	ASN	2.0
1	E	738	GLN	2.0
1	C	398	GLY	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	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.