



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 05:54 pm BST

PDB ID : 1LVC  
Title : Crystal structure of the adenylyl cyclase domain of anthrax edema factor (EF) in complex with calmodulin and 2' deoxy, 3' anthraniloyl ATP  
Authors : Shen, Y.; Lee, Y.-S.; Soelaiman, S.; Bergson, P.; Lu, D.; Chen, A.; Beckingham, K.; Grabarek, Z.; Mrksich, M.; Tang, W.-J.  
Deposited on : 2002-05-28  
Resolution : 3.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

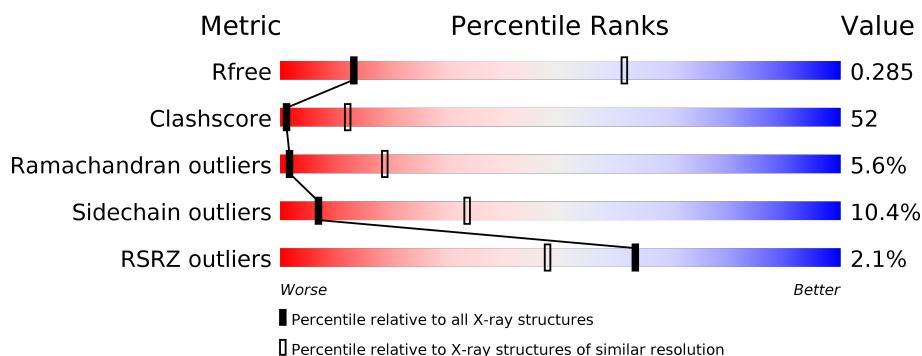
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	510	<div> <div></div> <div>38% 48% 9% 5%</div> </div>
1	B	510	<div> <div>3%</div> <div>22% 55% 14% 9%</div> </div>
1	C	510	<div> <div></div> <div>38% 51% 9% ..</div> </div>
2	D	149	<div> <div>3%</div> <div>34% 53% 9% .</div> </div>
2	E	149	<div> <div>7%</div> <div>38% 48% 9% .</div> </div>
2	F	149	<div> <div>5%</div> <div>36% 48% 11% .</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15302 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 calmodulin-sensitive adenylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	65	0	0
			3952	2528	673	748	3			
1	B	465	Total	C	N	O	S	113	0	0
			3794	2431	642	718	3			
1	C	503	Total	C	N	O	S	166	0	0
			4094	2616	696	779	3			

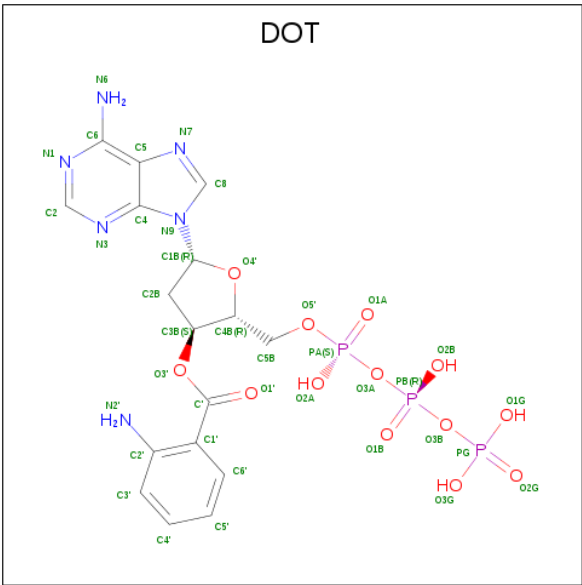
- Molecule 2 is a protein called calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	E	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	F	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			

- Molecule 3 is YTTERBIUM (III) ION (three-letter code: YB) (formula: Yb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Yb	0	0
			1	1		
3	A	1	Total	Yb	0	0
			1	1		
3	C	1	Total	Yb	0	0
			1	1		

- Molecule 4 is 3'ANTHRANILOYL-2'-DEOXY-ADENOSINE-5'-TRIPHOSPHATE (three-letter code: DOT) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			39	17	6	13	3		
4	C	1	Total	C	N	O	P	0	0
			39	17	6	13	3		

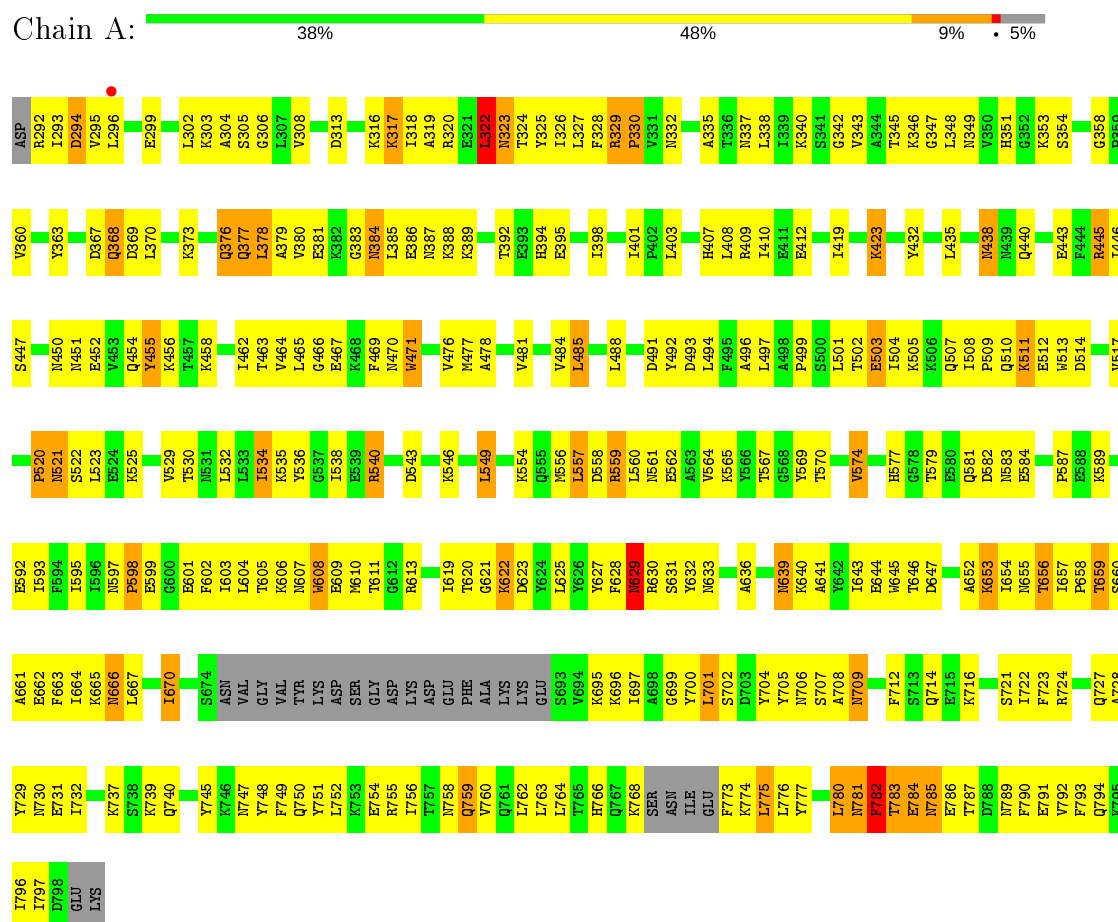
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	2	Total	Ca	0	0
			2	2		
5	F	2	Total	Ca	0	0
			2	2		
5	E	2	Total	Ca	0	0
			2	2		

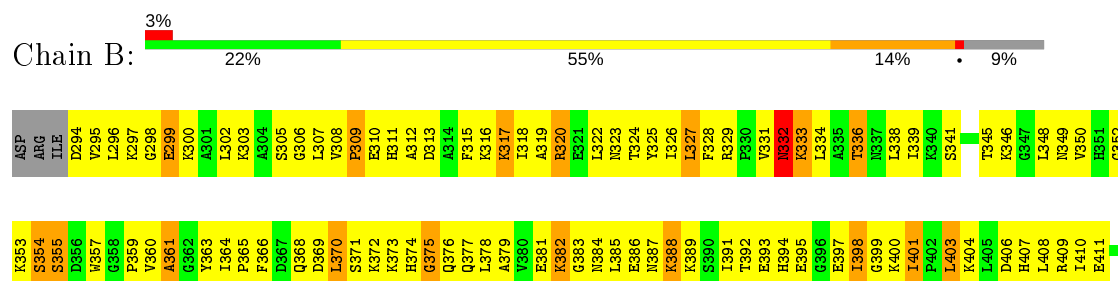
### 3 Residue-property plots

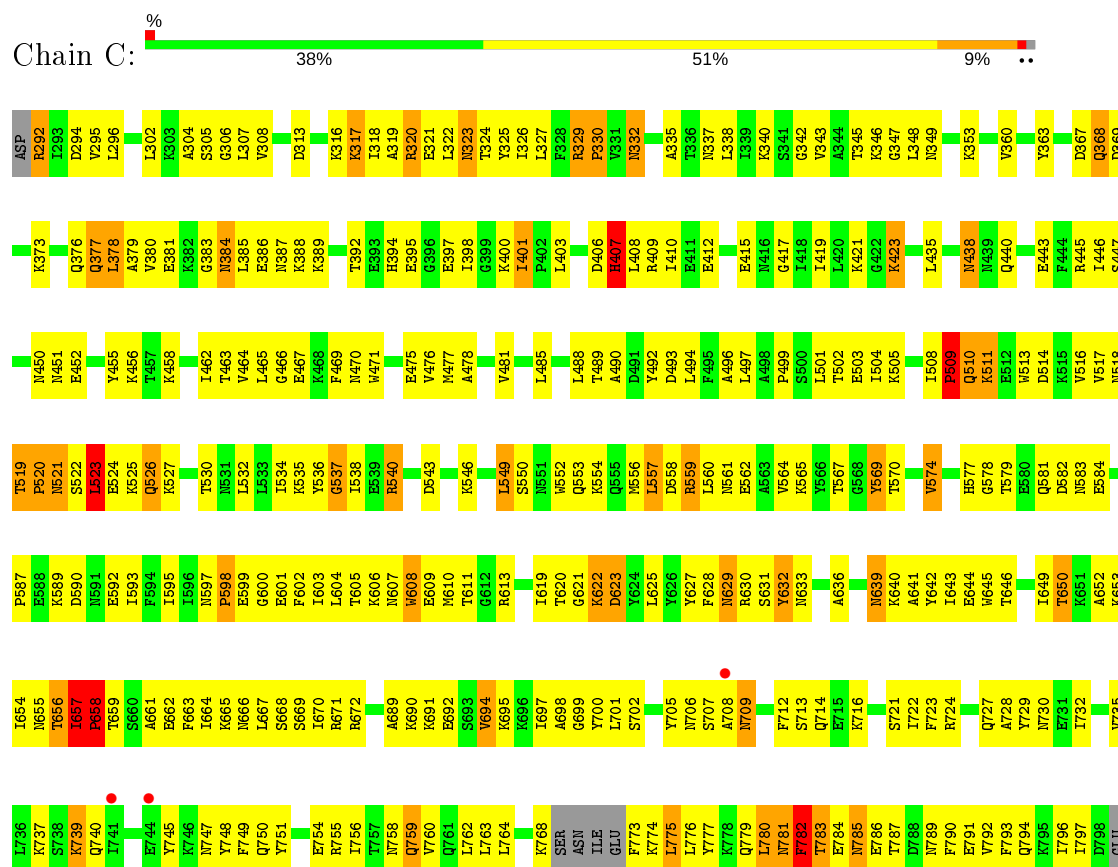
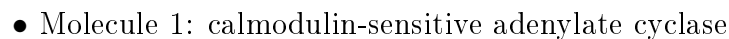
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: calmodulin-sensitive adenylate cyclase



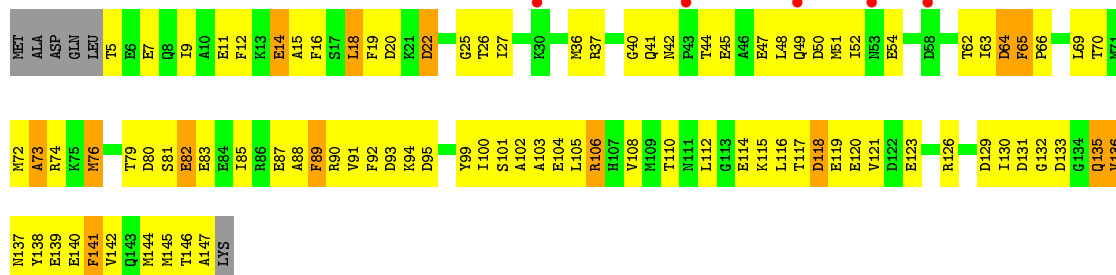
- Molecule 1: calmodulin-sensitive adenylate cyclase



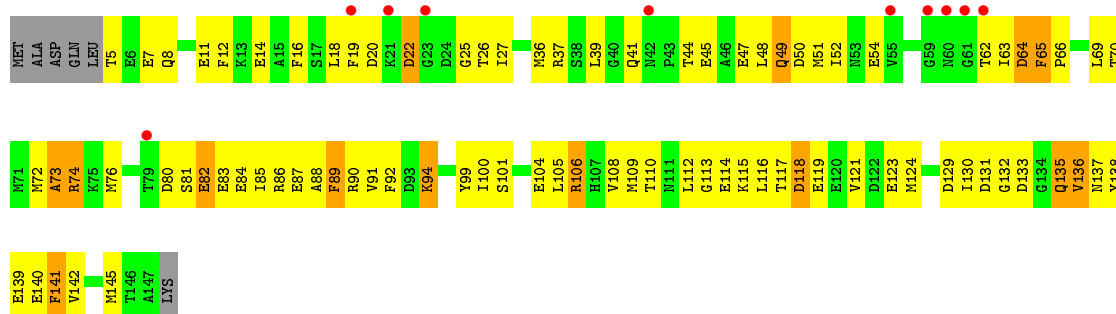


LYS

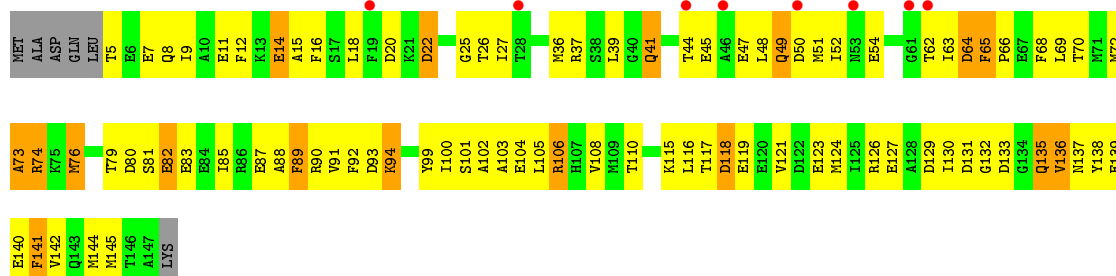
- Molecule 2: calmodulin



- Molecule 2: calmodulin



- Molecule 2: calmodulin



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.92Å 167.92Å 341.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.60 29.95 – 3.60	Depositor EDS
% Data completeness (in resolution range)	90.6 (29.96-3.60) 95.9 (29.95-3.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.00 (at 3.65Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.281 , 0.307 0.253 , 0.285	Depositor DCC
$R_{free}$ test set	1945 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	98.5	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 67.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	15302	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, YB, DOT

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	0.49	0/4027	0.82	13/5419 (0.2%)
1	B	0.51	0/3867	0.78	9/5204 (0.2%)
1	C	0.51	1/4172 (0.0%)	0.82	16/5613 (0.3%)
2	D	0.38	0/1137	0.59	2/1527 (0.1%)
2	E	0.40	0/1137	0.61	2/1527 (0.1%)
2	F	0.37	0/1137	0.74	3/1527 (0.2%)
All	All	0.48	1/15477 (0.0%)	0.78	45/20817 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	658	PRO	CA-C	-5.34	1.42	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	106	ARG	NE-CZ-NH1	-14.10	113.25	120.30
2	F	106	ARG	NE-CZ-NH2	13.51	127.06	120.30
1	A	613	ARG	NE-CZ-NH1	-11.05	114.77	120.30
1	C	613	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	C	613	ARG	NE-CZ-NH1	10.64	125.62	120.30
1	A	613	ARG	NE-CZ-NH2	10.42	125.51	120.30
1	A	785	ASN	CA-C-N	9.67	138.46	117.20
1	C	320	ARG	NE-CZ-NH1	-9.11	115.74	120.30
1	A	320	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	C	320	ARG	NE-CZ-NH2	8.95	124.78	120.30
1	A	320	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	B	538	ILE	CB-CA-C	-8.57	94.47	111.60
1	C	509	PRO	CA-N-CD	-8.35	99.81	111.50
1	A	785	ASN	O-C-N	-7.76	110.28	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	632	TYR	C-N-CA	-7.74	102.35	121.70
2	D	106	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	B	738	SER	N-CA-C	-7.36	91.12	111.00
2	E	106	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	A	785	ASN	C-N-CA	-7.33	103.38	121.70
2	E	106	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	C	785	ASN	N-CA-C	7.17	130.35	111.00
1	A	740	GLN	N-CA-C	-6.95	92.25	111.00
2	D	106	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	C	783	THR	C-N-CA	-6.65	105.07	121.70
1	A	322	LEU	N-CA-C	-6.58	93.24	111.00
1	C	658	PRO	CA-N-CD	-6.58	102.29	111.50
2	F	106	ARG	CD-NE-CZ	6.58	132.81	123.60
1	C	632	TYR	CA-C-N	6.50	131.50	117.20
1	B	470	ASN	CA-C-N	6.17	130.78	117.20
1	B	375	GLY	C-N-CA	-6.10	106.46	121.70
1	B	739	LYS	N-CA-C	5.85	126.80	111.00
1	A	783	THR	CA-C-N	5.84	130.05	117.20
1	C	613	ARG	CD-NE-CZ	5.55	131.37	123.60
1	C	689	ALA	N-CA-C	5.50	125.84	111.00
1	C	632	TYR	O-C-N	-5.47	113.94	122.70
1	B	470	ASN	O-C-N	-5.47	113.95	122.70
1	C	784	GLU	C-N-CA	-5.44	108.11	121.70
1	B	470	ASN	C-N-CA	-5.44	108.11	121.70
1	C	783	THR	CA-C-N	5.38	129.04	117.20
1	A	783	THR	C-N-CA	-5.36	108.29	121.70
1	A	783	THR	N-CA-C	5.28	125.25	111.00
1	B	542	PRO	CA-N-CD	-5.22	104.19	111.50
1	A	782	PHE	N-CA-C	-5.15	97.09	111.00
1	C	782	PHE	N-CA-C	-5.10	97.23	111.00
1	B	493	ASP	CB-CG-OD1	5.06	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3952	0	3999	403	0
1	B	3794	0	3828	500	0
1	C	4094	0	4134	394	0
2	D	1125	0	1049	113	0
2	E	1125	0	1049	103	0
2	F	1125	0	1049	109	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	39	0	17	8	0
4	C	39	0	17	5	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
All	All	15302	0	15142	1552	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 52.

All (1552) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:ASN:ND2	1:B:631:SER:H	1.14	1.44
1:C:456:LYS:HB2	1:C:470:ASN:O	1.22	1.34
1:C:456:LYS:CB	1:C:470:ASN:O	1.84	1.24
1:C:659:THR:HG22	1:C:661:ALA:H	1.08	1.14
1:A:456:LYS:HB2	1:A:470:ASN:O	1.46	1.11
1:B:629:ASN:ND2	1:B:631:SER:N	1.98	1.10
1:A:632:TYR:O	1:A:643:ILE:O	1.69	1.09
1:B:376:GLN:HB2	1:B:379:ALA:HB3	1.33	1.08
1:A:666:ASN:O	1:A:670:ILE:HB	1.52	1.07
1:B:538:ILE:HG22	1:B:538:ILE:O	1.52	1.06
1:A:456:LYS:CB	1:A:470:ASN:O	2.02	1.06
1:B:353:LYS:H	1:B:368:GLN:NE2	1.55	1.04
1:B:581:GLN:NE2	1:B:629:ASN:H	1.55	1.04
1:A:705:TYR:CE2	2:D:139:GLU:HB3	1.93	1.04
1:C:629:ASN:ND2	1:C:631:SER:H	1.56	1.03
1:A:759:GLN:HA	1:A:759:GLN:HE21	1.21	1.03
1:C:510:GLN:O	1:C:514:ASP:OD1	1.77	1.03
4:C:1999:DOT:O1'	4:C:1999:DOT:N2'	1.93	1.02
1:A:633:ASN:HD21	1:A:645:TRP:H	1.09	1.01
1:B:348:LEU:HD21	1:B:577:HIS:HB3	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:ASN:ND2	1:A:631:SER:H	1.57	1.00
1:A:605:THR:HG21	1:A:611:THR:HA	1.43	1.00
1:C:759:GLN:HA	1:C:759:GLN:HE21	1.21	0.99
1:C:605:THR:HG21	1:C:611:THR:HA	1.44	0.99
1:A:295:VAL:HG21	1:A:603:ILE:HG22	1.44	0.99
1:C:664:ILE:HG21	2:F:15:ALA:HB2	1.45	0.99
1:B:629:ASN:HD22	1:B:631:SER:N	1.60	0.98
1:B:456:LYS:HB2	1:B:470:ASN:O	1.63	0.98
1:B:353:LYS:N	1:B:368:GLN:HE22	1.62	0.97
1:B:657:ILE:HG12	1:B:658:PRO:HD2	1.47	0.96
1:C:295:VAL:HG21	1:C:603:ILE:HG22	1.45	0.96
4:A:999:DOT:O1'	4:A:999:DOT:N2'	1.92	0.96
1:B:777:TYR:HD1	1:B:780:LEU:HD12	1.30	0.95
1:B:581:GLN:HE21	1:B:629:ASN:H	1.10	0.95
1:C:510:GLN:C	1:C:514:ASP:OD1	2.05	0.95
1:B:456:LYS:CB	1:B:470:ASN:O	2.16	0.94
1:A:324:THR:HG21	1:A:556:MET:HE1	1.49	0.94
2:E:25:GLY:HA3	2:E:65:PHE:CE1	2.03	0.94
1:A:695:LYS:HB2	2:D:18:LEU:HD22	1.49	0.93
1:C:633:ASN:HD21	1:C:645:TRP:H	1.15	0.93
1:B:538:ILE:CG2	1:B:538:ILE:O	2.15	0.93
1:A:629:ASN:HD22	1:A:631:SER:H	1.10	0.93
1:A:324:THR:HG21	1:A:556:MET:CE	1.99	0.93
2:D:25:GLY:HA3	2:D:65:PHE:CE1	2.04	0.93
1:B:322:LEU:O	1:B:324:THR:HG23	1.70	0.91
1:B:376:GLN:HB2	1:B:379:ALA:CB	2.01	0.91
2:F:25:GLY:HA3	2:F:65:PHE:CE1	2.06	0.91
1:B:606:LYS:H	1:B:610:MET:HE2	1.34	0.90
1:C:657:ILE:HD13	1:C:756:ILE:HD13	1.54	0.89
1:B:360:VAL:HG11	1:B:365:PRO:HG3	1.54	0.89
1:B:587:PRO:HD2	1:B:639:ASN:HD21	1.36	0.89
1:A:559:ARG:HH11	1:A:559:ARG:HB3	1.38	0.89
1:A:639:ASN:ND2	1:A:641:ALA:H	1.70	0.89
1:B:516:VAL:HA	1:B:520:PRO:HG2	1.55	0.89
1:A:521:ASN:ND2	1:A:522:SER:H	1.69	0.89
1:C:705:TYR:CE2	2:F:139:GLU:HB3	2.08	0.88
1:B:296:LEU:HD12	1:B:604:LEU:HD22	1.55	0.88
1:B:509:PRO:HG2	1:B:512:GLU:HB3	1.55	0.88
1:C:659:THR:HG22	1:C:661:ALA:N	1.88	0.88
1:B:518:ASN:C	1:B:520:PRO:HD3	1.94	0.88
1:C:622:LYS:HA	1:C:622:LYS:HE3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:20:ASP:OD2	2:E:22:ASP:HB2	1.74	0.88
1:B:514:ASP:HA	1:B:517:VAL:HG12	1.56	0.87
1:B:709:ASN:HD21	1:B:720:ILE:HD11	1.38	0.87
1:B:654:ILE:HA	1:B:755:ARG:CD	2.04	0.87
1:B:561:ASN:O	1:B:564:VAL:HG22	1.74	0.87
2:D:20:ASP:OD2	2:D:22:ASP:HB2	1.75	0.87
1:A:712:PHE:HD2	1:A:716:LYS:HG2	1.38	0.86
2:E:100:ILE:HB	2:E:136:VAL:HG23	1.56	0.86
1:A:513:TRP:CD2	1:A:517:VAL:HG21	2.09	0.86
1:B:717:LYS:HD2	2:E:132:GLY:N	1.91	0.86
1:C:657:ILE:HG13	1:C:759:GLN:HG2	1.57	0.86
1:A:522:SER:O	1:A:525:LYS:HB3	1.76	0.86
1:C:639:ASN:ND2	1:C:641:ALA:H	1.73	0.86
2:F:100:ILE:HB	2:F:136:VAL:HG23	1.55	0.86
2:F:20:ASP:OD2	2:F:22:ASP:HB2	1.75	0.85
1:C:712:PHE:HD2	1:C:716:LYS:HG2	1.41	0.85
1:B:756:ILE:O	1:B:760:VAL:HG23	1.76	0.85
1:C:540:ARG:NH2	1:C:627:TYR:CD1	2.45	0.85
1:B:779:GLN:NE2	1:B:796:ILE:HG13	1.92	0.84
1:A:525:LYS:O	1:A:529:VAL:HG23	1.76	0.84
1:C:694:VAL:HG23	1:C:695:LYS:H	1.41	0.84
1:B:391:ILE:HD12	1:B:399:GLY:HA2	1.59	0.84
1:C:456:LYS:HB3	1:C:470:ASN:O	1.74	0.84
1:A:712:PHE:CD2	1:A:716:LYS:HG2	2.13	0.84
1:B:625:LEU:HD23	1:B:626:TYR:N	1.93	0.83
1:B:308:VAL:HB	1:B:311:HIS:CD2	2.13	0.83
2:D:100:ILE:HB	2:D:136:VAL:HG23	1.58	0.83
1:B:728:ALA:HA	1:B:731:GLU:HG3	1.60	0.83
1:B:734:ASN:C	1:B:736:LEU:H	1.77	0.83
1:B:629:ASN:HD21	1:B:631:SER:H	1.22	0.83
1:A:747:ASN:O	1:A:750:GLN:HG2	1.79	0.82
1:A:695:LYS:HG3	2:D:18:LEU:HD13	1.61	0.82
1:C:747:ASN:O	1:C:750:GLN:HG2	1.79	0.82
2:F:36:MET:O	2:F:41:GLN:HB2	1.79	0.82
1:A:445:ARG:CZ	1:A:471:TRP:NE1	2.43	0.81
1:B:629:ASN:HD21	1:B:631:SER:HB2	1.43	0.81
1:B:728:ALA:HA	1:B:731:GLU:CG	2.10	0.81
1:B:324:THR:HG22	1:B:499:PRO:HA	1.61	0.81
1:C:510:GLN:HG3	1:C:510:GLN:O	1.80	0.81
1:C:712:PHE:CD2	1:C:716:LYS:HG2	2.15	0.81
1:A:657:ILE:HD11	1:A:704:TYR:CE1	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:ASN:HD22	1:B:631:SER:H	0.83	0.81
1:B:649:ILE:O	1:B:649:ILE:HG22	1.80	0.81
1:A:445:ARG:HG3	1:A:471:TRP:CZ2	2.15	0.80
1:A:540:ARG:NH2	1:A:627:TYR:CD1	2.49	0.80
1:B:527:LYS:O	1:B:531:ASN:HB2	1.81	0.80
1:A:445:ARG:HH22	1:A:456:LYS:HD3	1.45	0.80
1:C:377:GLN:HA	1:C:380:VAL:HG12	1.64	0.80
2:E:36:MET:O	2:E:41:GLN:HB2	1.81	0.80
1:A:714:GLN:NE2	2:D:126:ARG:HG3	1.97	0.79
1:C:633:ASN:HD21	1:C:645:TRP:N	1.79	0.79
1:B:543:ASP:OD1	1:B:544:SER:N	2.14	0.79
1:B:577:HIS:CD2	1:B:577:HIS:H	1.99	0.79
1:B:706:ASN:ND2	1:B:708:ALA:HB3	1.97	0.79
1:A:445:ARG:NH2	1:A:456:LYS:HD3	1.96	0.79
1:A:622:LYS:HE3	1:A:622:LYS:HA	1.65	0.79
1:B:332:ASN:C	1:B:332:ASN:HD22	1.86	0.79
1:A:348:LEU:HD23	1:A:348:LEU:O	1.82	0.78
1:C:559:ARG:HH11	1:C:559:ARG:HB3	1.45	0.78
1:C:629:ASN:HD22	1:C:631:SER:H	1.26	0.78
1:B:654:ILE:HA	1:B:755:ARG:HD2	1.64	0.78
1:A:492:TYR:CD2	1:A:574:VAL:HG13	2.19	0.78
1:B:550:SER:H	1:B:553:GLN:HG3	1.47	0.78
1:B:391:ILE:CD1	1:B:399:GLY:HA2	2.14	0.78
1:C:318:ILE:HD12	1:C:318:ILE:H	1.48	0.78
1:B:706:ASN:HD21	1:B:708:ALA:HB3	1.48	0.78
1:A:629:ASN:HD22	1:A:631:SER:N	1.81	0.77
1:B:731:GLU:OE2	1:B:733:GLU:HB2	1.84	0.77
1:B:597:ASN:ND2	1:B:601:GLU:HB2	1.99	0.77
1:B:581:GLN:HE21	1:B:629:ASN:N	1.82	0.77
1:B:779:GLN:HE22	1:B:796:ILE:HG13	1.48	0.77
1:B:565:LYS:O	1:B:567:THR:N	2.18	0.77
1:B:626:TYR:CD2	1:B:627:TYR:N	2.53	0.77
1:A:445:ARG:HG3	1:A:471:TRP:CH2	2.20	0.77
1:B:394:HIS:O	1:B:397:GLU:HG2	1.85	0.77
2:D:36:MET:O	2:D:41:GLN:HB2	1.85	0.76
1:A:657:ILE:HD11	1:A:704:TYR:CZ	2.21	0.76
1:B:615:ILE:HD12	1:B:645:TRP:CH2	2.20	0.76
1:A:657:ILE:CG2	1:A:756:ILE:HD13	2.16	0.76
1:B:709:ASN:OD1	1:B:717:LYS:HG3	1.85	0.76
1:B:712:PHE:HD1	1:B:712:PHE:H	1.34	0.76
1:C:729:TYR:HB2	1:C:756:ILE:HG21	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:TYR:HB2	1:A:756:ILE:HG21	1.65	0.76
1:A:318:ILE:H	1:A:318:ILE:HD12	1.47	0.76
1:B:657:ILE:HG12	1:B:658:PRO:CD	2.16	0.76
1:A:492:TYR:HD2	1:A:574:VAL:HG13	1.51	0.76
1:A:377:GLN:HA	1:A:380:VAL:HG12	1.67	0.75
1:A:581:GLN:HE21	1:A:629:ASN:H	1.32	0.75
1:C:633:ASN:ND2	1:C:644:GLU:HA	2.02	0.75
1:C:492:TYR:CD2	1:C:574:VAL:HG13	2.21	0.75
1:C:794:GLN:O	1:C:797:ILE:HG13	1.85	0.75
1:C:348:LEU:O	1:C:348:LEU:HD23	1.85	0.75
1:A:794:GLN:O	1:A:797:ILE:HG13	1.87	0.75
1:B:353:LYS:H	1:B:368:GLN:HE22	0.81	0.75
1:B:463:THR:HG23	1:B:467:GLU:O	1.86	0.74
1:B:506:LYS:NZ	1:B:506:LYS:HB3	2.01	0.74
1:B:560:LEU:O	1:B:564:VAL:HG13	1.87	0.74
1:C:360:VAL:HG22	1:C:360:VAL:O	1.87	0.74
1:C:629:ASN:HD22	1:C:631:SER:N	1.84	0.74
1:C:493:ASP:OD2	1:C:577:HIS:HE1	1.70	0.74
1:C:629:ASN:ND2	1:C:631:SER:N	2.34	0.74
1:C:632:TYR:O	1:C:643:ILE:O	2.05	0.74
1:A:657:ILE:CG2	1:A:756:ILE:HA	2.17	0.74
1:B:308:VAL:HB	1:B:311:HIS:HD2	1.52	0.74
1:B:626:TYR:HD2	1:B:627:TYR:N	1.85	0.74
1:A:456:LYS:HB3	1:A:470:ASN:O	1.85	0.74
1:C:722:ILE:HD13	1:C:764:LEU:HD23	1.69	0.74
1:C:700:TYR:HB3	1:C:728:ALA:HB2	1.67	0.74
1:A:493:ASP:OD2	1:A:577:HIS:CE1	2.40	0.74
1:A:639:ASN:C	1:A:639:ASN:HD22	1.91	0.74
1:A:759:GLN:HE21	1:A:759:GLN:CA	1.97	0.74
1:B:710:HIS:CE1	1:B:711:ILE:HG23	2.23	0.74
1:A:360:VAL:O	1:A:360:VAL:HG22	1.85	0.74
1:A:581:GLN:NE2	1:A:628:PHE:HA	2.03	0.73
1:B:747:ASN:O	1:B:751:TYR:HB2	1.87	0.73
1:B:777:TYR:CD1	1:B:780:LEU:HD12	2.20	0.73
1:B:779:GLN:OE1	1:B:796:ILE:HG21	1.87	0.73
1:C:516:VAL:O	1:C:516:VAL:HG12	1.86	0.73
1:C:324:THR:HG21	1:C:556:MET:CE	2.17	0.73
1:B:745:TYR:HB3	1:B:749:PHE:HE1	1.51	0.73
1:A:722:ILE:HD13	1:A:764:LEU:HD23	1.68	0.73
1:B:366:PHE:HA	1:B:477:MET:CE	2.18	0.73
1:C:759:GLN:CA	1:C:759:GLN:HE21	1.97	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:70:THR:O	2:E:73:ALA:HB3	1.88	0.73
1:B:312:ALA:O	1:B:315:PHE:HB2	1.87	0.73
1:B:650:THR:HA	1:B:653:LYS:HB2	1.70	0.73
1:C:324:THR:HG21	1:C:556:MET:HE1	1.71	0.73
1:A:322:LEU:HD12	1:A:322:LEU:N	2.04	0.72
1:A:493:ASP:OD2	1:A:577:HIS:HE1	1.72	0.72
1:B:606:LYS:H	1:B:610:MET:CE	2.02	0.72
1:C:629:ASN:HB3	1:C:632:TYR:CD2	2.24	0.72
1:B:565:LYS:C	1:B:567:THR:H	1.90	0.72
2:E:25:GLY:HA3	2:E:65:PHE:HE1	1.51	0.72
2:F:106:ARG:O	2:F:110:THR:HG23	1.90	0.72
2:E:106:ARG:O	2:E:110:THR:HG23	1.89	0.72
1:C:581:GLN:HE21	1:C:629:ASN:H	1.35	0.72
1:C:581:GLN:NE2	1:C:629:ASN:H	1.86	0.72
1:C:639:ASN:HD22	1:C:639:ASN:C	1.91	0.72
2:D:44:THR:HG22	2:D:47:GLU:HG3	1.71	0.72
1:B:540:ARG:NH2	1:B:630:ARG:CZ	2.53	0.71
1:C:518:ASN:O	1:C:519:THR:HB	1.90	0.71
1:B:657:ILE:CG1	1:B:658:PRO:HD2	2.19	0.71
1:C:523:LEU:HD21	2:F:127:GLU:HB3	1.72	0.71
1:C:748:TYR:O	1:C:751:TYR:HB3	1.90	0.71
2:F:81:SER:O	2:F:83:GLU:N	2.23	0.71
1:C:621:GLY:O	2:F:94:LYS:HE3	1.90	0.71
1:A:657:ILE:HG22	1:A:756:ILE:HA	1.73	0.71
1:B:332:ASN:ND2	1:B:334:LEU:H	1.87	0.71
1:B:456:LYS:HB3	1:B:470:ASN:O	1.91	0.71
1:B:470:ASN:OD1	1:B:471:TRP:N	2.23	0.71
1:B:526:GLN:H	1:B:526:GLN:CD	1.94	0.71
1:B:530:THR:HG22	2:E:92:PHE:CZ	2.25	0.71
1:B:697:ILE:HD13	1:B:732:ILE:CD1	2.21	0.71
1:A:351:HIS:CD2	4:A:999:DOT:H3B	2.26	0.71
1:C:401:ILE:HD13	1:C:478:ALA:HB2	1.73	0.71
2:E:44:THR:HG22	2:E:47:GLU:HG3	1.72	0.71
1:A:581:GLN:NE2	1:A:629:ASN:H	1.88	0.71
2:E:81:SER:O	2:E:83:GLU:N	2.24	0.71
1:B:777:TYR:HD1	1:B:780:LEU:CD1	2.02	0.71
1:C:318:ILE:HG23	1:C:322:LEU:HD13	1.73	0.71
1:C:759:GLN:HA	1:C:759:GLN:NE2	2.01	0.70
1:A:445:ARG:HH12	1:A:456:LYS:HB3	1.56	0.70
1:A:513:TRP:O	1:A:517:VAL:HG23	1.91	0.70
2:E:65:PHE:HB2	2:E:66:PRO:HD3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:65:PHE:HB2	2:F:66:PRO:HD3	1.74	0.70
1:B:363:TYR:O	1:B:365:PRO:HD3	1.92	0.70
1:B:540:ARG:NH1	2:E:87:GLU:OE1	2.24	0.70
1:C:723:PHE:HB2	1:C:793:PHE:CE2	2.26	0.70
2:D:106:ARG:O	2:D:110:THR:HG23	1.92	0.70
2:D:25:GLY:HA3	2:D:65:PHE:HE1	1.54	0.70
1:C:633:ASN:HD22	1:C:644:GLU:HA	1.57	0.70
1:A:633:ASN:ND2	1:A:645:TRP:H	1.87	0.70
2:D:25:GLY:O	2:D:64:ASP:HA	1.92	0.70
2:D:70:THR:O	2:D:73:ALA:HB3	1.92	0.70
1:C:540:ARG:HB3	1:C:549:LEU:C	2.12	0.70
1:C:446:ILE:HG12	1:C:447:SER:N	2.07	0.69
2:D:65:PHE:HB2	2:D:66:PRO:HD3	1.73	0.69
2:E:89:PHE:CD2	2:E:89:PHE:C	2.65	0.69
2:F:44:THR:HG22	2:F:47:GLU:HG3	1.74	0.69
1:B:540:ARG:NH2	1:B:630:ARG:NH2	2.40	0.69
1:B:727:GLN:HG3	1:B:786:GLU:CD	2.13	0.69
1:A:445:ARG:HH22	1:A:456:LYS:CD	2.06	0.69
1:B:385:LEU:HA	1:B:388:LYS:HD3	1.74	0.69
1:B:585:GLU:O	1:B:638:GLY:HA3	1.93	0.69
1:B:349:ASN:OD1	1:B:350:VAL:HG23	1.93	0.69
1:A:782:PHE:H	1:A:782:PHE:HD1	1.39	0.69
1:B:376:GLN:CB	1:B:379:ALA:HB3	2.17	0.69
1:C:782:PHE:HD1	1:C:782:PHE:H	1.39	0.69
2:F:25:GLY:HA3	2:F:65:PHE:HE1	1.55	0.69
1:A:723:PHE:HB2	1:A:793:PHE:CE2	2.27	0.69
1:B:478:ALA:HB1	1:B:486:LYS:O	1.92	0.69
1:C:367:ASP:O	1:C:369:ASP:N	2.26	0.69
1:C:492:TYR:HD2	1:C:574:VAL:HG13	1.54	0.69
2:D:133:ASP:OD1	2:D:135:GLN:HG3	1.93	0.69
1:C:501:LEU:O	1:C:504:ILE:HG22	1.93	0.68
2:D:89:PHE:CD2	2:D:89:PHE:C	2.66	0.68
2:F:89:PHE:CD2	2:F:89:PHE:C	2.66	0.68
1:A:477:MET:O	1:A:488:LEU:HD12	1.93	0.68
1:A:657:ILE:HG22	1:A:756:ILE:HD13	1.75	0.68
1:B:525:LYS:HB2	1:B:526:GLN:NE2	2.07	0.68
1:B:653:LYS:O	1:B:755:ARG:HD3	1.93	0.68
2:D:48:LEU:O	2:D:52:ILE:HG22	1.92	0.68
2:F:25:GLY:O	2:F:64:ASP:HA	1.93	0.68
1:C:657:ILE:HD13	1:C:756:ILE:CD1	2.23	0.68
1:A:748:TYR:O	1:A:751:TYR:HB3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:GLN:HA	1:A:759:GLN:NE2	2.01	0.68
1:A:782:PHE:N	1:A:782:PHE:CD1	2.61	0.68
2:D:136:VAL:HA	2:D:140:GLU:OE1	1.92	0.68
1:B:454:GLN:HB3	1:B:472:ARG:O	1.93	0.68
1:C:782:PHE:N	1:C:782:PHE:CD1	2.62	0.68
1:C:793:PHE:O	1:C:796:ILE:HG12	1.94	0.68
2:F:70:THR:O	2:F:73:ALA:HB3	1.93	0.68
1:B:432:TYR:CD2	1:B:447:SER:HA	2.28	0.68
1:B:748:TYR:O	1:B:752:LEU:HG	1.92	0.68
1:C:508:ILE:HD13	1:C:532:LEU:HB3	1.75	0.68
1:B:720:ILE:HD12	1:B:721:SER:N	2.08	0.68
1:C:445:ARG:NH1	1:C:471:TRP:CD1	2.62	0.68
1:C:665:LYS:HE2	2:F:11:GLU:OE2	1.92	0.68
1:A:446:ILE:HG12	1:A:447:SER:N	2.09	0.68
1:A:501:LEU:O	1:A:504:ILE:HG22	1.94	0.68
1:C:514:ASP:HA	1:C:517:VAL:HG12	1.76	0.68
1:C:463:THR:HG22	1:C:465:LEU:H	1.59	0.68
1:C:690:LYS:HG2	1:C:691:LYS:O	1.94	0.68
1:B:615:ILE:HD13	1:B:626:TYR:CE1	2.28	0.67
1:B:596:ILE:HG12	1:B:602:PHE:CE2	2.29	0.67
2:F:48:LEU:O	2:F:52:ILE:HG22	1.95	0.67
1:A:313:ASP:HA	1:A:316:LYS:HE2	1.77	0.67
1:B:462:ILE:HD11	1:B:466:GLY:HA2	1.76	0.67
1:C:313:ASP:HA	1:C:316:LYS:HE2	1.77	0.67
2:F:136:VAL:HA	2:F:140:GLU:OE1	1.95	0.67
1:A:367:ASP:O	1:A:369:ASP:N	2.28	0.67
1:A:388:LYS:O	1:A:392:THR:HG23	1.95	0.67
1:B:366:PHE:HA	1:B:477:MET:HE3	1.77	0.67
1:B:734:ASN:O	1:B:736:LEU:N	2.28	0.67
1:B:747:ASN:O	1:B:751:TYR:CB	2.43	0.67
1:B:760:VAL:O	1:B:764:LEU:HG	1.95	0.67
1:C:712:PHE:HB3	1:C:716:LYS:HG2	1.75	0.67
1:B:388:LYS:O	1:B:392:THR:HG23	1.94	0.67
1:B:734:ASN:C	1:B:736:LEU:N	2.48	0.67
1:B:432:TYR:HE2	1:B:447:SER:HB2	1.59	0.66
1:A:793:PHE:O	1:A:796:ILE:HG12	1.94	0.66
1:C:561:ASN:O	1:C:565:LYS:HG3	1.96	0.66
2:E:48:LEU:O	2:E:52:ILE:HG22	1.95	0.66
1:A:295:VAL:HG21	1:A:603:ILE:CG2	2.22	0.66
1:B:746:LYS:O	1:B:750:GLN:N	2.29	0.66
1:C:654:ILE:O	1:C:755:ARG:HG2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:25:GLY:O	2:E:64:ASP:HA	1.94	0.66
1:A:463:THR:HG22	1:A:465:LEU:N	2.10	0.66
1:A:561:ASN:O	1:A:565:LYS:HG3	1.96	0.66
1:A:295:VAL:CG2	1:A:603:ILE:HG22	2.22	0.66
1:C:758:ASN:O	1:C:762:LEU:HB2	1.95	0.66
1:A:540:ARG:HB3	1:A:549:LEU:C	2.16	0.66
1:A:700:TYR:HD1	1:A:728:ALA:HA	1.58	0.66
1:A:337:ASN:HB3	1:A:412:GLU:OE2	1.95	0.66
1:C:463:THR:HG22	1:C:465:LEU:N	2.10	0.66
2:D:101:SER:OG	2:D:104:GLU:HG3	1.96	0.66
1:A:670:ILE:HD12	1:A:745:TYR:CE1	2.31	0.66
1:B:324:THR:CG2	1:B:499:PRO:HA	2.26	0.66
1:B:616:GLU:HA	1:B:620:THR:HG22	1.78	0.66
2:D:81:SER:O	2:D:83:GLU:N	2.29	0.66
1:B:792:VAL:O	1:B:792:VAL:HG12	1.96	0.65
1:C:388:LYS:O	1:C:392:THR:HG23	1.96	0.65
1:A:705:TYR:HE2	2:D:139:GLU:HB3	1.58	0.65
1:C:705:TYR:HE2	2:F:139:GLU:HB3	1.55	0.65
1:B:562:GLU:HA	1:B:565:LYS:HG3	1.77	0.65
1:C:302:LEU:C	1:C:302:LEU:HD23	2.16	0.65
1:C:540:ARG:NH2	1:C:627:TYR:CE1	2.65	0.65
2:E:115:LYS:O	2:E:116:LEU:HD23	1.95	0.65
1:A:758:ASN:O	1:A:762:LEU:HB2	1.96	0.65
2:E:101:SER:OG	2:E:104:GLU:HG3	1.97	0.65
1:A:377:GLN:O	1:A:379:ALA:N	2.29	0.65
1:A:521:ASN:ND2	1:A:522:SER:N	2.44	0.65
1:A:639:ASN:HD22	1:A:641:ALA:H	1.45	0.65
1:B:513:TRP:HH2	2:E:113:GLY:HA3	1.61	0.65
1:A:302:LEU:C	1:A:302:LEU:HD23	2.17	0.65
1:A:401:ILE:HD13	1:A:478:ALA:HB2	1.78	0.65
2:F:81:SER:O	2:F:82:GLU:C	2.35	0.65
1:B:577:HIS:N	1:B:577:HIS:CD2	2.65	0.65
1:A:481:VAL:HG23	1:A:481:VAL:O	1.97	0.65
1:A:633:ASN:HD21	1:A:645:TRP:N	1.88	0.65
1:A:659:THR:OG1	1:A:660:SER:N	2.31	0.65
1:B:629:ASN:HD21	1:B:631:SER:N	1.84	0.65
1:B:722:ILE:HD13	1:B:764:LEU:HD21	1.78	0.65
2:E:92:PHE:CE2	2:E:108:VAL:HG11	2.32	0.65
2:E:81:SER:O	2:E:82:GLU:C	2.35	0.65
1:C:295:VAL:HG21	1:C:603:ILE:CG2	2.24	0.64
1:C:337:ASN:HB3	1:C:412:GLU:OE2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:TRP:CE3	1:A:517:VAL:HG21	2.32	0.64
1:A:656:THR:O	1:A:755:ARG:HD2	1.97	0.64
1:B:306:GLY:O	1:B:336:THR:HB	1.96	0.64
1:C:530:THR:HG21	2:F:145:MET:CE	2.27	0.64
1:C:692:GLU:O	1:C:735:VAL:HG22	1.96	0.64
1:B:615:ILE:HD12	1:B:645:TRP:HH2	1.60	0.64
1:C:353:LYS:HG3	1:C:373:LYS:HD3	1.78	0.64
2:E:92:PHE:CD2	2:E:108:VAL:HG21	2.32	0.64
2:F:140:GLU:O	2:F:142:VAL:N	2.30	0.64
1:C:349:ASN:HD21	1:C:398:ILE:HG13	1.62	0.64
1:C:463:THR:HB	1:C:467:GLU:H	1.63	0.64
1:A:445:ARG:NH2	1:A:471:TRP:NE1	2.45	0.64
1:B:377:GLN:HG2	1:B:378:LEU:HD22	1.80	0.64
1:B:654:ILE:HA	1:B:755:ARG:CG	2.26	0.64
1:C:522:SER:O	1:C:525:LYS:N	2.30	0.64
1:A:353:LYS:HG3	1:A:373:LYS:HD3	1.78	0.64
1:A:663:PHE:CE1	1:A:752:LEU:HD11	2.32	0.64
1:B:332:ASN:C	1:B:332:ASN:ND2	2.49	0.64
1:A:658:PRO:O	1:A:701:LEU:HD13	1.98	0.64
1:B:597:ASN:HD21	1:B:601:GLU:HB2	1.62	0.64
1:A:463:THR:HG22	1:A:465:LEU:H	1.61	0.63
1:A:696:LYS:HA	1:A:696:LYS:HE2	1.80	0.63
1:B:697:ILE:HD13	1:B:732:ILE:HD13	1.80	0.63
2:E:136:VAL:HA	2:E:140:GLU:OE1	1.98	0.63
1:A:633:ASN:HD22	1:A:644:GLU:HA	1.63	0.63
1:C:349:ASN:ND2	1:C:398:ILE:HG13	2.13	0.63
2:E:5:THR:OG1	2:E:8:GLN:HB2	1.98	0.63
1:A:445:ARG:NH2	1:A:471:TRP:HE1	1.95	0.63
1:B:619:ILE:C	1:B:621:GLY:H	2.00	0.63
1:B:712:PHE:CD1	1:B:712:PHE:N	2.66	0.63
1:B:712:PHE:HD1	1:B:712:PHE:N	1.97	0.63
1:B:722:ILE:HD13	1:B:764:LEU:CD2	2.29	0.63
1:B:728:ALA:CA	1:B:731:GLU:HG3	2.28	0.63
1:A:722:ILE:HD13	1:A:764:LEU:CD2	2.28	0.63
1:C:622:LYS:O	1:C:623:ASP:HB2	1.97	0.63
1:B:320:ARG:HG3	1:B:320:ARG:HH21	1.64	0.63
1:B:360:VAL:CG1	1:B:365:PRO:HG3	2.28	0.63
1:B:407:HIS:H	1:B:407:HIS:CD2	2.16	0.63
1:B:711:ILE:HG13	1:B:712:PHE:CD1	2.34	0.63
1:A:349:ASN:HD21	1:A:398:ILE:HG13	1.62	0.63
1:A:653:LYS:O	1:A:755:ARG:HD3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:TYR:HD2	1:B:447:SER:HA	1.61	0.63
1:B:656:THR:O	1:B:705:TYR:HE1	1.80	0.63
1:A:697:ILE:N	1:A:697:ILE:HD12	2.14	0.63
1:C:508:ILE:HG12	1:C:536:TYR:CD2	2.34	0.63
1:C:653:LYS:O	1:C:656:THR:HG23	1.99	0.63
2:D:99:TYR:CD2	2:D:137:ASN:HB3	2.34	0.62
2:F:115:LYS:O	2:F:116:LEU:HD23	1.99	0.62
1:A:385:LEU:HD13	1:A:385:LEU:O	1.99	0.62
1:B:424:LYS:HE2	1:B:433:TYR:OH	1.98	0.62
1:C:722:ILE:HD13	1:C:764:LEU:CD2	2.29	0.62
1:C:722:ILE:HG23	1:C:760:VAL:HG13	1.81	0.62
1:C:327:LEU:HG	1:C:595:ILE:HG23	1.81	0.62
2:D:115:LYS:O	2:D:116:LEU:HD23	1.99	0.62
1:B:376:GLN:CB	1:B:379:ALA:CB	2.77	0.62
1:B:525:LYS:O	1:B:529:VAL:HG22	1.99	0.62
1:B:777:TYR:CD1	1:B:780:LEU:HB2	2.34	0.62
1:C:324:THR:HG23	1:C:324:THR:O	1.99	0.62
1:C:581:GLN:NE2	1:C:628:PHE:HA	2.14	0.62
2:E:133:ASP:OD1	2:E:135:GLN:HG3	2.00	0.62
2:F:133:ASP:OD1	2:F:135:GLN:HG3	1.99	0.62
1:A:318:ILE:N	1:A:318:ILE:HD12	2.14	0.62
1:B:649:ILE:O	1:B:649:ILE:CG2	2.48	0.62
2:E:140:GLU:O	2:E:142:VAL:N	2.31	0.62
1:B:310:GLU:CD	1:B:310:GLU:H	2.03	0.62
1:B:333:LYS:O	1:B:336:THR:HG22	1.99	0.62
1:C:319:ALA:O	1:C:598:PRO:HA	1.99	0.62
1:C:602:PHE:O	1:C:603:ILE:HD13	1.99	0.62
1:C:700:TYR:CE1	1:C:727:GLN:HG2	2.35	0.62
2:D:81:SER:O	2:D:82:GLU:C	2.37	0.62
1:B:633:ASN:O	1:B:634:LYS:HG3	2.00	0.62
1:B:361:ALA:O	1:B:409:ARG:NH2	2.30	0.62
1:B:419:ILE:HD12	1:B:435:LEU:HD22	1.81	0.62
1:B:445:ARG:HB3	1:B:471:TRP:CZ3	2.35	0.62
1:A:630:ARG:HE	2:D:87:GLU:CD	2.03	0.62
2:F:99:TYR:CD2	2:F:137:ASN:HB3	2.35	0.62
1:B:519:THR:N	1:B:520:PRO:HD3	2.15	0.61
1:B:723:PHE:O	1:B:727:GLN:N	2.30	0.61
1:C:525:LYS:HB2	2:F:124:MET:CE	2.30	0.61
1:A:622:LYS:O	1:A:623:ASP:HB2	2.00	0.61
1:B:514:ASP:HA	1:B:517:VAL:CG1	2.29	0.61
2:F:65:PHE:O	2:F:69:LEU:HG	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:ILE:CD1	2:E:86:ARG:HG3	2.29	0.61
1:B:653:LYS:O	1:B:653:LYS:HG3	1.99	0.61
1:C:481:VAL:HG23	1:C:481:VAL:O	2.00	0.61
1:A:605:THR:CG2	1:A:611:THR:HA	2.25	0.61
1:A:712:PHE:HB3	1:A:716:LYS:HG2	1.81	0.61
1:C:543:ASP:OD2	1:C:546:LYS:HG3	1.99	0.61
1:B:639:ASN:H	1:B:639:ASN:ND2	1.98	0.61
1:B:501:LEU:HB2	1:B:623:ASP:O	2.01	0.61
1:B:722:ILE:HG22	1:B:726:ILE:HD12	1.81	0.61
1:C:377:GLN:O	1:C:379:ALA:N	2.33	0.61
2:E:99:TYR:CD2	2:E:137:ASN:HB3	2.36	0.61
1:B:508:ILE:HG21	1:B:532:LEU:HD22	1.83	0.61
1:C:653:LYS:O	1:C:755:ARG:HD3	2.01	0.61
1:C:385:LEU:HD13	1:C:385:LEU:O	2.01	0.61
1:C:649:ILE:HD13	2:F:90:ARG:HE	1.66	0.61
1:C:663:PHE:HD2	1:C:664:ILE:HD12	1.66	0.61
1:A:349:ASN:ND2	1:A:398:ILE:HG13	2.16	0.61
1:A:792:VAL:HG12	1:A:796:ILE:HD11	1.83	0.61
1:C:657:ILE:HG22	1:C:658:PRO:N	2.16	0.61
1:C:776:LEU:HD12	1:C:776:LEU:N	2.15	0.61
2:F:63:ILE:N	2:F:63:ILE:HD12	2.16	0.61
1:B:535:LYS:C	1:B:536:TYR:HD2	2.03	0.60
1:B:339:ILE:HG12	1:B:489:THR:HG21	1.83	0.60
1:C:535:LYS:HE2	1:C:536:TYR:CZ	2.36	0.60
1:B:459:GLU:O	1:B:461:LYS:N	2.27	0.60
1:C:659:THR:HB	1:C:662:GLU:HG3	1.82	0.60
1:B:565:LYS:C	1:B:567:THR:N	2.55	0.60
1:C:368:GLN:HB2	1:C:384:ASN:OD1	2.02	0.60
2:F:130:ILE:O	2:F:130:ILE:HG22	2.01	0.60
1:A:408:LEU:C	1:A:408:LEU:HD23	2.20	0.60
1:C:324:THR:CG2	1:C:324:THR:O	2.50	0.60
1:C:438:ASN:C	1:C:438:ASN:HD22	2.05	0.60
1:A:299:GLU:HG3	1:A:303:LYS:NZ	2.16	0.60
1:A:445:ARG:CZ	1:A:471:TRP:CD1	2.83	0.60
1:B:319:ALA:HB2	1:B:326:ILE:HD12	1.83	0.60
1:B:346:LYS:NZ	1:B:352:GLY:O	2.34	0.60
1:B:516:VAL:CA	1:B:520:PRO:HG2	2.28	0.60
1:A:538:ILE:HD11	2:D:91:VAL:HG21	1.83	0.60
2:F:7:GLU:O	2:F:11:GLU:HG3	2.02	0.60
1:A:776:LEU:HD12	1:A:776:LEU:N	2.17	0.60
1:A:462:ILE:HD11	1:A:466:GLY:HA2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ARG:HD3	1:A:582:ASP:OD1	2.01	0.59
1:A:587:PRO:HB2	1:A:643:ILE:HD12	1.83	0.59
1:B:318:ILE:HD12	1:B:319:ALA:N	2.18	0.59
1:B:498:ALA:CB	1:B:619:ILE:HD13	2.32	0.59
1:B:615:ILE:HD12	1:B:645:TRP:CZ2	2.37	0.59
2:E:7:GLU:O	2:E:11:GLU:HG3	2.01	0.59
1:A:589:LYS:HE2	1:A:643:ILE:HG23	1.85	0.59
1:B:711:ILE:HG13	1:B:712:PHE:HD1	1.67	0.59
1:C:639:ASN:HD22	1:C:641:ALA:H	1.51	0.59
1:A:787:THR:O	1:A:791:GLU:HG2	2.02	0.59
1:B:369:ASP:OD2	1:B:442:TYR:OH	2.19	0.59
1:B:432:TYR:CE2	1:B:447:SER:HB2	2.37	0.59
1:C:655:ASN:HD22	1:C:655:ASN:N	1.97	0.59
1:A:670:ILE:HG23	1:A:745:TYR:CE1	2.38	0.59
1:C:605:THR:CG2	1:C:611:THR:HA	2.27	0.59
1:C:740:GLN:CD	1:C:740:GLN:H	2.05	0.59
1:B:554:LYS:O	1:B:557:LEU:N	2.35	0.59
1:C:583:ASN:ND2	4:C:1999:DOT:H1'	2.18	0.59
1:C:587:PRO:HB2	1:C:643:ILE:HD12	1.83	0.59
1:A:695:LYS:CB	2:D:18:LEU:HD22	2.30	0.59
1:A:432:TYR:CE1	1:A:471:TRP:HZ3	2.20	0.59
1:B:540:ARG:HH22	1:B:630:ARG:CZ	2.15	0.59
1:C:639:ASN:HD22	1:C:640:LYS:N	2.00	0.59
1:A:592:GLU:HB3	1:A:604:LEU:HD21	1.85	0.59
1:B:629:ASN:HD21	1:B:631:SER:CB	2.14	0.59
1:B:752:LEU:O	1:B:756:ILE:HG13	2.02	0.59
1:A:722:ILE:HG23	1:A:760:VAL:HG13	1.83	0.59
1:B:322:LEU:HA	1:B:503:GLU:OE1	2.02	0.59
1:B:546:LYS:N	1:B:546:LYS:HD2	2.18	0.59
1:B:540:ARG:HD2	1:B:627:TYR:CE1	2.38	0.59
1:B:733:GLU:O	1:B:735:VAL:N	2.35	0.59
1:A:438:ASN:HD22	1:A:438:ASN:C	2.05	0.58
1:A:697:ILE:H	1:A:697:ILE:HD12	1.67	0.58
4:C:1999:DOT:O1'	4:C:1999:DOT:H2'1	2.01	0.58
1:B:606:LYS:N	1:B:610:MET:CE	2.65	0.58
1:C:698:ALA:O	1:C:701:LEU:HB2	2.02	0.58
1:C:792:VAL:HG12	1:C:796:ILE:HD11	1.84	0.58
1:B:605:THR:HG22	1:B:606:LYS:N	2.18	0.58
1:C:295:VAL:HG23	1:C:604:LEU:O	2.02	0.58
1:C:363:TYR:HD1	1:C:403:LEU:HD11	1.68	0.58
1:C:477:MET:O	1:C:488:LEU:HD12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ARG:HG3	1:C:598:PRO:O	2.02	0.58
1:B:761:GLN:OE1	1:B:765:THR:HG23	2.04	0.58
1:C:294:ASP:O	1:C:610:MET:HE1	2.04	0.58
2:D:65:PHE:O	2:D:69:LEU:HG	2.04	0.58
1:A:621:GLY:O	2:D:94:LYS:HE3	2.03	0.58
1:A:454:GLN:OE1	1:A:471:TRP:CE3	2.56	0.58
1:B:728:ALA:HA	1:B:731:GLU:HG2	1.86	0.58
1:C:318:ILE:N	1:C:318:ILE:HD12	2.17	0.58
1:C:659:THR:O	1:C:701:LEU:HD13	2.04	0.58
2:D:63:ILE:N	2:D:63:ILE:HD12	2.19	0.58
1:C:326:ILE:C	1:C:327:LEU:HD12	2.24	0.58
1:C:519:THR:O	1:C:525:LYS:HE2	2.04	0.58
1:C:664:ILE:CG2	2:F:15:ALA:HB2	2.24	0.58
1:B:621:GLY:O	2:E:94:LYS:HE3	2.04	0.58
1:A:322:LEU:HD12	1:A:322:LEU:H	1.68	0.58
1:B:761:GLN:HA	1:B:761:GLN:OE1	2.03	0.58
1:C:450:ASN:O	1:C:451:ASN:HB2	2.04	0.58
2:D:140:GLU:O	2:D:142:VAL:N	2.37	0.58
1:C:558:ASP:O	1:C:562:GLU:HG3	2.03	0.58
2:F:5:THR:O	2:F:9:ILE:HG13	2.03	0.58
1:B:354:SER:O	1:B:371:SER:HB2	2.04	0.57
1:C:304:ALA:HB3	1:C:604:LEU:HD13	1.86	0.57
1:C:584:GLU:OE1	1:C:630:ARG:HG3	2.04	0.57
2:D:133:ASP:OD1	2:D:135:GLN:O	2.22	0.57
1:B:550:SER:N	1:B:553:GLN:HG3	2.19	0.57
1:C:324:THR:OG1	1:C:499:PRO:HA	2.04	0.57
1:C:408:LEU:C	1:C:408:LEU:HD23	2.25	0.57
1:C:697:ILE:HD11	1:C:735:VAL:HG21	1.85	0.57
1:A:295:VAL:HG23	1:A:604:LEU:O	2.04	0.57
1:A:540:ARG:NH1	1:A:630:ARG:HH21	2.03	0.57
1:B:307:LEU:HD21	1:B:328:PHE:CD1	2.40	0.57
1:C:302:LEU:HD12	1:C:602:PHE:HE1	1.69	0.57
2:F:131:ASP:OD1	2:F:133:ASP:OD2	2.22	0.57
1:A:790:PHE:O	1:A:793:PHE:HB3	2.05	0.57
1:C:462:ILE:HD11	1:C:466:GLY:HA2	1.85	0.57
1:B:586:PHE:N	1:B:587:PRO:HD3	2.20	0.57
1:B:657:ILE:CG1	1:B:658:PRO:CD	2.81	0.57
1:B:605:THR:HG21	1:B:611:THR:OG1	2.03	0.57
2:E:65:PHE:O	2:E:69:LEU:HG	2.05	0.57
1:A:583:ASN:ND2	4:A:999:DOT:H1'	2.19	0.57
1:C:450:ASN:OD1	1:C:452:GLU:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:787:THR:O	1:C:791:GLU:HG2	2.05	0.57
1:B:513:TRP:CH2	2:E:113:GLY:HA3	2.40	0.57
1:C:714:GLN:NE2	2:F:126:ARG:HG2	2.20	0.57
1:A:574:VAL:O	1:A:574:VAL:HG13	2.05	0.56
1:C:363:TYR:CD1	1:C:403:LEU:HD11	2.40	0.56
1:C:324:THR:OG1	1:C:499:PRO:CA	2.53	0.56
2:F:137:ASN:OD1	2:F:139:GLU:HB2	2.05	0.56
1:A:781:ASN:ND2	1:A:783:THR:OG1	2.38	0.56
1:B:307:LEU:HD21	1:B:328:PHE:CE1	2.40	0.56
1:B:385:LEU:CD2	1:B:389:LYS:HE2	2.36	0.56
1:C:518:ASN:O	1:C:519:THR:CB	2.54	0.56
1:C:606:LYS:O	1:C:607:ASN:HB3	2.05	0.56
1:C:712:PHE:CD2	1:C:716:LYS:HE2	2.39	0.56
1:A:505:LYS:HD3	2:D:112:LEU:O	2.05	0.56
2:F:92:PHE:CD2	2:F:108:VAL:HG21	2.40	0.56
1:A:712:PHE:CD2	1:A:716:LYS:HE2	2.41	0.56
1:B:327:LEU:HG	1:B:595:ILE:HG23	1.88	0.56
1:B:509:PRO:HD2	1:B:536:TYR:HE1	1.69	0.56
1:B:773:PHE:C	1:B:775:LEU:H	2.08	0.56
1:C:377:GLN:O	1:C:378:LEU:C	2.42	0.56
2:E:133:ASP:OD1	2:E:135:GLN:O	2.23	0.56
1:B:331:VAL:O	1:B:332:ASN:C	2.44	0.56
1:B:562:GLU:O	1:B:564:VAL:N	2.38	0.56
1:B:597:ASN:HB2	1:B:598:PRO:HD2	1.87	0.56
1:B:526:GLN:HE21	2:E:124:MET:HE2	1.67	0.56
1:C:295:VAL:HG22	1:C:296:LEU:N	2.19	0.56
1:A:318:ILE:H	1:A:318:ILE:CD1	2.17	0.56
1:A:378:LEU:HD22	1:B:378:LEU:HD11	1.87	0.56
1:A:318:ILE:HG23	1:A:322:LEU:HD13	1.86	0.56
1:A:509:PRO:HD3	1:A:536:TYR:HE1	1.70	0.56
1:A:581:GLN:HE21	1:A:629:ASN:N	2.03	0.56
1:B:554:LYS:O	1:B:555:GLN:C	2.43	0.56
1:C:639:ASN:ND2	1:C:641:ALA:N	2.50	0.56
1:A:385:LEU:CD1	1:A:389:LYS:HD2	2.36	0.56
1:B:506:LYS:HZ3	1:B:506:LYS:HB3	1.68	0.56
1:B:751:TYR:O	1:B:754:GLU:N	2.39	0.56
1:C:607:ASN:HD21	1:C:609:GLU:HB2	1.71	0.56
2:E:63:ILE:HD12	2:E:63:ILE:N	2.20	0.56
1:A:377:GLN:O	1:A:378:LEU:C	2.44	0.56
1:B:308:VAL:O	1:B:311:HIS:HB2	2.06	0.56
1:A:308:VAL:HG23	1:A:492:TYR:OH	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:TRP:CE2	1:A:517:VAL:HG21	2.41	0.56
1:B:324:THR:HG22	1:B:499:PRO:CA	2.35	0.56
1:B:332:ASN:ND2	1:B:334:LEU:N	2.53	0.56
1:B:720:ILE:HD12	1:B:720:ILE:C	2.26	0.56
2:E:130:ILE:HG22	2:E:130:ILE:O	2.06	0.56
1:C:603:ILE:HG22	1:C:604:LEU:H	1.70	0.55
1:C:697:ILE:HD13	1:C:732:ILE:HG12	1.88	0.55
2:D:7:GLU:O	2:D:11:GLU:HG3	2.05	0.55
1:C:523:LEU:CD2	2:F:127:GLU:HB3	2.36	0.55
1:B:400:LYS:HD2	1:B:475:GLU:OE2	2.05	0.55
1:B:454:GLN:CB	1:B:472:ARG:O	2.54	0.55
1:B:733:GLU:C	1:B:735:VAL:H	2.10	0.55
2:D:92:PHE:CE2	2:D:108:VAL:HG11	2.41	0.55
2:F:117:THR:C	2:F:119:GLU:H	2.08	0.55
1:A:368:GLN:HB2	1:A:384:ASN:OD1	2.07	0.55
1:A:450:ASN:O	1:A:451:ASN:HB2	2.06	0.55
1:B:616:GLU:HG3	1:B:617:LYS:N	2.20	0.55
1:B:654:ILE:HA	1:B:755:ARG:HG2	1.87	0.55
1:A:293:ILE:HG13	1:A:293:ILE:O	2.06	0.55
1:A:322:LEU:HB3	1:A:503:GLU:OE2	2.05	0.55
1:A:540:ARG:NH1	1:A:630:ARG:NH2	2.54	0.55
1:B:536:TYR:CD2	1:B:536:TYR:N	2.73	0.55
1:C:652:ALA:O	1:C:656:THR:HG22	2.07	0.55
1:C:775:LEU:HB2	1:C:776:LEU:HD12	1.87	0.55
1:C:527:LYS:NZ	2:F:145:MET:O	2.39	0.55
1:A:463:THR:HB	1:A:467:GLU:H	1.70	0.55
1:A:521:ASN:CG	1:A:522:SER:N	2.60	0.55
1:A:581:GLN:HE21	1:A:628:PHE:HA	1.70	0.55
1:A:639:ASN:HD22	1:A:640:LYS:N	2.05	0.55
1:A:632:TYR:C	1:A:643:ILE:O	2.42	0.55
1:B:529:VAL:HG23	1:B:530:THR:H	1.71	0.55
1:C:534:ILE:HA	1:C:538:ILE:HB	1.88	0.55
1:C:589:LYS:HE2	1:C:643:ILE:HG23	1.87	0.55
1:C:667:LEU:HA	1:C:670:ILE:HG22	1.88	0.55
2:E:105:LEU:O	2:E:105:LEU:HD23	2.06	0.55
1:A:602:PHE:O	1:A:603:ILE:HD13	2.07	0.55
1:A:670:ILE:HG23	1:A:745:TYR:CZ	2.41	0.55
1:B:549:LEU:HD23	1:B:549:LEU:N	2.22	0.55
1:C:540:ARG:HD3	1:C:582:ASP:OD1	2.07	0.55
1:C:694:VAL:HG23	1:C:695:LYS:N	2.15	0.55
1:C:706:ASN:O	1:C:709:ASN:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:LEU:HD23	1:A:497:LEU:HG	1.89	0.55
1:A:517:VAL:C	1:A:525:LYS:HZ1	2.09	0.55
1:A:327:LEU:HG	1:A:595:ILE:HG23	1.89	0.55
1:B:400:LYS:NZ	1:B:475:GLU:OE2	2.35	0.55
1:B:616:GLU:CG	1:B:617:LYS:N	2.68	0.55
2:D:20:ASP:C	2:D:22:ASP:H	2.11	0.55
1:A:540:ARG:HH12	1:A:630:ARG:NH2	2.05	0.55
1:B:332:ASN:HD22	1:B:333:LYS:N	2.04	0.55
1:B:427:ASP:C	1:B:429:GLY:H	2.11	0.55
1:B:557:LEU:HD11	1:B:575:VAL:HG12	1.89	0.55
1:C:295:VAL:CG2	1:C:603:ILE:HG22	2.27	0.55
1:C:667:LEU:HB2	2:F:14:GLU:OE2	2.07	0.55
1:B:445:ARG:HB2	1:B:471:TRP:CH2	2.42	0.54
1:B:527:LYS:O	1:B:527:LYS:HG2	2.07	0.54
1:B:616:GLU:O	1:B:621:GLY:HA3	2.07	0.54
1:B:726:ILE:HA	1:B:729:TYR:HB2	1.88	0.54
2:D:130:ILE:HG22	2:D:130:ILE:O	2.06	0.54
2:E:117:THR:C	2:E:119:GLU:H	2.09	0.54
1:B:775:LEU:H	1:B:775:LEU:HD22	1.72	0.54
1:C:629:ASN:HB3	1:C:632:TYR:CE2	2.42	0.54
1:A:664:ILE:HD13	2:D:15:ALA:HB2	1.88	0.54
2:F:100:ILE:HB	2:F:136:VAL:CG2	2.33	0.54
1:C:669:SER:HA	1:C:672:ARG:HG2	1.90	0.54
1:C:790:PHE:O	1:C:793:PHE:HB3	2.07	0.54
2:D:44:THR:CG2	2:D:47:GLU:HG3	2.37	0.54
2:E:20:ASP:C	2:E:22:ASP:H	2.10	0.54
1:A:295:VAL:HG22	1:A:296:LEU:N	2.23	0.54
1:A:445:ARG:NE	1:A:471:TRP:CE2	2.75	0.54
1:A:663:PHE:HE1	1:A:752:LEU:HD11	1.73	0.54
1:A:768:LYS:HG2	1:A:768:LYS:O	2.08	0.54
1:C:661:ALA:C	1:C:663:PHE:H	2.11	0.54
2:E:87:GLU:O	2:E:91:VAL:HG23	2.08	0.54
1:A:456:LYS:HD3	1:A:471:TRP:CD1	2.43	0.54
1:A:603:ILE:HG22	1:A:604:LEU:H	1.72	0.54
1:A:700:TYR:CE1	1:A:731:GLU:HG2	2.42	0.54
1:B:753:LYS:O	1:B:757:THR:OG1	2.23	0.54
1:C:318:ILE:CD1	1:C:318:ILE:H	2.18	0.54
1:C:631:SER:O	1:C:632:TYR:C	2.44	0.54
1:B:530:THR:HG22	2:E:92:PHE:HZ	1.70	0.54
1:A:408:LEU:O	1:A:408:LEU:HD23	2.08	0.54
1:A:583:ASN:O	1:A:629:ASN:OD1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:THR:HG21	1:A:556:MET:HE3	1.85	0.54
1:A:706:ASN:O	1:A:709:ASN:HB2	2.08	0.54
1:B:592:GLU:HG2	1:B:605:THR:O	2.08	0.54
1:C:462:ILE:CD1	1:C:466:GLY:HA2	2.38	0.54
2:E:137:ASN:OD1	2:E:139:GLU:HB2	2.08	0.54
1:B:415:GLU:C	1:B:417:GLY:N	2.61	0.54
1:B:606:LYS:N	1:B:610:MET:HE2	2.11	0.54
1:C:494:LEU:HD23	1:C:497:LEU:HG	1.90	0.54
1:A:387:ASN:CB	1:A:477:MET:HE1	2.38	0.54
1:B:774:LYS:HG3	1:B:774:LYS:O	2.08	0.54
1:B:785:ASN:HD22	1:B:787:THR:HG22	1.73	0.54
1:C:505:LYS:HE3	1:C:513:TRP:CG	2.43	0.54
1:C:521:ASN:O	1:C:524:GLU:HB2	2.08	0.54
1:A:652:ALA:O	1:A:653:LYS:C	2.46	0.54
1:B:732:ILE:HG22	1:B:732:ILE:O	2.07	0.54
1:C:385:LEU:CD1	1:C:389:LYS:HD2	2.37	0.54
1:A:775:LEU:HB2	1:A:776:LEU:HD12	1.89	0.53
1:B:761:GLN:O	1:B:765:THR:N	2.38	0.53
1:A:450:ASN:OD1	1:A:452:GLU:HG3	2.08	0.53
1:A:462:ILE:CD1	1:A:466:GLY:HA2	2.38	0.53
1:B:654:ILE:HG13	1:B:654:ILE:O	2.08	0.53
1:B:727:GLN:HG3	1:B:786:GLU:OE2	2.08	0.53
2:D:117:THR:C	2:D:119:GLU:H	2.11	0.53
1:A:324:THR:OG1	1:A:499:PRO:HB3	2.08	0.53
1:A:639:ASN:ND2	1:A:641:ALA:N	2.50	0.53
1:A:665:LYS:HG3	2:D:11:GLU:OE1	2.08	0.53
1:A:764:LEU:O	1:A:768:LYS:N	2.40	0.53
1:B:502:THR:O	1:B:505:LYS:HG2	2.08	0.53
1:B:654:ILE:HG22	1:B:755:ARG:HG2	1.90	0.53
1:B:721:SER:O	1:B:723:PHE:N	2.41	0.53
1:C:327:LEU:N	1:C:327:LEU:HD12	2.22	0.53
1:B:581:GLN:NE2	1:B:629:ASN:N	2.39	0.53
1:C:581:GLN:HE21	1:C:629:ASN:N	2.05	0.53
1:C:707:SER:C	1:C:709:ASN:H	2.12	0.53
2:F:44:THR:CG2	2:F:47:GLU:HG3	2.38	0.53
1:A:540:ARG:HH12	1:A:630:ARG:HH21	1.57	0.53
1:B:381:GLU:HG2	1:B:465:LEU:HD11	1.90	0.53
2:D:137:ASN:OD1	2:D:139:GLU:HB2	2.08	0.53
1:A:383:GLY:O	1:A:386:GLU:HB2	2.08	0.53
1:B:443:GLU:OE1	1:B:456:LYS:HE2	2.09	0.53
1:B:654:ILE:O	1:B:655:ASN:ND2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:732:ILE:O	1:B:735:VAL:HG12	2.09	0.53
1:C:317:LYS:HB3	1:C:318:ILE:HD12	1.91	0.53
2:F:92:PHE:CE2	2:F:108:VAL:HG11	2.43	0.53
2:F:62:THR:C	2:F:63:ILE:HD12	2.29	0.53
2:F:101:SER:OG	2:F:104:GLU:HG3	2.09	0.53
2:F:105:LEU:O	2:F:105:LEU:HD23	2.08	0.53
2:F:27:ILE:CG1	2:F:63:ILE:HB	2.39	0.53
1:A:445:ARG:HH22	1:A:456:LYS:CG	2.21	0.53
1:A:509:PRO:O	1:A:511:LYS:N	2.40	0.53
1:A:697:ILE:HD11	1:A:731:GLU:O	2.09	0.53
2:D:105:LEU:HD23	2:D:105:LEU:O	2.08	0.53
1:A:523:LEU:C	1:A:525:LYS:N	2.62	0.53
1:A:319:ALA:O	1:A:598:PRO:HA	2.09	0.53
1:B:574:VAL:O	1:B:575:VAL:HG23	2.09	0.53
1:B:793:PHE:HA	1:B:796:ILE:HG12	1.91	0.53
1:A:385:LEU:HD13	1:A:385:LEU:C	2.29	0.53
1:A:440:GLN:H	1:A:440:GLN:CD	2.13	0.53
1:B:596:ILE:HG12	1:B:602:PHE:CD2	2.44	0.53
1:C:384:ASN:N	1:C:384:ASN:OD1	2.42	0.53
1:A:535:LYS:HZ3	1:A:536:TYR:HE2	1.57	0.52
1:B:629:ASN:HD22	1:B:629:ASN:C	2.11	0.52
1:A:534:ILE:HG22	1:A:535:LYS:N	2.24	0.52
1:C:338:LEU:O	1:C:343:VAL:HG23	2.09	0.52
1:A:324:THR:O	1:A:324:THR:HG23	2.07	0.52
1:A:338:LEU:O	1:A:343:VAL:HG23	2.10	0.52
1:A:360:VAL:CG2	1:A:360:VAL:O	2.57	0.52
1:A:707:SER:C	1:A:709:ASN:H	2.12	0.52
1:B:296:LEU:HB2	1:B:604:LEU:HB3	1.92	0.52
1:C:574:VAL:O	1:C:574:VAL:HG13	2.09	0.52
2:E:44:THR:CG2	2:E:47:GLU:HG3	2.37	0.52
2:E:72:MET:C	2:E:74:ARG:H	2.12	0.52
1:C:669:SER:C	1:C:671:ARG:H	2.13	0.52
2:F:89:PHE:C	2:F:89:PHE:HD2	2.13	0.52
1:A:523:LEU:C	1:A:525:LYS:H	2.13	0.52
1:B:391:ILE:HD13	1:B:398:ILE:HG22	1.90	0.52
1:B:415:GLU:C	1:B:417:GLY:H	2.11	0.52
1:B:557:LEU:CD1	1:B:575:VAL:HG12	2.40	0.52
1:B:714:GLN:OE1	1:B:718:ARG:NH2	2.42	0.52
1:A:540:ARG:NH2	1:A:627:TYR:CE1	2.77	0.52
1:B:744:GLU:OE1	1:B:744:GLU:HA	2.08	0.52
1:C:308:VAL:HG23	1:C:492:TYR:OH	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:509:PRO:HD2	1:C:536:TYR:CZ	2.45	0.52
1:C:781:ASN:ND2	1:C:783:THR:OG1	2.42	0.52
2:E:37:ARG:HG2	2:E:41:GLN:O	2.10	0.52
1:A:633:ASN:ND2	1:A:644:GLU:HA	2.25	0.52
1:B:309:PRO:O	1:B:312:ALA:N	2.42	0.52
1:A:636:ALA:O	1:A:640:LYS:HA	2.10	0.52
1:B:298:GLY:O	1:B:300:LYS:N	2.43	0.52
1:B:306:GLY:O	1:B:336:THR:CB	2.57	0.52
1:B:423:LYS:HB3	1:B:434:LEU:CD2	2.39	0.52
1:B:516:VAL:O	1:B:520:PRO:HD2	2.10	0.52
1:B:311:HIS:ND1	1:B:564:VAL:HB	2.24	0.52
1:B:540:ARG:HD2	1:B:627:TYR:CZ	2.44	0.52
1:B:728:ALA:C	1:B:730:ASN:H	2.13	0.52
1:B:785:ASN:ND2	1:B:787:THR:CG2	2.73	0.52
1:C:636:ALA:O	1:C:640:LYS:HA	2.10	0.52
2:D:92:PHE:CD2	2:D:108:VAL:HG21	2.44	0.52
2:E:85:ILE:O	2:E:88:ALA:HB3	2.10	0.52
2:F:20:ASP:C	2:F:22:ASP:H	2.11	0.52
2:F:65:PHE:CD1	2:F:65:PHE:N	2.77	0.52
2:F:72:MET:C	2:F:74:ARG:H	2.14	0.52
1:A:299:GLU:HG3	1:A:303:LYS:HZ2	1.74	0.52
1:B:509:PRO:CD	1:B:536:TYR:HE1	2.21	0.52
1:B:748:TYR:O	1:B:752:LEU:CG	2.58	0.52
1:C:530:THR:HG21	2:F:145:MET:HE1	1.92	0.52
1:B:536:TYR:N	1:B:536:TYR:HD2	2.09	0.51
1:B:749:PHE:O	1:B:752:LEU:HB2	2.11	0.51
1:C:292:ARG:NE	1:C:292:ARG:HA	2.25	0.51
1:A:384:ASN:O	1:A:385:LEU:C	2.48	0.51
1:C:657:ILE:CG1	1:C:759:GLN:HG2	2.37	0.51
2:D:37:ARG:HG2	2:D:41:GLN:O	2.11	0.51
2:E:131:ASP:OD1	2:E:133:ASP:OD2	2.27	0.51
2:E:36:MET:C	2:E:41:GLN:HB2	2.31	0.51
2:E:89:PHE:HD2	2:E:89:PHE:C	2.11	0.51
1:A:509:PRO:HD3	1:A:536:TYR:CE1	2.44	0.51
1:A:517:VAL:HA	1:A:525:LYS:NZ	2.25	0.51
1:B:525:LYS:NZ	2:E:114:GLU:OE2	2.43	0.51
1:B:540:ARG:NH1	1:B:627:TYR:CD1	2.79	0.51
1:B:785:ASN:O	1:B:786:GLU:C	2.48	0.51
1:C:346:LYS:O	1:C:346:LYS:HG3	2.10	0.51
1:A:318:ILE:HG23	1:A:322:LEU:CD1	2.41	0.51
1:A:607:ASN:O	1:A:610:MET:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:LYS:HG2	1:B:393:GLU:OE2	2.11	0.51
1:C:440:GLN:CD	1:C:440:GLN:H	2.14	0.51
1:C:666:ASN:O	1:C:670:ILE:HG22	2.10	0.51
2:F:140:GLU:C	2:F:142:VAL:N	2.64	0.51
1:A:324:THR:O	1:A:324:THR:CG2	2.58	0.51
1:A:384:ASN:O	1:A:387:ASN:N	2.44	0.51
1:A:394:HIS:O	1:A:395:GLU:C	2.49	0.51
1:A:607:ASN:HD21	1:A:609:GLU:HB2	1.75	0.51
1:B:513:TRP:O	1:B:517:VAL:HG12	2.10	0.51
1:B:730:ASN:HA	1:B:733:GLU:HB3	1.93	0.51
1:B:787:THR:HG23	1:B:788:ASP:N	2.25	0.51
1:C:657:ILE:HG23	1:C:658:PRO:HD2	1.91	0.51
2:E:27:ILE:CG1	2:E:63:ILE:HB	2.40	0.51
1:A:558:ASP:O	1:A:562:GLU:HG3	2.11	0.51
1:A:606:LYS:O	1:A:607:ASN:HB3	2.11	0.51
1:B:355:SER:HB2	1:B:371:SER:HA	1.91	0.51
1:B:327:LEU:CG	1:B:595:ILE:HG23	2.40	0.51
1:C:510:GLN:CG	1:C:510:GLN:O	2.57	0.51
1:C:608:TRP:O	1:C:609:GLU:C	2.47	0.51
1:C:774:LYS:O	1:C:777:TYR:N	2.38	0.51
1:A:419:ILE:O	1:A:419:ILE:HG13	2.11	0.51
1:A:445:ARG:NE	1:A:471:TRP:NE1	2.59	0.51
1:A:697:ILE:O	1:A:701:LEU:HG	2.10	0.51
1:A:705:TYR:CE2	2:D:139:GLU:CB	2.81	0.51
1:C:383:GLY:O	1:C:386:GLU:HB2	2.10	0.51
1:B:717:LYS:CD	2:E:132:GLY:N	2.70	0.51
2:F:37:ARG:HG2	2:F:41:GLN:O	2.10	0.51
1:A:652:ALA:O	1:A:654:ILE:N	2.44	0.51
1:C:628:PHE:CD1	1:C:628:PHE:C	2.84	0.51
2:E:44:THR:HG23	2:E:47:GLU:H	1.76	0.51
2:D:44:THR:HG23	2:D:47:GLU:H	1.75	0.51
1:B:298:GLY:O	1:B:299:GLU:C	2.48	0.50
1:B:508:ILE:HA	1:B:536:TYR:HD1	1.75	0.50
1:A:502:THR:O	1:A:505:LYS:N	2.44	0.50
1:B:309:PRO:O	1:B:310:GLU:C	2.50	0.50
1:B:622:LYS:O	1:B:623:ASP:HB2	2.12	0.50
1:C:639:ASN:C	1:C:639:ASN:ND2	2.59	0.50
1:B:300:LYS:HA	1:B:303:LYS:NZ	2.25	0.50
1:B:576:ASN:N	1:B:576:ASN:OD1	2.44	0.50
1:B:722:ILE:O	1:B:726:ILE:HG13	2.11	0.50
2:F:44:THR:HG23	2:F:47:GLU:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:LEU:HB3	1:A:579:THR:HG22	1.93	0.50
1:A:667:LEU:HA	1:A:670:ILE:CG2	2.41	0.50
1:A:774:LYS:O	1:A:777:TYR:N	2.39	0.50
1:B:616:GLU:HA	1:B:620:THR:CG2	2.40	0.50
2:D:27:ILE:CG1	2:D:63:ILE:HB	2.42	0.50
2:E:65:PHE:N	2:E:65:PHE:CD1	2.75	0.50
1:A:697:ILE:H	1:A:697:ILE:CD1	2.25	0.50
1:B:649:ILE:HD12	2:E:86:ARG:HG3	1.92	0.50
1:B:746:LYS:CG	1:B:750:GLN:HB2	2.41	0.50
1:C:409:ARG:O	1:C:410:ILE:C	2.49	0.50
1:C:540:ARG:HB3	1:C:549:LEU:O	2.11	0.50
2:E:117:THR:C	2:E:119:GLU:N	2.64	0.50
1:C:668:SER:HA	2:F:14:GLU:HG3	1.94	0.50
2:F:36:MET:C	2:F:41:GLN:HB2	2.31	0.50
1:A:377:GLN:C	1:A:379:ALA:N	2.64	0.50
1:B:404:LYS:HG3	1:B:452:GLU:HA	1.93	0.50
1:B:625:LEU:C	1:B:625:LEU:HD23	2.32	0.50
1:A:324:THR:HA	1:A:499:PRO:HA	1.94	0.50
2:D:72:MET:C	2:D:74:ARG:H	2.13	0.50
1:A:346:LYS:O	1:A:346:LYS:HG3	2.12	0.50
1:C:385:LEU:HD13	1:C:385:LEU:C	2.31	0.50
2:D:140:GLU:C	2:D:142:VAL:N	2.65	0.50
2:F:117:THR:C	2:F:119:GLU:N	2.64	0.50
2:F:5:THR:N	2:F:8:GLN:HB2	2.27	0.50
1:B:453:VAL:CG1	1:B:474:ILE:HD12	2.42	0.50
1:C:360:VAL:CG2	1:C:360:VAL:O	2.57	0.49
1:C:387:ASN:CB	1:C:477:MET:HE1	2.42	0.49
1:C:400:LYS:HD2	1:C:475:GLU:OE1	2.12	0.49
1:C:650:THR:C	1:C:652:ALA:N	2.63	0.49
2:E:100:ILE:HB	2:E:136:VAL:CG2	2.37	0.49
1:A:348:LEU:HD12	1:A:577:HIS:CB	2.42	0.49
1:B:489:THR:HG23	1:B:490:ALA:O	2.12	0.49
1:C:363:TYR:CD1	1:C:403:LEU:CD1	2.95	0.49
1:C:592:GLU:HB3	1:C:604:LEU:HD21	1.93	0.49
1:C:739:LYS:HE2	1:C:739:LYS:HA	1.94	0.49
1:A:722:ILE:HG21	1:A:764:LEU:HD21	1.94	0.49
1:C:318:ILE:CG2	1:C:322:LEU:HD13	2.42	0.49
2:D:117:THR:C	2:D:119:GLU:N	2.65	0.49
1:A:780:LEU:HD12	1:A:780:LEU:O	2.12	0.49
1:B:530:THR:OG1	2:E:145:MET:SD	2.70	0.49
1:C:340:LYS:C	1:C:342:GLY:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ARG:HH21	1:C:600:GLY:HA3	1.77	0.49
1:C:602:PHE:C	1:C:603:ILE:HD13	2.33	0.49
1:C:655:ASN:N	1:C:655:ASN:ND2	2.60	0.49
2:D:42:ASN:ND2	2:D:147:ALA:HB2	2.27	0.49
2:E:37:ARG:HA	2:E:41:GLN:O	2.12	0.49
1:A:597:ASN:OD1	1:A:601:GLU:HB2	2.13	0.49
1:B:315:PHE:CE2	1:B:560:LEU:HD23	2.47	0.49
1:B:524:GLU:O	1:B:525:LYS:C	2.51	0.49
1:B:605:THR:CG2	1:B:606:LYS:N	2.76	0.49
1:B:709:ASN:O	1:B:709:ASN:OD1	2.30	0.49
1:B:709:ASN:ND2	1:B:720:ILE:HD11	2.19	0.49
1:B:773:PHE:O	1:B:775:LEU:N	2.46	0.49
1:C:381:GLU:C	1:C:383:GLY:N	2.66	0.49
1:C:525:LYS:HB2	2:F:124:MET:HE3	1.94	0.49
1:B:629:ASN:ND2	1:B:631:SER:HB2	2.21	0.49
1:C:540:ARG:HH12	1:C:630:ARG:NH2	2.10	0.49
1:A:325:TYR:CE1	1:A:619:ILE:HG12	2.47	0.49
1:A:608:TRP:O	1:A:609:GLU:C	2.50	0.49
1:C:322:LEU:O	1:C:323:ASN:C	2.50	0.49
1:C:502:THR:O	1:C:505:LYS:N	2.45	0.49
1:A:557:LEU:O	1:A:560:LEU:HB2	2.11	0.49
1:A:629:ASN:ND2	1:A:631:SER:N	2.41	0.49
1:B:587:PRO:CD	1:B:639:ASN:HD21	2.18	0.49
1:B:639:ASN:ND2	1:B:639:ASN:N	2.58	0.49
1:B:655:ASN:H	1:B:755:ARG:HD2	1.78	0.49
1:C:305:SER:OG	1:C:306:GLY:N	2.45	0.49
1:C:325:TYR:CE2	1:C:598:PRO:HD2	2.48	0.49
1:C:561:ASN:O	1:C:564:VAL:HG22	2.12	0.49
1:C:581:GLN:HE21	1:C:628:PHE:HA	1.77	0.49
2:F:117:THR:O	2:F:119:GLU:N	2.46	0.49
1:C:335:ALA:O	1:C:338:LEU:HB2	2.12	0.49
1:C:557:LEU:O	1:C:560:LEU:HB2	2.12	0.49
1:C:607:ASN:O	1:C:610:MET:N	2.44	0.49
2:E:117:THR:O	2:E:119:GLU:N	2.46	0.49
2:F:140:GLU:C	2:F:142:VAL:H	2.16	0.49
1:A:326:ILE:C	1:A:327:LEU:HD12	2.33	0.49
1:A:639:ASN:C	1:A:639:ASN:ND2	2.60	0.49
1:B:338:LEU:O	1:B:339:ILE:C	2.50	0.49
1:B:294:ASP:O	1:B:606:LYS:HE3	2.12	0.49
1:B:795:LYS:O	1:B:797:ILE:HG12	2.12	0.49
1:C:670:ILE:O	1:C:745:TYR:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:MET:C	2:D:41:GLN:HB2	2.33	0.49
2:D:62:THR:C	2:D:63:ILE:HD12	2.33	0.49
1:A:403:LEU:HD13	1:A:476:VAL:HG21	1.93	0.48
1:A:602:PHE:C	1:A:603:ILE:HD13	2.34	0.48
1:A:700:TYR:HE1	1:A:731:GLU:HG2	1.77	0.48
1:C:318:ILE:HG23	1:C:322:LEU:CD1	2.41	0.48
1:C:438:ASN:ND2	1:C:438:ASN:C	2.66	0.48
1:C:780:LEU:HD12	1:C:780:LEU:O	2.12	0.48
2:D:65:PHE:CD1	2:D:65:PHE:N	2.78	0.48
1:A:438:ASN:ND2	1:A:438:ASN:C	2.66	0.48
1:B:315:PHE:O	1:B:316:LYS:C	2.51	0.48
1:C:401:ILE:HD13	1:C:478:ALA:CB	2.42	0.48
2:E:140:GLU:C	2:E:142:VAL:N	2.64	0.48
1:A:325:TYR:CE2	1:A:598:PRO:HD2	2.49	0.48
1:B:315:PHE:HA	1:B:318:ILE:HD11	1.95	0.48
1:B:722:ILE:HG23	1:B:760:VAL:HG13	1.95	0.48
1:A:432:TYR:CD1	1:A:471:TRP:CZ3	3.01	0.48
1:B:359:PRO:HG2	1:B:444:PHE:CD2	2.49	0.48
2:E:50:ASP:OD1	2:E:51:MET:N	2.47	0.48
1:A:304:ALA:HB3	1:A:604:LEU:HD13	1.95	0.48
1:A:587:PRO:HB2	1:A:643:ILE:CD1	2.44	0.48
1:B:717:LYS:HD2	2:E:132:GLY:CA	2.43	0.48
2:D:89:PHE:C	2:D:89:PHE:HD2	2.14	0.48
1:B:331:VAL:O	1:B:331:VAL:HG12	2.13	0.48
1:B:423:LYS:O	1:B:434:LEU:CD2	2.62	0.48
1:C:667:LEU:O	1:C:671:ARG:HB2	2.14	0.48
1:A:508:ILE:HG21	1:A:532:LEU:HD13	1.96	0.48
1:B:338:LEU:HD11	1:B:409:ARG:NE	2.28	0.48
1:C:583:ASN:ND2	4:C:1999:DOT:C1B	2.77	0.48
1:A:401:ILE:HD13	1:A:478:ALA:CB	2.44	0.48
1:A:543:ASP:OD2	1:A:546:LYS:HG3	2.13	0.48
1:A:604:LEU:HD23	1:A:604:LEU:C	2.33	0.48
1:B:535:LYS:HB3	1:B:536:TYR:CD2	2.48	0.48
1:B:626:TYR:C	1:B:626:TYR:CD2	2.87	0.48
1:B:737:LYS:C	1:B:738:SER:O	2.47	0.48
1:B:746:LYS:HG3	1:B:750:GLN:HB2	1.95	0.48
1:C:419:ILE:O	1:C:419:ILE:HG13	2.12	0.48
2:D:100:ILE:HB	2:D:136:VAL:CG2	2.37	0.48
1:A:423:LYS:HB3	1:A:423:LYS:NZ	2.28	0.48
1:A:477:MET:C	1:A:488:LEU:HD12	2.34	0.48
1:B:333:LYS:O	1:B:336:THR:CG2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:ASP:HB3	1:B:546:LYS:O	2.14	0.48
1:C:377:GLN:C	1:C:379:ALA:N	2.66	0.48
1:C:394:HIS:O	1:C:395:GLU:C	2.53	0.48
2:D:117:THR:O	2:D:119:GLU:N	2.46	0.48
2:E:140:GLU:C	2:E:142:VAL:H	2.17	0.48
1:A:652:ALA:O	1:A:655:ASN:N	2.38	0.48
1:B:400:LYS:HA	1:B:476:VAL:O	2.14	0.48
1:B:526:GLN:HE21	2:E:124:MET:CE	2.27	0.48
1:B:529:VAL:HG23	1:B:530:THR:N	2.28	0.48
1:B:619:ILE:C	1:B:621:GLY:N	2.67	0.48
1:C:304:ALA:HB3	1:C:604:LEU:CD1	2.43	0.48
1:A:540:ARG:NH2	2:D:87:GLU:OE1	2.45	0.48
2:E:65:PHE:HD1	2:E:65:PHE:H	1.56	0.48
1:B:726:ILE:O	1:B:729:TYR:CB	2.62	0.47
1:A:559:ARG:NH1	1:A:559:ARG:HB3	2.19	0.47
1:B:497:LEU:HD13	1:B:556:MET:HG2	1.96	0.47
1:B:720:ILE:O	1:B:724:ARG:HG2	2.14	0.47
1:C:403:LEU:CD1	1:C:476:VAL:HG21	2.44	0.47
1:C:527:LYS:HZ3	2:F:145:MET:HA	1.79	0.47
1:A:462:ILE:HD11	1:A:466:GLY:CA	2.43	0.47
1:A:583:ASN:HD21	4:A:999:DOT:H1'	1.79	0.47
1:A:493:ASP:OD2	4:A:999:DOT:O1A	2.33	0.47
2:F:45:GLU:O	2:F:49:GLN:HG2	2.15	0.47
1:A:561:ASN:O	1:A:564:VAL:HG22	2.14	0.47
1:A:657:ILE:HG21	1:A:756:ILE:HD13	1.92	0.47
1:A:789:ASN:N	1:A:789:ASN:HD22	2.11	0.47
1:B:574:VAL:C	1:B:575:VAL:HG23	2.35	0.47
1:A:317:LYS:HB3	1:A:318:ILE:HD12	1.97	0.47
1:A:340:LYS:C	1:A:342:GLY:H	2.18	0.47
1:A:419:ILE:HD12	1:A:435:LEU:HD22	1.97	0.47
1:B:587:PRO:HD2	1:B:639:ASN:ND2	2.18	0.47
1:B:735:VAL:HG22	1:B:735:VAL:O	2.15	0.47
1:B:773:PHE:HE1	1:B:777:TYR:HB2	1.78	0.47
1:C:445:ARG:NH1	1:C:471:TRP:NE1	2.61	0.47
1:A:504:ILE:CG2	1:A:505:LYS:N	2.77	0.47
1:A:534:ILE:HA	1:A:538:ILE:HB	1.96	0.47
1:A:628:PHE:HD1	1:A:629:ASN:O	1.98	0.47
1:B:313:ASP:C	1:B:315:PHE:N	2.68	0.47
1:B:456:LYS:HG3	1:B:457:THR:O	2.14	0.47
1:B:615:ILE:HD13	1:B:626:TYR:CZ	2.50	0.47
1:B:785:ASN:ND2	1:B:787:THR:HG22	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:699:GLY:O	1:C:702:SER:N	2.46	0.47
1:A:538:ILE:CD1	2:D:88:ALA:HA	2.45	0.47
1:A:370:LEU:HD11	1:A:455:TYR:CE1	2.49	0.47
1:B:357:TRP:CZ2	1:B:370:LEU:HA	2.49	0.47
1:B:750:GLN:O	1:B:753:LYS:HB3	2.15	0.47
1:B:785:ASN:HD22	1:B:787:THR:CG2	2.27	0.47
2:D:140:GLU:C	2:D:142:VAL:H	2.18	0.47
2:D:45:GLU:O	2:D:49:GLN:HG2	2.15	0.47
1:B:514:ASP:CA	1:B:517:VAL:HG12	2.38	0.47
1:C:408:LEU:O	1:C:408:LEU:HD23	2.14	0.47
1:C:540:ARG:NH1	1:C:630:ARG:NH2	2.63	0.47
1:C:789:ASN:HD22	1:C:789:ASN:N	2.12	0.47
2:D:22:ASP:HB3	2:D:26:THR:OG1	2.15	0.47
1:B:338:LEU:O	1:B:341:SER:N	2.47	0.47
1:B:377:GLN:HG3	1:B:465:LEU:HD23	1.97	0.47
1:B:574:VAL:O	1:B:575:VAL:CG2	2.63	0.47
1:B:721:SER:C	1:B:723:PHE:N	2.68	0.47
1:B:733:GLU:C	1:B:735:VAL:N	2.68	0.47
1:C:349:ASN:HD21	1:C:398:ILE:CG1	2.27	0.47
2:D:5:THR:O	2:D:9:ILE:HG13	2.15	0.47
2:E:62:THR:C	2:E:63:ILE:HD12	2.35	0.47
2:F:37:ARG:HA	2:F:41:GLN:O	2.15	0.47
1:A:329:ARG:O	1:A:330:PRO:O	2.33	0.47
1:A:443:GLU:HB2	1:A:458:LYS:HG2	1.97	0.47
1:B:498:ALA:HB3	1:B:619:ILE:HD13	1.95	0.47
1:C:363:TYR:HD1	1:C:403:LEU:CD1	2.27	0.47
1:C:583:ASN:O	1:C:629:ASN:OD1	2.32	0.47
1:C:657:ILE:CG2	1:C:658:PRO:N	2.78	0.47
1:B:327:LEU:HA	1:B:594:PHE:O	2.14	0.47
1:B:328:PHE:HB2	1:B:594:PHE:HB3	1.97	0.47
1:C:597:ASN:OD1	1:C:601:GLU:HB2	2.14	0.46
1:C:629:ASN:HD21	1:C:631:SER:H	1.52	0.46
1:A:327:LEU:HB2	1:A:496:ALA:O	2.14	0.46
1:B:327:LEU:HD13	1:B:496:ALA:HB3	1.96	0.46
1:B:758:ASN:HA	1:B:761:GLN:HB2	1.97	0.46
1:C:517:VAL:O	1:C:517:VAL:HG22	2.13	0.46
1:C:722:ILE:HG21	1:C:764:LEU:HD21	1.97	0.46
1:A:299:GLU:CG	1:A:303:LYS:NZ	2.79	0.46
1:A:628:PHE:C	1:A:628:PHE:CD1	2.88	0.46
1:C:302:LEU:HD12	1:C:602:PHE:CE1	2.48	0.46
1:C:384:ASN:O	1:C:385:LEU:C	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:ILE:HD12	1:C:435:LEU:HD22	1.97	0.46
1:C:658:PRO:HB2	1:C:701:LEU:CD1	2.44	0.46
2:D:37:ARG:HA	2:D:41:GLN:O	2.15	0.46
1:A:700:TYR:HD1	1:A:728:ALA:CA	2.28	0.46
1:A:722:ILE:HG12	1:A:763:LEU:HB2	1.98	0.46
1:B:418:ILE:HG22	1:B:419:ILE:HG23	1.96	0.46
1:B:450:ASN:O	1:B:451:ASN:HB2	2.15	0.46
1:B:470:ASN:CG	1:B:471:TRP:N	2.69	0.46
1:B:476:VAL:HG12	1:B:477:MET:N	2.30	0.46
1:B:480:ASN:HA	1:B:485:LEU:HD12	1.97	0.46
2:E:22:ASP:HB3	2:E:26:THR:OG1	2.15	0.46
1:B:327:LEU:HD23	1:B:595:ILE:HG23	1.98	0.46
1:B:368:GLN:H	1:B:384:ASN:ND2	2.13	0.46
1:C:381:GLU:C	1:C:383:GLY:H	2.19	0.46
1:C:462:ILE:HD11	1:C:466:GLY:CA	2.45	0.46
1:C:663:PHE:O	1:C:667:LEU:HG	2.16	0.46
2:D:42:ASN:HD21	2:D:147:ALA:HB2	1.80	0.46
1:A:345:THR:HB	1:A:491:ASP:HA	1.97	0.46
1:A:657:ILE:HD11	1:A:704:TYR:CD1	2.50	0.46
1:B:346:LYS:HD3	1:B:364:ILE:CD1	2.46	0.46
1:B:324:THR:CB	1:B:499:PRO:HA	2.46	0.46
1:B:501:LEU:HA	1:B:504:ILE:HG12	1.98	0.46
1:B:509:PRO:HD2	1:B:536:TYR:CE1	2.51	0.46
1:C:325:TYR:CD2	1:C:597:ASN:HA	2.51	0.46
2:D:87:GLU:O	2:D:91:VAL:HG23	2.15	0.46
1:A:324:THR:OG1	1:A:499:PRO:CA	2.64	0.46
1:A:663:PHE:CE1	1:A:752:LEU:CD1	2.98	0.46
1:B:332:ASN:HD21	1:B:334:LEU:H	1.62	0.46
1:B:368:GLN:H	1:B:384:ASN:HD21	1.64	0.46
1:B:622:LYS:O	1:B:623:ASP:CB	2.64	0.46
1:C:340:LYS:C	1:C:342:GLY:N	2.68	0.46
1:B:350:VAL:HG22	1:B:398:ILE:HG13	1.98	0.46
1:B:423:LYS:HB3	1:B:434:LEU:HD22	1.97	0.46
1:B:613:ARG:O	1:B:616:GLU:HG2	2.15	0.46
1:B:791:GLU:C	1:B:793:PHE:H	2.19	0.46
1:C:385:LEU:HD11	1:C:389:LYS:HD2	1.97	0.46
1:C:593:ILE:O	1:C:604:LEU:HA	2.15	0.46
1:C:650:THR:C	1:C:652:ALA:H	2.19	0.46
2:F:65:PHE:H	2:F:65:PHE:HD1	1.58	0.46
1:A:292:ARG:HH11	1:A:292:ARG:HG3	1.79	0.46
1:A:349:ASN:HD21	1:A:398:ILE:CG1	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:THR:CG2	1:A:465:LEU:H	2.28	0.46
1:A:789:ASN:ND2	1:A:789:ASN:N	2.63	0.46
1:B:745:TYR:HB3	1:B:749:PHE:CE1	2.41	0.46
1:C:504:ILE:CG2	1:C:505:LYS:N	2.78	0.46
2:D:50:ASP:OD1	2:D:51:MET:N	2.48	0.46
2:F:50:ASP:OD1	2:F:51:MET:N	2.48	0.46
1:B:315:PHE:O	1:B:318:ILE:CD1	2.64	0.46
2:D:118:ASP:N	2:D:118:ASP:OD2	2.48	0.46
2:F:22:ASP:HB3	2:F:26:THR:OG1	2.16	0.46
1:B:777:TYR:HA	1:B:780:LEU:HD12	1.97	0.45
1:C:463:THR:CG2	1:C:465:LEU:H	2.28	0.45
1:C:583:ASN:HD21	4:C:1999:DOT:H1'	1.79	0.45
1:A:714:GLN:HE22	2:D:126:ARG:HG3	1.75	0.45
2:F:76:MET:HE2	2:F:79:THR:HG23	1.98	0.45
2:F:87:GLU:O	2:F:91:VAL:HG23	2.15	0.45
1:A:432:TYR:CD1	1:A:471:TRP:HZ3	2.33	0.45
1:A:654:ILE:O	1:A:654:ILE:HG13	2.14	0.45
1:A:655:ASN:OD1	1:A:758:ASN:HB3	2.16	0.45
1:A:697:ILE:N	1:A:697:ILE:CD1	2.80	0.45
1:B:408:LEU:O	1:B:411:GLU:HB3	2.16	0.45
1:B:549:LEU:CD2	1:B:549:LEU:N	2.79	0.45
1:C:403:LEU:HD13	1:C:476:VAL:HG21	1.97	0.45
2:E:12:PHE:O	2:E:16:PHE:HB2	2.16	0.45
2:E:89:PHE:HE1	2:E:138:TYR:N	2.14	0.45
1:B:744:GLU:HG2	1:C:397:GLU:HG2	1.99	0.45
1:C:639:ASN:HD21	1:C:641:ALA:CB	2.29	0.45
2:E:129:ASP:OD1	2:E:132:GLY:N	2.44	0.45
2:F:99:TYR:HD2	2:F:137:ASN:HB3	1.79	0.45
1:A:327:LEU:N	1:A:327:LEU:HD12	2.32	0.45
1:A:456:LYS:HD3	1:A:471:TRP:HD1	1.81	0.45
1:A:625:LEU:HD12	1:A:625:LEU:HA	1.64	0.45
1:B:302:LEU:HD13	1:B:594:PHE:CZ	2.52	0.45
1:B:716:LYS:O	1:B:720:ILE:HG23	2.17	0.45
1:B:717:LYS:HE3	1:B:717:LYS:HB3	1.67	0.45
1:B:787:THR:HG23	1:B:788:ASP:H	1.81	0.45
1:B:790:PHE:O	1:B:794:GLN:HB2	2.17	0.45
1:C:322:LEU:N	1:C:322:LEU:HD12	2.31	0.45
1:C:423:LYS:HB3	1:C:423:LYS:NZ	2.32	0.45
2:D:12:PHE:O	2:D:16:PHE:HB2	2.16	0.45
2:E:105:LEU:O	2:E:109:MET:HG2	2.16	0.45
2:E:45:GLU:O	2:E:49:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:92:PHE:O	2:F:94:LYS:N	2.38	0.45
1:A:607:ASN:O	1:A:608:TRP:C	2.54	0.45
1:B:387:ASN:C	1:B:389:LYS:N	2.69	0.45
1:B:308:VAL:HG23	1:B:492:TYR:OH	2.16	0.45
1:B:581:GLN:O	1:B:629:ASN:HA	2.15	0.45
1:B:703:ASP:O	1:B:705:TYR:O	2.35	0.45
1:B:723:PHE:O	1:B:726:ILE:N	2.49	0.45
1:C:522:SER:O	1:C:524:GLU:N	2.49	0.45
1:C:789:ASN:ND2	1:C:789:ASN:N	2.63	0.45
2:F:89:PHE:CE1	2:F:138:TYR:N	2.85	0.45
2:F:144:MET:SD	2:F:144:MET:C	2.95	0.45
1:A:535:LYS:NZ	1:A:536:TYR:HE2	2.14	0.45
1:B:455:TYR:H	1:B:455:TYR:HD2	1.64	0.45
1:B:462:ILE:HG12	1:B:463:THR:O	2.17	0.45
1:B:589:LYS:HA	1:B:608:TRP:CZ3	2.51	0.45
1:C:669:SER:C	1:C:671:ARG:N	2.70	0.45
1:A:530:THR:HG21	2:D:145:MET:HE1	1.99	0.45
2:E:89:PHE:HD2	2:E:90:ARG:N	2.14	0.45
1:A:367:ASP:C	1:A:369:ASP:H	2.20	0.45
1:A:513:TRP:CD2	1:A:517:VAL:CG2	2.92	0.45
1:A:325:TYR:CD2	1:A:597:ASN:HA	2.52	0.45
1:B:636:ALA:O	1:B:640:LYS:HA	2.17	0.45
1:C:721:SER:O	1:C:724:ARG:N	2.50	0.45
2:E:89:PHE:CE1	2:E:138:TYR:N	2.85	0.45
1:A:663:PHE:HE1	1:A:752:LEU:CD1	2.30	0.45
1:A:667:LEU:HA	1:A:670:ILE:HG21	1.99	0.45
1:C:658:PRO:HB2	1:C:701:LEU:HD13	1.98	0.45
1:C:776:LEU:CD1	1:C:776:LEU:N	2.79	0.45
1:A:335:ALA:O	1:A:338:LEU:HB2	2.16	0.45
1:B:408:LEU:O	1:B:411:GLU:N	2.48	0.45
1:C:537:GLY:HA2	1:C:552:TRP:NE1	2.31	0.45
2:F:130:ILE:CG2	2:F:130:ILE:O	2.65	0.45
1:A:340:LYS:C	1:A:342:GLY:N	2.67	0.45
1:A:409:ARG:O	1:A:410:ILE:C	2.54	0.45
1:A:520:PRO:O	1:A:521:ASN:O	2.36	0.45
1:A:581:GLN:O	1:A:629:ASN:HA	2.17	0.45
1:B:422:GLY:O	1:B:433:TYR:CD2	2.70	0.45
1:B:312:ALA:HB1	1:B:602:PHE:CZ	2.52	0.45
1:B:629:ASN:C	1:B:629:ASN:ND2	2.70	0.45
1:B:786:GLU:O	1:B:789:ASN:N	2.44	0.45
1:C:329:ARG:O	1:C:330:PRO:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:THR:HB	1:C:662:GLU:H	1.82	0.45
1:A:695:LYS:CG	2:D:18:LEU:HD13	2.39	0.45
2:F:121:VAL:C	2:F:123:GLU:N	2.70	0.45
1:A:323:ASN:O	1:A:323:ASN:ND2	2.50	0.44
1:A:667:LEU:O	1:A:670:ILE:HG22	2.16	0.44
1:A:722:ILE:CG1	1:A:763:LEU:HB2	2.47	0.44
1:B:345:THR:HG21	1:B:574:VAL:HG23	1.99	0.44
1:B:508:ILE:HA	1:B:536:TYR:CD1	2.52	0.44
1:B:540:ARG:CZ	1:B:627:TYR:CE1	3.00	0.44
1:B:793:PHE:C	1:B:795:LYS:H	2.20	0.44
1:C:478:ALA:HA	1:C:488:LEU:HD12	1.99	0.44
1:C:768:LYS:HD2	1:C:797:ILE:O	2.17	0.44
1:C:776:LEU:H	1:C:776:LEU:HD12	1.80	0.44
2:D:138:TYR:O	2:D:139:GLU:C	2.55	0.44
1:A:305:SER:OG	1:A:306:GLY:N	2.50	0.44
1:B:517:VAL:O	1:B:517:VAL:HG22	2.17	0.44
1:C:522:SER:C	1:C:524:GLU:N	2.71	0.44
1:C:722:ILE:CG1	1:C:763:LEU:HB2	2.47	0.44
1:C:776:LEU:H	1:C:776:LEU:CD1	2.31	0.44
2:F:100:ILE:HD12	2:F:141:PHE:CD1	2.52	0.44
1:A:445:ARG:N	1:A:445:ARG:HD2	2.32	0.44
1:A:509:PRO:HG2	1:A:512:GLU:HB2	2.00	0.44
1:A:584:GLU:OE1	1:A:630:ARG:HG3	2.17	0.44
1:B:550:SER:H	1:B:553:GLN:CG	2.24	0.44
1:B:732:ILE:O	1:B:735:VAL:HB	2.17	0.44
1:C:663:PHE:CD2	1:C:664:ILE:HD12	2.49	0.44
1:A:760:VAL:HG11	1:A:773:PHE:HE1	1.83	0.44
1:B:348:LEU:HD22	1:B:348:LEU:N	2.32	0.44
1:B:391:ILE:CD1	1:B:399:GLY:CA	2.90	0.44
1:B:478:ALA:HB2	1:B:487:PRO:HA	1.99	0.44
1:C:527:LYS:NZ	2:F:145:MET:HA	2.31	0.44
2:D:26:THR:HA	2:D:63:ILE:O	2.17	0.44
2:E:99:TYR:HD2	2:E:137:ASN:HB3	1.82	0.44
2:E:99:TYR:CE2	2:E:137:ASN:HB3	2.52	0.44
1:A:639:ASN:HD21	1:A:641:ALA:CB	2.30	0.44
1:A:667:LEU:HB3	2:D:14:GLU:OE2	2.17	0.44
1:B:353:LYS:N	1:B:368:GLN:NE2	2.40	0.44
1:B:728:ALA:C	1:B:731:GLU:HG3	2.37	0.44
1:B:773:PHE:C	1:B:775:LEU:N	2.71	0.44
1:C:625:LEU:HD12	1:C:625:LEU:HA	1.66	0.44
2:D:42:ASN:ND2	2:D:147:ALA:CB	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:105:LEU:HD23	2:E:109:MET:HG2	2.00	0.44
2:E:100:ILE:HD12	2:E:141:PHE:CD1	2.52	0.44
1:A:700:TYR:CE1	1:A:727:GLN:O	2.71	0.44
1:A:721:SER:O	1:A:722:ILE:C	2.55	0.44
1:C:400:LYS:CE	1:C:475:GLU:OE1	2.66	0.44
1:C:327:LEU:HB2	1:C:496:ALA:O	2.18	0.44
1:C:712:PHE:HB3	1:C:716:LYS:CG	2.44	0.44
2:D:146:THR:HG22	2:D:147:ALA:N	2.31	0.44
2:F:89:PHE:HE1	2:F:138:TYR:N	2.16	0.44
1:B:562:GLU:C	1:B:564:VAL:N	2.70	0.44
2:D:121:VAL:C	2:D:123:GLU:N	2.71	0.44
2:D:141:PHE:CD2	2:D:141:PHE:O	2.70	0.44
2:D:145:MET:O	2:D:145:MET:HG3	2.18	0.44
2:D:19:PHE:C	2:D:19:PHE:CD2	2.89	0.44
1:B:403:LEU:HD23	1:B:453:VAL:HB	1.99	0.44
1:B:489:THR:HG23	1:B:490:ALA:N	2.31	0.44
1:C:384:ASN:O	1:C:387:ASN:N	2.51	0.44
1:C:749:PHE:C	1:C:751:TYR:N	2.71	0.44
2:D:65:PHE:HB2	2:D:66:PRO:CD	2.46	0.44
1:A:299:GLU:CG	1:A:303:LYS:HZ2	2.31	0.44
1:A:499:PRO:HD2	1:A:625:LEU:HB3	1.99	0.44
1:A:597:ASN:HB2	1:A:598:PRO:HD2	1.99	0.44
1:A:776:LEU:H	1:A:776:LEU:HD12	1.81	0.44
1:B:562:GLU:C	1:B:564:VAL:H	2.22	0.44
1:B:606:LYS:HG3	1:B:610:MET:HE1	2.00	0.44
1:C:550:SER:OG	1:C:553:GLN:HB2	2.17	0.44
1:C:659:THR:HB	1:C:662:GLU:CG	2.47	0.44
1:C:700:TYR:HD1	1:C:728:ALA:HA	1.82	0.44
2:D:131:ASP:OD1	2:D:133:ASP:OD2	2.35	0.44
2:D:65:PHE:H	2:D:65:PHE:HD1	1.59	0.44
1:B:649:ILE:HD12	2:E:86:ARG:CG	2.48	0.44
2:F:121:VAL:C	2:F:123:GLU:H	2.22	0.44
2:F:141:PHE:CD2	2:F:141:PHE:O	2.70	0.44
1:A:385:LEU:HD11	1:A:389:LYS:HD2	1.99	0.43
1:A:768:LYS:CG	1:A:768:LYS:O	2.65	0.43
1:B:727:GLN:O	1:B:730:ASN:O	2.35	0.43
1:B:773:PHE:O	1:B:773:PHE:CD1	2.71	0.43
1:C:325:TYR:CE1	1:C:619:ILE:HG12	2.53	0.43
1:C:712:PHE:HD2	1:C:716:LYS:HE2	1.81	0.43
2:D:26:THR:HG22	2:D:64:ASP:OD1	2.18	0.43
2:D:99:TYR:CE2	2:D:137:ASN:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:26:THR:HA	2:E:63:ILE:O	2.18	0.43
1:A:322:LEU:HA	1:A:503:GLU:OE2	2.18	0.43
1:A:294:ASP:O	1:A:610:MET:HE1	2.18	0.43
1:C:332:ASN:O	1:C:335:ALA:N	2.39	0.43
1:C:597:ASN:HB2	1:C:598:PRO:HD2	2.00	0.43
2:E:26:THR:HG22	2:E:64:ASP:OD1	2.19	0.43
1:A:381:GLU:C	1:A:383:GLY:N	2.71	0.43
1:A:384:ASN:N	1:A:384:ASN:OD1	2.49	0.43
1:A:793:PHE:O	1:A:794:GLN:C	2.56	0.43
1:B:553:GLN:O	1:B:556:MET:HB3	2.18	0.43
1:B:607:ASN:OD1	1:B:610:MET:CB	2.66	0.43
1:B:639:ASN:HD22	1:B:639:ASN:N	2.16	0.43
1:B:721:SER:O	1:B:722:ILE:C	2.56	0.43
1:C:527:LYS:HZ1	2:F:145:MET:C	2.22	0.43
2:D:129:ASP:OD1	2:D:132:GLY:N	2.47	0.43
2:E:19:PHE:C	2:E:19:PHE:CD2	2.91	0.43
2:F:12:PHE:O	2:F:16:PHE:HB2	2.18	0.43
1:C:367:ASP:C	1:C:369:ASP:H	2.22	0.43
1:C:519:THR:OG1	1:C:520:PRO:HD2	2.18	0.43
2:D:137:ASN:O	2:D:138:TYR:C	2.56	0.43
2:F:26:THR:HG22	2:F:64:ASP:OD1	2.19	0.43
1:C:630:ARG:HE	2:F:87:GLU:CD	2.21	0.43
2:F:99:TYR:CE2	2:F:137:ASN:HB3	2.54	0.43
1:A:345:THR:HG21	1:A:574:VAL:CG2	2.49	0.43
1:A:514:ASP:HA	1:A:517:VAL:HB	2.01	0.43
1:B:383:GLY:O	1:B:386:GLU:HB2	2.19	0.43
1:B:437:SER:C	1:B:439:ASN:H	2.21	0.43
1:B:508:ILE:HG22	1:B:509:PRO:HD2	2.01	0.43
1:B:549:LEU:HD11	1:B:554:LYS:HG2	1.99	0.43
1:C:721:SER:O	1:C:722:ILE:C	2.55	0.43
2:D:144:MET:C	2:D:144:MET:SD	2.97	0.43
1:A:323:ASN:HD22	1:A:323:ASN:C	2.22	0.43
1:A:408:LEU:C	1:A:408:LEU:CD2	2.86	0.43
1:A:370:LEU:HD11	1:A:455:TYR:CD1	2.53	0.43
1:A:504:ILE:O	1:A:505:LYS:C	2.55	0.43
1:B:441:VAL:HA	1:B:461:LYS:HG2	2.01	0.43
1:B:326:ILE:HG23	1:B:497:LEU:HD21	2.00	0.43
1:B:607:ASN:O	1:B:610:MET:N	2.52	0.43
1:B:747:ASN:O	1:B:751:TYR:HB3	2.17	0.43
1:C:722:ILE:HG12	1:C:763:LEU:HB2	1.99	0.43
2:E:39:LEU:HG	2:E:39:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:102:ALA:O	2:F:103:ALA:C	2.56	0.43
1:A:302:LEU:HD12	1:A:602:PHE:HE1	1.84	0.43
1:A:712:PHE:CE2	1:A:716:LYS:HE2	2.54	0.43
1:A:700:TYR:HB3	1:A:728:ALA:HB2	2.00	0.43
1:A:730:ASN:C	1:A:732:ILE:H	2.22	0.43
1:A:762:LEU:O	1:A:766:HIS:HB2	2.19	0.43
1:B:744:GLU:HG2	1:C:397:GLU:CG	2.48	0.43
1:C:516:VAL:O	1:C:516:VAL:CG1	2.58	0.43
2:D:79:THR:C	2:D:81:SER:H	2.22	0.43
2:E:44:THR:HG22	2:E:47:GLU:CG	2.45	0.43
2:F:26:THR:HA	2:F:63:ILE:O	2.17	0.43
1:A:345:THR:HG21	1:A:574:VAL:HG22	2.00	0.43
1:A:445:ARG:HH22	1:A:456:LYS:HG2	1.83	0.43
1:A:387:ASN:HB3	1:A:477:MET:HE1	1.99	0.43
1:B:320:ARG:HH21	1:B:320:ARG:CG	2.31	0.43
1:B:323:ASN:ND2	1:B:500:SER:CB	2.82	0.43
1:B:570:THR:O	1:B:572:GLY:N	2.51	0.43
1:B:727:GLN:HG3	1:B:786:GLU:CG	2.48	0.43
1:B:745:TYR:O	1:B:749:PHE:CD1	2.72	0.43
1:C:329:ARG:HD2	1:C:590:ASP:OD2	2.18	0.43
1:C:463:THR:CG2	1:C:464:VAL:N	2.82	0.43
1:C:320:ARG:HA	1:C:598:PRO:O	2.19	0.43
2:D:95:ASP:OD1	2:D:104:GLU:OE2	2.36	0.43
1:A:304:ALA:HB3	1:A:604:LEU:CD1	2.49	0.43
1:A:385:LEU:HD23	1:C:640:LYS:HB3	2.00	0.43
1:A:337:ASN:CB	1:A:412:GLU:OE2	2.64	0.43
1:A:354:SER:N	4:A:999:DOT:O2G	2.42	0.43
1:B:318:ILE:HD12	1:B:319:ALA:H	1.83	0.43
1:B:629:ASN:ND2	1:B:631:SER:CA	2.79	0.43
1:C:324:THR:OG1	1:C:499:PRO:HB3	2.18	0.43
1:C:773:PHE:CD2	1:C:774:LYS:N	2.87	0.43
1:C:793:PHE:O	1:C:794:GLN:C	2.57	0.43
2:E:92:PHE:CZ	2:E:108:VAL:HG11	2.53	0.43
1:A:647:ASP:OD2	2:D:90:ARG:NE	2.52	0.43
1:A:663:PHE:CD1	1:A:752:LEU:HD11	2.54	0.43
1:B:313:ASP:O	1:B:315:PHE:N	2.52	0.43
1:B:555:GLN:O	1:B:558:ASP:HB2	2.19	0.43
1:B:327:LEU:CD2	1:B:595:ILE:HG23	2.48	0.43
1:C:321:GLU:HB3	1:C:322:LEU:HD12	2.00	0.43
1:C:332:ASN:O	1:C:335:ALA:HB3	2.19	0.43
1:C:522:SER:HA	1:C:525:LYS:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:712:PHE:CE2	1:C:716:LYS:HE2	2.54	0.43
1:C:754:GLU:O	1:C:758:ASN:ND2	2.52	0.43
2:F:118:ASP:N	2:F:118:ASP:OD2	2.52	0.43
2:F:9:ILE:HG22	2:F:9:ILE:O	2.19	0.43
1:A:700:TYR:CD1	1:A:728:ALA:HA	2.47	0.42
1:A:747:ASN:O	1:A:748:TYR:C	2.56	0.42
1:A:773:PHE:CD2	1:A:774:LYS:N	2.86	0.42
1:A:776:LEU:CD1	1:A:776:LEU:N	2.81	0.42
1:B:381:GLU:O	1:B:382:LYS:C	2.55	0.42
2:E:118:ASP:N	2:E:118:ASP:OD2	2.52	0.42
2:E:145:MET:HE2	2:E:145:MET:HB2	1.72	0.42
2:F:145:MET:HG3	2:F:145:MET:O	2.19	0.42
1:B:317:LYS:O	1:B:320:ARG:N	2.51	0.42
1:B:415:GLU:O	1:B:417:GLY:N	2.52	0.42
1:B:434:LEU:HA	1:B:445:ARG:HA	2.01	0.42
1:B:726:ILE:O	1:B:729:TYR:HB2	2.19	0.42
1:B:774:LYS:O	1:B:774:LYS:CG	2.66	0.42
2:E:27:ILE:HG13	2:E:63:ILE:HB	2.01	0.42
1:A:340:LYS:O	1:A:342:GLY:N	2.52	0.42
1:A:440:GLN:O	1:A:458:LYS:HE2	2.20	0.42
1:A:721:SER:O	1:A:724:ARG:N	2.53	0.42
1:B:315:PHE:O	1:B:318:ILE:HD12	2.19	0.42
1:B:648:PRO:C	1:B:650:THR:H	2.22	0.42
1:C:666:ASN:HD22	1:C:666:ASN:N	2.15	0.42
1:C:712:PHE:N	1:C:712:PHE:CD1	2.87	0.42
2:D:89:PHE:HD2	2:D:90:ARG:N	2.17	0.42
2:F:27:ILE:HG13	2:F:63:ILE:HB	2.00	0.42
1:A:665:LYS:HE2	2:D:11:GLU:OE1	2.19	0.42
1:B:728:ALA:CA	1:B:731:GLU:CG	2.90	0.42
1:C:549:LEU:CD1	1:C:554:LYS:HE2	2.49	0.42
1:C:691:LYS:HB2	1:C:694:VAL:HG13	2.02	0.42
2:D:89:PHE:CE1	2:D:138:TYR:N	2.87	0.42
2:F:5:THR:O	2:F:9:ILE:CG1	2.66	0.42
1:A:318:ILE:CG2	1:A:322:LEU:HD13	2.49	0.42
1:A:376:GLN:HG3	1:A:376:GLN:H	1.68	0.42
1:A:403:LEU:CD1	1:A:476:VAL:HG21	2.49	0.42
1:B:401:ILE:O	1:B:401:ILE:HG12	2.19	0.42
1:B:757:THR:O	1:B:760:VAL:N	2.52	0.42
1:C:295:VAL:CG2	1:C:296:LEU:N	2.81	0.42
1:C:307:LEU:HA	1:C:492:TYR:HE1	1.85	0.42
1:C:607:ASN:O	1:C:608:TRP:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:121:VAL:C	2:D:123:GLU:H	2.22	0.42
2:E:65:PHE:HB2	2:E:66:PRO:CD	2.45	0.42
2:F:65:PHE:HB2	2:F:66:PRO:CD	2.46	0.42
1:A:699:GLY:O	1:A:702:SER:N	2.53	0.42
1:B:773:PHE:HA	1:B:775:LEU:HD22	2.00	0.42
1:C:415:GLU:C	1:C:417:GLY:H	2.23	0.42
1:C:489:THR:OG1	1:C:490:ALA:N	2.53	0.42
1:A:508:ILE:CG2	1:A:532:LEU:HD13	2.49	0.42
1:B:530:THR:HG22	2:E:92:PHE:CE1	2.54	0.42
1:B:614:PHE:CD2	1:B:614:PHE:C	2.93	0.42
1:C:628:PHE:O	1:C:628:PHE:CD1	2.73	0.42
1:C:664:ILE:N	1:C:664:ILE:HD12	2.35	0.42
2:F:92:PHE:CB	2:F:100:ILE:HD13	2.50	0.42
1:A:463:THR:CG2	1:A:464:VAL:N	2.82	0.42
1:A:523:LEU:O	1:A:525:LYS:N	2.52	0.42
1:B:715:GLU:O	1:B:719:LYS:HB2	2.19	0.42
1:C:502:THR:OG1	1:C:503:GLU:N	2.52	0.42
1:C:667:LEU:HA	1:C:670:ILE:CG2	2.49	0.42
1:C:700:TYR:CD1	1:C:728:ALA:HA	2.55	0.42
1:A:387:ASN:OD1	1:A:477:MET:HE2	2.20	0.42
1:A:484:VAL:CG1	1:A:485:LEU:N	2.82	0.42
1:A:776:LEU:CD1	1:A:776:LEU:H	2.32	0.42
1:A:351:HIS:NE2	4:A:999:DOT:H3B	2.34	0.42
1:B:556:MET:O	1:B:560:LEU:HD12	2.19	0.42
1:B:732:ILE:O	1:B:735:VAL:CG1	2.67	0.42
1:C:740:GLN:N	1:C:740:GLN:CD	2.72	0.42
1:B:525:LYS:NZ	2:E:114:GLU:HG2	2.35	0.42
2:F:129:ASP:OD1	2:F:132:GLY:N	2.44	0.42
2:F:144:MET:SD	2:F:144:MET:O	2.77	0.42
1:C:527:LYS:NZ	2:F:145:MET:C	2.74	0.42
1:A:593:ILE:HB	1:A:605:THR:OG1	2.20	0.42
1:A:712:PHE:N	1:A:712:PHE:CD1	2.88	0.42
1:B:360:VAL:O	1:B:361:ALA:C	2.58	0.42
1:B:751:TYR:CE2	1:B:755:ARG:HG3	2.55	0.42
1:C:363:TYR:HB3	1:C:476:VAL:HG11	2.02	0.42
1:C:387:ASN:OD1	1:C:477:MET:HE2	2.19	0.42
1:C:478:ALA:CA	1:C:488:LEU:HD12	2.50	0.42
1:C:659:THR:C	1:C:701:LEU:HD13	2.40	0.42
2:D:44:THR:HG22	2:D:47:GLU:CG	2.44	0.42
2:F:137:ASN:O	2:F:138:TYR:C	2.57	0.42
1:A:363:TYR:HB3	1:A:476:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:THR:OG1	1:A:503:GLU:N	2.52	0.41
1:B:453:VAL:HG12	1:B:474:ILE:HD12	2.02	0.41
1:B:546:LYS:O	1:B:547:GLY:O	2.38	0.41
1:B:629:ASN:ND2	1:B:630:ARG:N	2.67	0.41
1:B:722:ILE:O	1:B:726:ILE:CG1	2.68	0.41
1:C:593:ILE:HB	1:C:605:THR:OG1	2.20	0.41
2:F:89:PHE:HD2	2:F:90:ARG:N	2.18	0.41
1:A:540:ARG:CZ	1:A:627:TYR:CE1	3.03	0.41
1:A:658:PRO:HG3	1:A:752:LEU:HD22	2.02	0.41
1:A:749:PHE:C	1:A:751:TYR:N	2.72	0.41
1:A:754:GLU:O	1:A:758:ASN:ND2	2.53	0.41
1:B:374:HIS:ND1	1:B:375:GLY:N	2.68	0.41
1:B:629:ASN:HB3	1:B:632:TYR:CZ	2.55	0.41
1:B:762:LEU:O	1:B:766:HIS:HB2	2.20	0.41
1:C:511:LYS:N	1:C:514:ASP:OD1	2.51	0.41
2:D:130:ILE:O	2:D:130:ILE:CG2	2.68	0.41
2:F:68:PHE:CE1	2:F:72:MET:HG2	2.55	0.41
1:A:540:ARG:HB3	1:A:549:LEU:O	2.20	0.41
1:B:410:ILE:HD13	1:B:419:ILE:HD11	2.01	0.41
1:B:461:LYS:HG3	1:B:462:ILE:H	1.85	0.41
1:B:445:ARG:CB	1:B:471:TRP:CZ3	3.02	0.41
1:B:728:ALA:C	1:B:730:ASN:N	2.73	0.41
2:D:99:TYR:HD2	2:D:137:ASN:HB3	1.79	0.41
2:E:137:ASN:O	2:E:138:TYR:C	2.58	0.41
2:F:39:LEU:HG	2:F:39:LEU:O	2.20	0.41
1:A:505:LYS:O	1:A:507:GLN:N	2.54	0.41
1:A:662:GLU:O	1:A:666:ASN:HB2	2.20	0.41
1:B:350:VAL:CG2	1:B:398:ILE:HG13	2.51	0.41
1:B:707:SER:C	1:B:709:ASN:H	2.24	0.41
1:C:340:LYS:O	1:C:342:GLY:N	2.54	0.41
1:C:713:SER:O	1:C:716:LYS:HB3	2.19	0.41
1:A:517:VAL:HG13	2:D:114:GLU:OE2	2.20	0.41
1:A:670:ILE:HD12	1:A:745:TYR:CD1	2.54	0.41
1:B:403:LEU:HB2	1:B:476:VAL:HG23	2.01	0.41
1:B:656:THR:O	1:B:705:TYR:CE1	2.69	0.41
1:C:522:SER:C	1:C:524:GLU:H	2.24	0.41
2:E:121:VAL:C	2:E:123:GLU:H	2.24	0.41
2:F:85:ILE:O	2:F:88:ALA:HB3	2.20	0.41
1:A:583:ASN:ND2	4:A:999:DOT:C1B	2.82	0.41
1:A:661:ALA:O	1:A:662:GLU:C	2.58	0.41
1:B:410:ILE:HD12	1:B:435:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:ASN:CG	1:B:601:GLU:HB2	2.41	0.41
1:B:784:GLU:HB2	1:B:788:ASP:HB2	2.03	0.41
1:C:415:GLU:C	1:C:417:GLY:N	2.74	0.41
1:C:540:ARG:HD3	1:C:582:ASP:CG	2.41	0.41
1:C:581:GLN:O	1:C:629:ASN:HA	2.20	0.41
2:D:92:PHE:O	2:D:94:LYS:N	2.44	0.41
1:A:388:LYS:HD3	1:C:642:TYR:HB2	2.02	0.41
1:B:775:LEU:N	1:B:775:LEU:HD13	2.35	0.41
1:C:540:ARG:CZ	1:C:627:TYR:CE1	3.03	0.41
1:C:691:LYS:HB2	1:C:694:VAL:CG1	2.51	0.41
1:C:747:ASN:O	1:C:748:TYR:C	2.56	0.41
1:B:629:ASN:HD22	1:B:630:ARG:N	2.19	0.41
1:C:463:THR:HB	1:C:467:GLU:N	2.33	0.41
2:D:121:VAL:O	2:D:123:GLU:N	2.54	0.41
2:D:40:GLY:O	2:D:41:GLN:HG2	2.21	0.41
2:D:76:MET:HE2	2:D:79:THR:HG23	2.02	0.41
2:D:79:THR:O	2:D:81:SER:N	2.53	0.41
2:F:44:THR:HG22	2:F:47:GLU:CG	2.45	0.41
1:A:302:LEU:C	1:A:302:LEU:CD2	2.88	0.41
1:A:712:PHE:HD2	1:A:716:LYS:HE2	1.83	0.41
1:A:768:LYS:HD2	1:A:797:ILE:O	2.21	0.41
1:B:616:GLU:CG	1:B:617:LYS:H	2.33	0.41
1:B:745:TYR:HD2	1:B:749:PHE:CZ	2.39	0.41
1:C:407:HIS:CD2	1:C:407:HIS:H	2.35	0.41
1:C:456:LYS:HD3	1:C:471:TRP:CE2	2.56	0.41
1:C:540:ARG:NH1	1:C:630:ARG:HH21	2.18	0.41
1:C:569:TYR:CE2	1:C:574:VAL:HG23	2.56	0.41
2:D:120:GLU:O	2:D:123:GLU:HB2	2.21	0.41
1:B:630:ARG:HE	2:E:87:GLU:CD	2.24	0.41
1:A:323:ASN:ND2	1:A:323:ASN:C	2.74	0.41
1:A:530:THR:CB	2:D:145:MET:HE1	2.51	0.41
1:B:457:THR:HG21	1:B:468:LYS:HA	2.01	0.41
1:B:785:ASN:O	1:B:787:THR:N	2.54	0.41
1:C:421:LYS:HA	1:C:435:LEU:HD23	2.02	0.41
1:C:628:PHE:HD1	1:C:629:ASN:O	2.03	0.41
2:D:92:PHE:CB	2:D:100:ILE:HD13	2.51	0.41
1:A:295:VAL:CG2	1:A:296:LEU:N	2.84	0.41
1:B:574:VAL:O	1:B:574:VAL:HG13	2.21	0.41
1:B:703:ASP:OD1	1:B:703:ASP:O	2.38	0.41
1:B:746:LYS:HG2	1:B:750:GLN:HB2	2.03	0.41
1:C:597:ASN:C	1:C:599:GLU:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:604:LEU:C	1:C:604:LEU:HD23	2.42	0.41
1:C:621:GLY:HA2	2:F:94:LYS:O	2.21	0.41
1:C:540:ARG:HH12	1:C:630:ARG:HH21	1.69	0.41
1:C:657:ILE:CG2	1:C:658:PRO:HD2	2.51	0.41
1:C:777:TYR:CD1	1:C:780:LEU:HD21	2.56	0.41
2:D:108:VAL:O	2:D:112:LEU:HG	2.21	0.41
2:F:121:VAL:O	2:F:123:GLU:N	2.54	0.41
1:A:326:ILE:HG22	1:A:328:PHE:CE1	2.57	0.40
1:A:593:ILE:HG13	1:A:611:THR:HG21	2.03	0.40
1:B:338:LEU:HD11	1:B:409:ARG:CZ	2.51	0.40
1:B:501:LEU:O	1:B:501:LEU:HD23	2.20	0.40
1:B:508:ILE:CG2	1:B:532:LEU:HD22	2.50	0.40
1:B:626:TYR:HD2	1:B:626:TYR:C	2.21	0.40
1:C:324:THR:HG21	1:C:556:MET:HE3	1.98	0.40
1:C:504:ILE:O	1:C:505:LYS:C	2.58	0.40
1:C:629:ASN:CB	1:C:632:TYR:CE2	3.03	0.40
1:C:654:ILE:HG13	1:C:654:ILE:H	1.59	0.40
1:C:773:PHE:O	1:C:774:LYS:C	2.60	0.40
2:D:85:ILE:O	2:D:88:ALA:HB3	2.20	0.40
2:E:108:VAL:O	2:E:112:LEU:HG	2.21	0.40
2:E:115:LYS:HA	2:E:115:LYS:HD2	1.96	0.40
1:A:556:MET:HB2	1:A:556:MET:HE2	1.98	0.40
1:A:777:TYR:CD1	1:A:780:LEU:HD21	2.55	0.40
1:B:322:LEU:O	1:B:323:ASN:C	2.59	0.40
1:B:394:HIS:O	1:B:395:GLU:C	2.59	0.40
1:B:509:PRO:HG2	1:B:512:GLU:CB	2.40	0.40
1:C:494:LEU:HB3	1:C:579:THR:HG22	2.04	0.40
1:C:509:PRO:C	1:C:511:LYS:H	2.25	0.40
1:C:785:ASN:OD1	1:C:786:GLU:HG2	2.22	0.40
1:A:549:LEU:CD1	1:A:554:LYS:HE2	2.51	0.40
1:B:297:LYS:HA	1:B:602:PHE:O	2.21	0.40
1:B:717:LYS:HD2	2:E:132:GLY:H	1.78	0.40
1:C:510:GLN:HE21	1:C:510:GLN:HA	1.86	0.40
1:C:526:GLN:HB3	2:F:144:MET:CE	2.52	0.40
1:C:587:PRO:HB2	1:C:643:ILE:CD1	2.49	0.40
1:C:779:GLN:O	1:C:779:GLN:HG3	2.22	0.40
2:D:145:MET:HB2	2:D:145:MET:HE2	1.83	0.40
2:E:41:GLN:HA	2:E:41:GLN:HE21	1.86	0.40
1:A:597:ASN:C	1:A:599:GLU:H	2.24	0.40
1:A:785:ASN:OD1	1:A:786:GLU:HG2	2.22	0.40
1:B:310:GLU:CB	1:B:567:THR:HG21	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ARG:HB3	1:B:329:ARG:HE	1.61	0.40
1:C:317:LYS:HB2	1:C:317:LYS:HE2	1.96	0.40
1:C:730:ASN:C	1:C:732:ILE:H	2.24	0.40
2:D:102:ALA:O	2:D:103:ALA:C	2.59	0.40
2:E:89:PHE:CD1	2:E:138:TYR:HA	2.57	0.40
1:A:432:TYR:CE1	1:A:471:TRP:CZ3	3.07	0.40
1:A:517:VAL:CA	1:A:525:LYS:NZ	2.85	0.40
1:B:325:TYR:HB2	1:B:498:ALA:HB3	2.03	0.40
1:B:717:LYS:CD	2:E:132:GLY:H	2.32	0.40
1:B:777:TYR:CD1	1:B:780:LEU:CD1	2.92	0.40
1:C:443:GLU:HB2	1:C:458:LYS:HG2	2.02	0.40
1:C:440:GLN:O	1:C:458:LYS:HE2	2.21	0.40
1:C:671:ARG:C	1:C:672:ARG:HE	2.25	0.40
2:E:121:VAL:C	2:E:123:GLU:N	2.72	0.40
2:E:83:GLU:O	2:E:84:GLU:C	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	479/510 (94%)	386 (81%)	71 (15%)	22 (5%)	2	23
1	B	457/510 (90%)	335 (73%)	89 (20%)	33 (7%)	1	13
1	C	499/510 (98%)	384 (77%)	93 (19%)	22 (4%)	2	23
2	D	141/149 (95%)	105 (74%)	28 (20%)	8 (6%)	1	18
2	E	141/149 (95%)	108 (77%)	24 (17%)	9 (6%)	1	17
2	F	141/149 (95%)	108 (77%)	23 (16%)	10 (7%)	1	14
All	All	1858/1977 (94%)	1426 (77%)	328 (18%)	104 (6%)	2	19

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	GLN
1	A	521	ASN
1	B	566	TYR
1	B	571	GLY
1	B	757	THR
1	C	368	GLN
1	C	519	THR
1	C	521	ASN
2	D	82	GLU
2	E	82	GLU
2	F	82	GLU
1	A	378	LEU
1	A	629	ASN
1	A	653	LYS
1	B	299	GLU
1	B	460	GLY
1	B	525	LYS
1	B	547	GLY
1	B	575	VAL
1	B	722	ILE
1	B	734	ASN
1	B	735	VAL
1	B	736	LEU
1	B	739	LYS
1	B	774	LYS
1	B	786	GLU
1	B	796	ILE
1	C	378	LEU
1	C	569	TYR
2	D	93	ASP
2	D	141	PHE
2	E	141	PHE
2	F	93	ASP
2	F	141	PHE
1	A	294	ASP
1	A	317	LYS
1	A	347	GLY
1	A	377	GLN
1	A	510	GLN
1	B	309	PRO
1	B	317	LYS
1	B	354	SER
1	B	463	THR

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Mol	Chain	Res	Type
1	B	563	ALA
1	B	591	ASN
1	B	702	SER
1	B	706	ASN
1	B	793	PHE
1	C	317	LYS
1	C	332	ASN
1	C	623	ASP
2	D	73	ALA
2	D	76	MET
2	D	80	ASP
2	E	73	ALA
2	E	76	MET
2	F	73	ALA
2	F	76	MET
2	F	80	ASP
1	A	330	PRO
1	A	332	ASN
1	A	511	LYS
1	A	520	PRO
1	A	708	ALA
1	B	332	ASN
1	B	361	ALA
1	B	629	ASN
1	B	794	GLN
1	C	347	GLY
1	C	407	HIS
1	C	523	LEU
1	C	708	ALA
2	D	118	ASP
2	E	80	ASP
2	E	118	ASP
2	F	94	LYS
2	F	118	ASP
1	A	503	GLU
1	A	569	TYR
1	A	608	TRP
1	B	694	VAL
1	B	792	VAL
1	C	330	PRO
1	C	377	GLN
1	C	658	PRO

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Mol	Chain	Res	Type
2	D	54	GLU
2	E	49	GLN
2	E	54	GLU
2	E	94	LYS
2	F	54	GLU
1	A	598	PRO
1	A	784	GLU
1	B	295	VAL
1	B	373	LYS
1	C	578	GLY
1	C	608	TRP
2	F	49	GLN
1	A	358	GLY
1	C	537	GLY
1	C	598	PRO
1	C	694	VAL
1	A	534	ILE
1	C	520	PRO
1	C	657	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	433/455 (95%)	394 (91%)	39 (9%)	9	39
1	B	414/455 (91%)	351 (85%)	63 (15%)	3	19
1	C	448/455 (98%)	405 (90%)	43 (10%)	8	37
2	D	121/127 (95%)	113 (93%)	8 (7%)	16	51
2	E	121/127 (95%)	112 (93%)	9 (7%)	13	46
2	F	121/127 (95%)	111 (92%)	10 (8%)	11	42
All	All	1658/1746 (95%)	1486 (90%)	172 (10%)	7	33

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	LEU
1	A	323	ASN
1	A	329	ARG
1	A	376	GLN
1	A	384	ASN
1	A	407	HIS
1	A	423	LYS
1	A	438	ASN
1	A	445	ARG
1	A	455	TYR
1	A	469	PHE
1	A	471	TRP
1	A	485	LEU
1	A	540	ARG
1	A	549	LEU
1	A	557	LEU
1	A	559	ARG
1	A	567	THR
1	A	570	THR
1	A	574	VAL
1	A	620	THR
1	A	622	LYS
1	A	629	ASN
1	A	639	ASN
1	A	646	THR
1	A	656	THR
1	A	659	THR
1	A	666	ASN
1	A	670	ILE
1	A	701	LEU
1	A	709	ASN
1	A	737	LYS
1	A	739	LYS
1	A	759	GLN
1	A	775	LEU
1	A	780	LEU
1	A	781	ASN
1	A	782	PHE
1	A	784	GLU
1	B	305	SER
1	B	320	ARG
1	B	327	LEU
1	B	332	ASN

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Mol	Chain	Res	Type
1	B	333	LYS
1	B	336	THR
1	B	355	SER
1	B	370	LEU
1	B	372	LYS
1	B	382	LYS
1	B	388	LYS
1	B	398	ILE
1	B	401	ILE
1	B	403	LEU
1	B	406	ASP
1	B	425	GLU
1	B	433	TYR
1	B	440	GLN
1	B	447	SER
1	B	455	TYR
1	B	458	LYS
1	B	462	ILE
1	B	463	THR
1	B	477	MET
1	B	480	ASN
1	B	485	LEU
1	B	493	ASP
1	B	501	LEU
1	B	503	GLU
1	B	524	GLU
1	B	531	ASN
1	B	535	LYS
1	B	539	GLU
1	B	540	ARG
1	B	541	LYS
1	B	544	SER
1	B	545	THR
1	B	549	LEU
1	B	552	TRP
1	B	562	GLU
1	B	576	ASN
1	B	577	HIS
1	B	590	ASP
1	B	595	ILE
1	B	611	THR
1	B	626	TYR

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Mol	Chain	Res	Type
1	B	629	ASN
1	B	631	SER
1	B	639	ASN
1	B	646	THR
1	B	711	ILE
1	B	712	PHE
1	B	723	PHE
1	B	724	ARG
1	B	729	TYR
1	B	730	ASN
1	B	731	GLU
1	B	741	ILE
1	B	744	GLU
1	B	775	LEU
1	B	785	ASN
1	B	790	PHE
1	B	794	GLN
1	C	292	ARG
1	C	323	ASN
1	C	329	ARG
1	C	345	THR
1	C	376	GLN
1	C	384	ASN
1	C	401	ILE
1	C	406	ASP
1	C	407	HIS
1	C	423	LYS
1	C	438	ASN
1	C	455	TYR
1	C	469	PHE
1	C	485	LEU
1	C	509	PRO
1	C	510	GLN
1	C	511	LYS
1	C	523	LEU
1	C	526	GLN
1	C	540	ARG
1	C	549	LEU
1	C	557	LEU
1	C	559	ARG
1	C	567	THR
1	C	570	THR

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Mol	Chain	Res	Type
1	C	574	VAL
1	C	620	THR
1	C	622	LYS
1	C	629	ASN
1	C	639	ASN
1	C	646	THR
1	C	650	THR
1	C	656	THR
1	C	657	ILE
1	C	658	PRO
1	C	709	ASN
1	C	737	LYS
1	C	739	LYS
1	C	759	GLN
1	C	775	LEU
1	C	780	LEU
1	C	781	ASN
1	C	782	PHE
2	D	14	GLU
2	D	18	LEU
2	D	22	ASP
2	D	64	ASP
2	D	65	PHE
2	D	89	PHE
2	D	135	GLN
2	D	136	VAL
2	E	14	GLU
2	E	18	LEU
2	E	22	ASP
2	E	64	ASP
2	E	65	PHE
2	E	74	ARG
2	E	89	PHE
2	E	135	GLN
2	E	136	VAL
2	F	14	GLU
2	F	18	LEU
2	F	22	ASP
2	F	41	GLN
2	F	64	ASP
2	F	65	PHE
2	F	74	ARG

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Mol	Chain	Res	Type
2	F	89	PHE
2	F	135	GLN
2	F	136	VAL

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	323	ASN
1	A	349	ASN
1	A	376	GLN
1	A	407	HIS
1	A	438	ASN
1	A	451	ASN
1	A	507	GLN
1	A	510	GLN
1	A	521	ASN
1	A	555	GLN
1	A	581	GLN
1	A	583	ASN
1	A	607	ASN
1	A	629	ASN
1	A	633	ASN
1	A	639	ASN
1	A	666	ASN
1	A	714	GLN
1	A	727	GLN
1	A	730	ASN
1	A	747	ASN
1	A	758	ASN
1	A	759	GLN
1	A	781	ASN
1	B	323	ASN
1	B	332	ASN
1	B	368	GLN
1	B	384	ASN
1	B	407	HIS
1	B	439	ASN
1	B	507	GLN
1	B	518	ASN
1	B	526	GLN
1	B	551	ASN
1	B	553	GLN

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Mol	Chain	Res	Type
1	B	555	GLN
1	B	581	GLN
1	B	629	ASN
1	B	639	ASN
1	B	655	ASN
1	B	706	ASN
1	B	709	ASN
1	B	730	ASN
1	B	734	ASN
1	B	750	GLN
1	B	785	ASN
1	C	323	ASN
1	C	349	ASN
1	C	376	GLN
1	C	377	GLN
1	C	438	ASN
1	C	507	GLN
1	C	510	GLN
1	C	518	ASN
1	C	555	GLN
1	C	581	GLN
1	C	583	ASN
1	C	607	ASN
1	C	629	ASN
1	C	633	ASN
1	C	639	ASN
1	C	655	ASN
1	C	714	GLN
1	C	727	GLN
1	C	730	ASN
1	C	747	ASN
1	C	758	ASN
1	C	759	GLN
1	C	781	ASN
2	D	41	GLN
2	D	42	ASN
2	E	41	GLN
2	F	41	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

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$
4	DOT	A	999	3	36,42,42	5.12	20 (55%)	44,64,64	7.86	22 (50%)
4	DOT	C	1999	3	36,42,42	5.11	20 (55%)	44,64,64	7.86	24 (54%)

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
4	DOT	A	999	3	-	6/26/42/42	0/4/4/4
4	DOT	C	1999	3	-	3/26/42/42	0/4/4/4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	DOT	C1'-C2'	20.34	1.70	1.41
4	C	1999	DOT	C1'-C2'	20.22	1.70	1.41
4	A	999	DOT	C3'-C2'	15.16	1.74	1.40
4	C	1999	DOT	C3'-C2'	15.15	1.74	1.40
4	C	1999	DOT	C8-N7	6.62	1.46	1.34
4	A	999	DOT	C8-N7	6.57	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	DOT	C6'-C1'	6.49	1.50	1.39
4	C	1999	DOT	C6'-C1'	6.48	1.50	1.39
4	A	999	DOT	C2-N1	5.02	1.43	1.33
4	C	1999	DOT	C2-N1	5.00	1.43	1.33
4	A	999	DOT	C2B-C3B	-4.69	1.42	1.52
4	C	1999	DOT	C2B-C3B	-4.65	1.42	1.52
4	C	1999	DOT	C5'-C4'	4.35	1.49	1.38
4	A	999	DOT	C5'-C4'	4.35	1.49	1.38
4	A	999	DOT	C5'-C6'	4.14	1.47	1.38
4	C	1999	DOT	C5'-C6'	4.13	1.47	1.38
4	C	1999	DOT	O3'-C3B	4.11	1.53	1.46
4	A	999	DOT	O3'-C3B	4.05	1.53	1.46
4	A	999	DOT	C2-N3	3.98	1.38	1.32
4	C	1999	DOT	C2-N3	3.98	1.38	1.32
4	A	999	DOT	C5-C4	3.39	1.49	1.40
4	C	1999	DOT	C5-C4	3.33	1.49	1.40
4	A	999	DOT	PA-O1A	3.24	1.62	1.50
4	C	1999	DOT	PA-O1A	3.23	1.62	1.50
4	A	999	DOT	O3'-C'	3.18	1.41	1.34
4	C	1999	DOT	O3'-C'	3.17	1.41	1.34
4	A	999	DOT	C4'-C3'	3.14	1.45	1.38
4	C	1999	DOT	C4'-C3'	3.07	1.45	1.38
4	C	1999	DOT	C3B-C4B	2.89	1.63	1.52
4	A	999	DOT	C3B-C4B	2.87	1.63	1.52
4	C	1999	DOT	C1'-C'	2.79	1.56	1.50
4	A	999	DOT	C1'-C'	2.79	1.56	1.50
4	C	1999	DOT	C1B-N9	2.56	1.57	1.49
4	A	999	DOT	C1B-N9	2.55	1.56	1.49
4	C	1999	DOT	C5B-C4B	2.54	1.59	1.51
4	A	999	DOT	C5B-C4B	2.53	1.59	1.51
4	C	1999	DOT	PB-O1B	-2.40	1.42	1.50
4	A	999	DOT	PB-O1B	-2.39	1.42	1.50
4	A	999	DOT	O1'-C'	2.15	1.28	1.22
4	C	1999	DOT	O1'-C'	2.14	1.28	1.22

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	DOT	C3'-C2'-N2'	26.73	171.91	120.13
4	C	1999	DOT	C3'-C2'-N2'	26.72	171.90	120.13
4	A	999	DOT	C3'-C2'-C1'	-24.77	94.08	118.10
4	C	1999	DOT	C3'-C2'-C1'	-24.72	94.13	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	DOT	C1'-C2'-N2'	-24.51	90.26	122.67
4	C	1999	DOT	C1'-C2'-N2'	-24.48	90.30	122.67
4	C	1999	DOT	C2'-C1'-C'	-12.11	104.95	121.02
4	A	999	DOT	C2'-C1'-C'	-12.11	104.95	121.02
4	C	1999	DOT	C6'-C1'-C2'	11.96	131.62	118.93
4	A	999	DOT	C6'-C1'-C2'	11.96	131.61	118.93
4	C	1999	DOT	O3'-C'-O1'	-10.36	106.63	123.53
4	A	999	DOT	O3'-C'-O1'	-10.33	106.67	123.53
4	A	999	DOT	C4'-C3'-C2'	9.67	134.54	121.04
4	C	1999	DOT	C4'-C3'-C2'	9.64	134.50	121.04
4	C	1999	DOT	O3'-C'-C1'	7.98	124.12	111.69
4	A	999	DOT	O3'-C'-C1'	7.97	124.10	111.69
4	C	1999	DOT	N6-C6-N1	-6.97	104.11	118.57
4	A	999	DOT	N6-C6-N1	-6.91	104.23	118.57
4	C	1999	DOT	C6'-C1'-C'	-4.37	109.69	118.66
4	A	999	DOT	C2B-C1B-N9	4.36	124.32	114.27
4	A	999	DOT	C6'-C1'-C'	-4.35	109.72	118.66
4	A	999	DOT	C3B-O3'-C'	4.32	124.89	117.38
4	C	1999	DOT	C3B-O3'-C'	4.32	124.88	117.38
4	A	999	DOT	O3'-C3B-C4B	4.07	118.83	109.42
4	C	1999	DOT	O3'-C3B-C4B	4.06	118.80	109.42
4	C	1999	DOT	C3B-C2B-C1B	3.95	110.52	102.93
4	A	999	DOT	C3B-C2B-C1B	3.93	110.49	102.93
4	A	999	DOT	O3'-C3B-C2B	3.88	118.44	109.18
4	C	1999	DOT	O3'-C3B-C2B	3.88	118.43	109.18
4	C	1999	DOT	O3G-PG-O3B	-3.62	92.50	104.64
4	A	999	DOT	O5'-PA-O1A	-3.29	96.21	109.07
4	C	1999	DOT	O5'-PA-O1A	-3.28	96.23	109.07
4	C	1999	DOT	C4-C5-N7	3.27	112.81	109.40
4	C	1999	DOT	C5-C6-N6	3.27	125.32	120.35
4	A	999	DOT	C5-C6-N6	3.26	125.30	120.35
4	A	999	DOT	C4-C5-N7	3.20	112.73	109.40
4	C	1999	DOT	O2A-PA-O1A	3.08	127.44	112.24
4	A	999	DOT	O2A-PA-O1A	3.07	127.44	112.24
4	C	1999	DOT	C5-C6-N1	-3.04	113.45	120.35
4	A	999	DOT	C5-C6-N1	-3.03	113.48	120.35
4	C	1999	DOT	C2B-C1B-N9	2.49	120.01	114.27
4	A	999	DOT	C5B-C4B-C3B	2.46	120.14	114.53
4	C	1999	DOT	C5B-C4B-C3B	2.44	120.10	114.53
4	C	1999	DOT	O1G-PG-O3B	2.15	111.83	104.64
4	A	999	DOT	C4'-C5'-C6'	-2.13	116.94	120.19
4	C	1999	DOT	C4'-C5'-C6'	-2.13	116.95	120.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

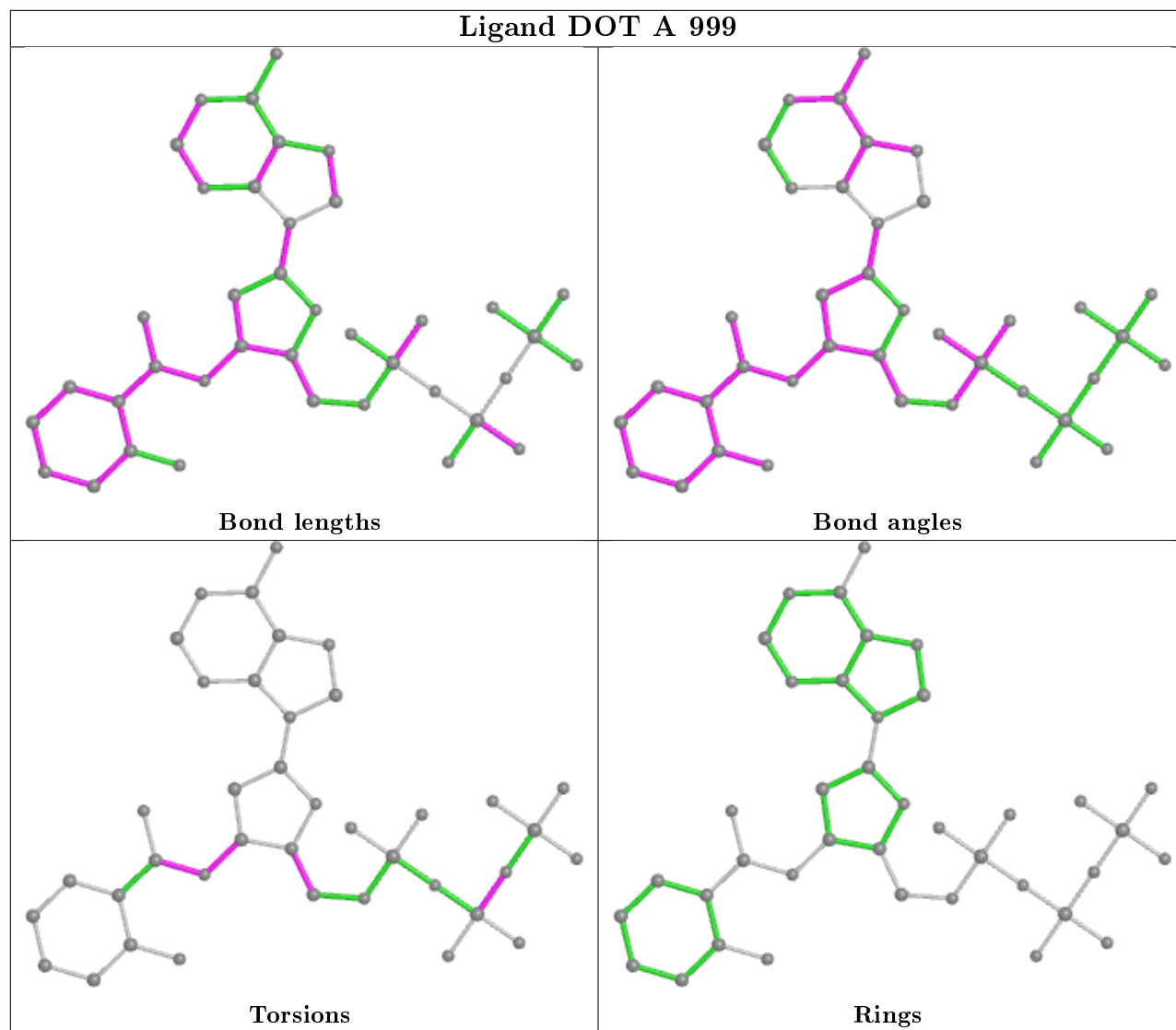
Mol	Chain	Res	Type	Atoms
4	C	1999	DOT	O4'-C4B-C5B-O5'
4	C	1999	DOT	C2B-C3B-O3'-C'
4	A	999	DOT	O4'-C4B-C5B-O5'
4	A	999	DOT	O1'-C'-O3'-C3B
4	A	999	DOT	C1'-C'-O3'-C3B
4	A	999	DOT	C3B-C4B-C5B-O5'
4	C	1999	DOT	O1'-C'-O3'-C3B
4	A	999	DOT	PG-O3B-PB-O2B
4	A	999	DOT	C2B-C3B-O3'-C'

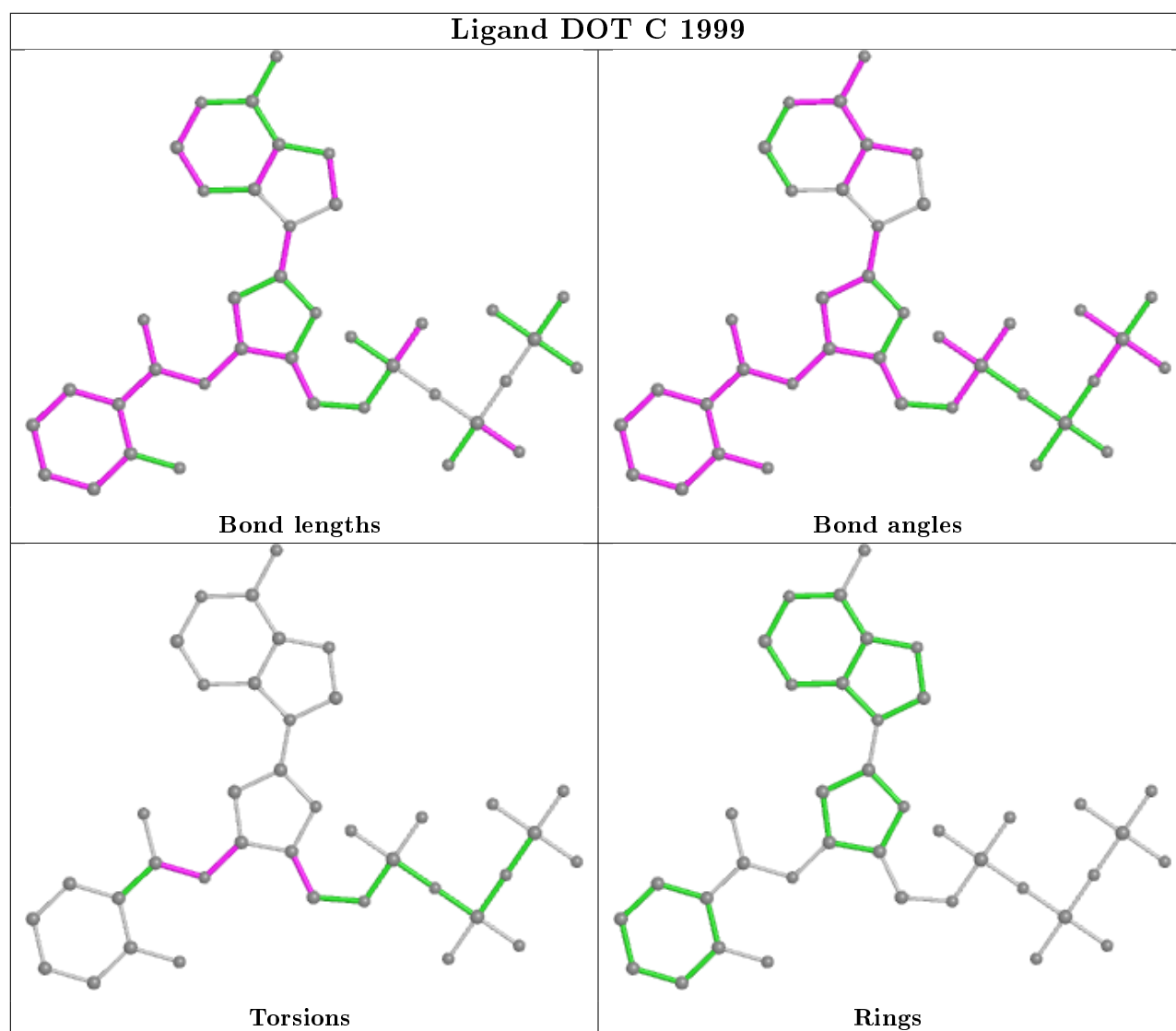
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	DOT	8	0
4	C	1999	DOT	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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	485/510 (95%)	-0.44	1 (0%) 95 91	14, 58, 137, 162	16 (3%)
1	B	457/510 (89%)	-0.28	13 (2%) 53 37	13, 58, 158, 165	12 (2%)
1	C	491/510 (96%)	-0.38	3 (0%) 89 81	13, 61, 137, 162	19 (3%)
2	D	143/149 (95%)	0.13	5 (3%) 44 29	49, 143, 180, 183	0
2	E	143/149 (95%)	0.17	10 (6%) 16 9	48, 144, 180, 182	0
2	F	143/149 (95%)	0.16	8 (5%) 24 14	49, 143, 180, 183	0
All	All	1862/1977 (94%)	-0.25	40 (2%) 63 48	13, 66, 166, 183	47 (2%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	697	ILE	5.4
2	F	62	THR	4.1
2	E	79	THR	3.5
2	E	21	LYS	3.3
2	E	19	PHE	3.3
2	F	46	ALA	3.2
1	B	778	LYS	3.2
2	E	62	THR	3.1
2	E	61	GLY	3.0
1	C	744	GLU	3.0
1	B	702	SER	2.9
2	D	58	ASP	2.7
1	B	741	ILE	2.7
1	C	708	ALA	2.7
1	B	740	GLN	2.6
2	F	61	GLY	2.6
2	E	60	ASN	2.6
2	E	55	VAL	2.5
2	F	53	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	658	PRO	2.5
1	C	741	ILE	2.5
1	B	776	LEU	2.5
2	F	50	ASP	2.5
2	F	19	PHE	2.5
2	F	28	THR	2.5
2	E	23	GLY	2.4
2	E	59	GLY	2.4
2	D	43	PRO	2.4
1	B	774	LYS	2.3
1	B	783	THR	2.2
1	B	779	GLN	2.2
2	D	49	GLN	2.2
2	F	44	THR	2.1
1	B	737	LYS	2.1
2	D	53	ASN	2.1
2	D	30	LYS	2.1
2	E	42	ASN	2.1
1	A	296	LEU	2.1
1	B	521	ASN	2.1
1	B	773	PHE	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

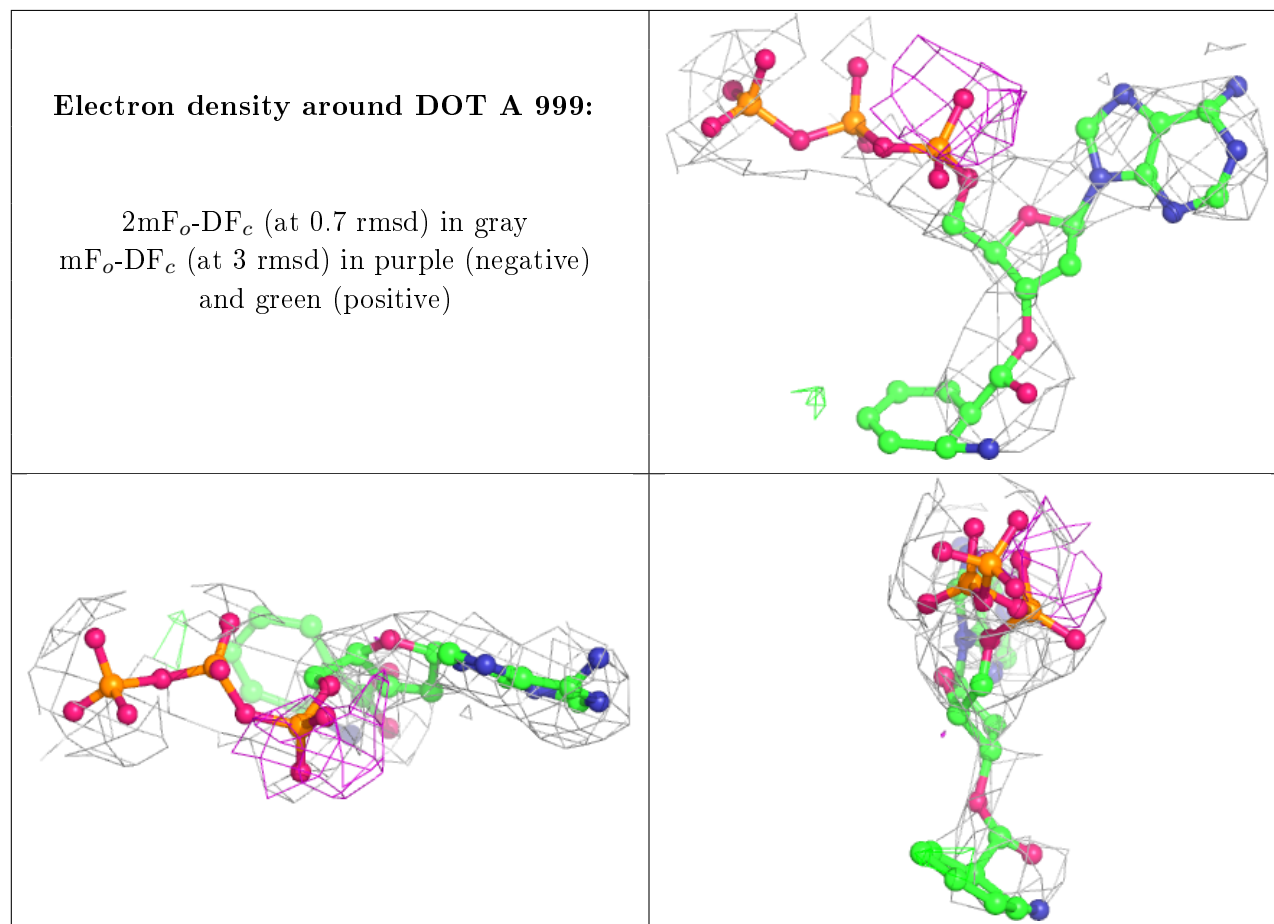
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CA	F	805	1/1	0.86	0.12	82,82,82,82	0
5	CA	E	802	1/1	0.86	0.04	75,75,75,75	0

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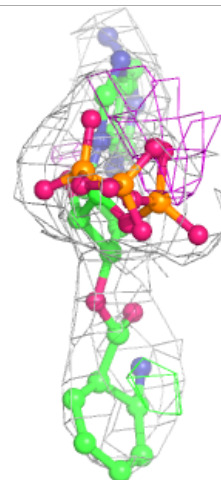
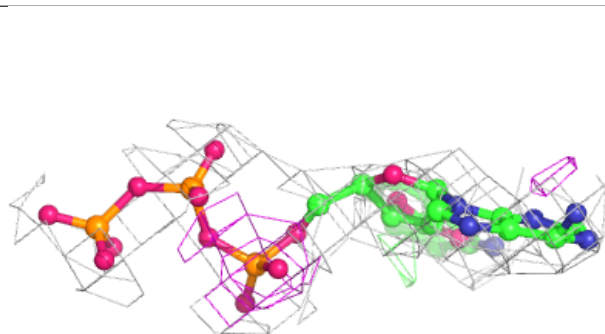
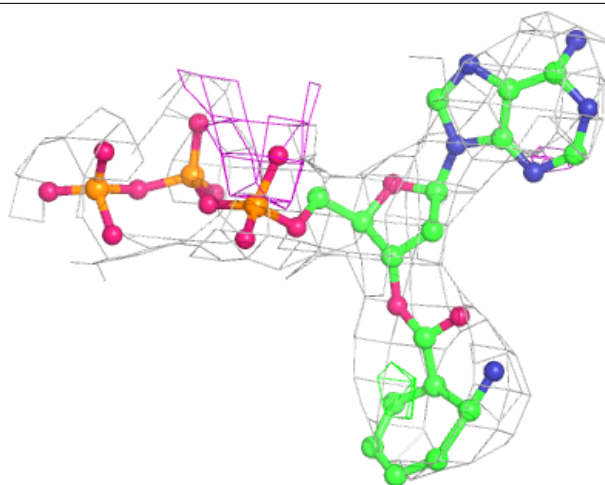
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DOT	A	999	39/39	0.87	0.29	52,80,92,92	0
3	YB	A	901	1/1	0.87	0.08	135,135,135,135	0
5	CA	F	804	1/1	0.88	0.14	70,70,70,70	0
4	DOT	C	1999	39/39	0.88	0.26	45,80,83,84	0
5	CA	D	800	1/1	0.94	0.11	65,65,65,65	0
3	YB	C	903	1/1	0.96	0.04	124,124,124,124	0
5	CA	D	801	1/1	0.98	0.04	51,51,51,51	0
3	YB	B	902	1/1	0.98	0.09	142,142,142,142	0
5	CA	E	803	1/1	0.99	0.06	70,70,70,70	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around DOT C 1999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.