



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:27 PM GMT

PDB ID : 4LNK  
Title : B. subtilis glutamine synthetase structures reveal large active site conformational changes and basis for isoenzyme specific regulation: structure of GS-glutamate-AMPPCP complex  
Authors : Schumacher, M.A.; Chinnam, N.; Tonthat, N.; Fisher, S.; Wray, L.  
Deposited on : 2013-07-11  
Resolution : 2.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

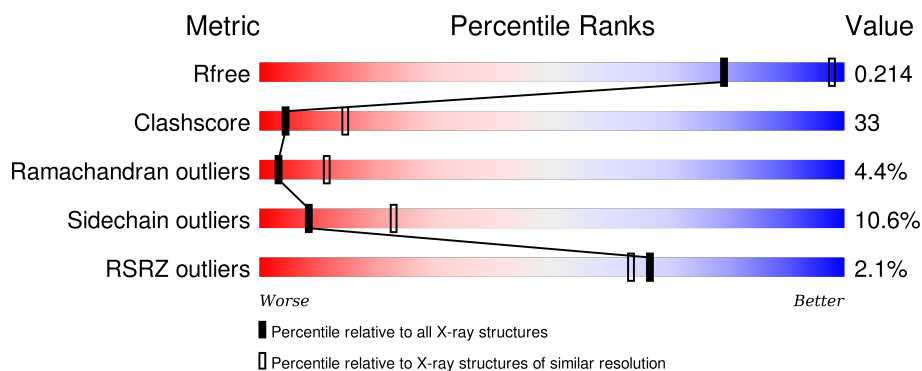
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.87 Å.

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



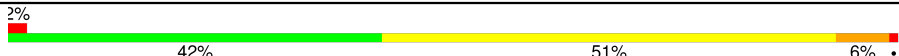
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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

Mol	Chain	Length	Quality of chain
1	A	443	<div> <div>2%</div> <div> <div></div> <div>47%</div> <div>43%</div> <div>9%</div> </div> </div>
1	B	443	<div> <div>2%</div> <div> <div></div> <div>44%</div> <div>50%</div> <div>6%</div> </div> </div>
1	C	443	<div> <div>2%</div> <div> <div></div> <div>44%</div> <div>47%</div> <div>9%</div> </div> </div>
1	D	443	<div> <div>2%</div> <div> <div></div> <div>46%</div> <div>43%</div> <div>10%</div> </div> </div>
1	E	443	<div> <div>3%</div> <div> <div></div> <div>47%</div> <div>43%</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	443	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLU	B	501	-	-	-	X
2	GLU	C	501	-	-	X	X
2	GLU	D	501	-	-	X	X
2	GLU	E	501	-	-	-	X
2	GLU	F	501	-	-	-	X
3	ADP	A	502	-	-	-	X
3	ADP	D	502	-	-	-	X
3	ADP	E	502	-	-	-	X
4	MG	B	503	-	-	-	X
4	MG	C	503	-	-	-	X
4	MG	D	503	-	-	-	X
5	SO4	A	506	-	-	-	X

## 2 Entry composition [i](#)

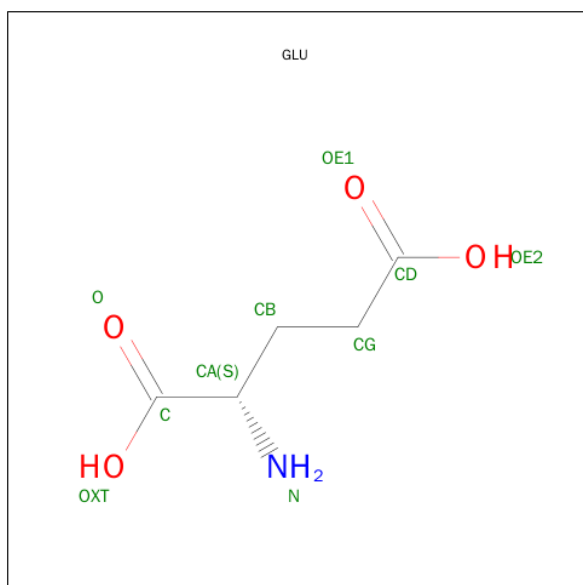
There are 6 unique types of molecules in this entry. The entry contains 21514 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamine synthetase.

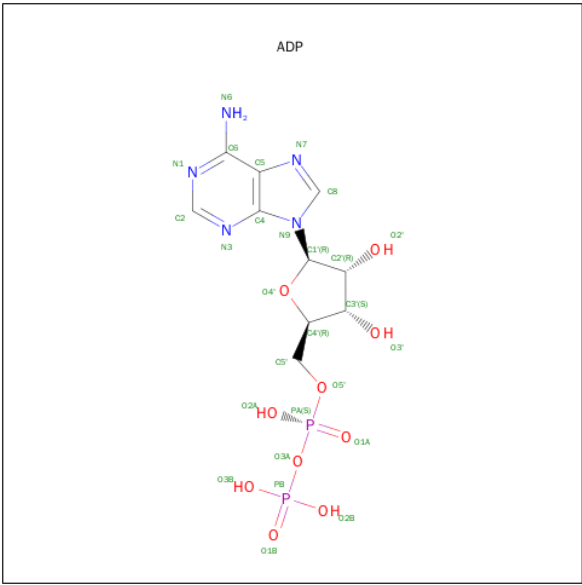
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	B	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	C	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	D	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	E	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	F	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			9	5	1	3		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0

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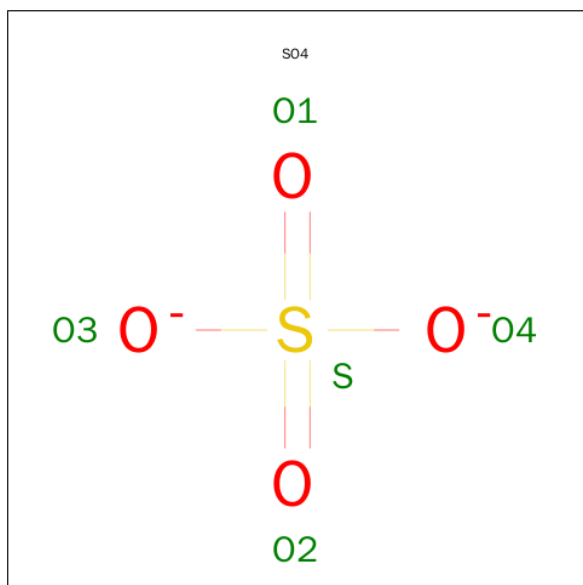
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Mg	0	0
			2	2		
4	E	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		
4	F	2	Total	Mg	0	0
			2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	O	S	0	0
			5	4	1		

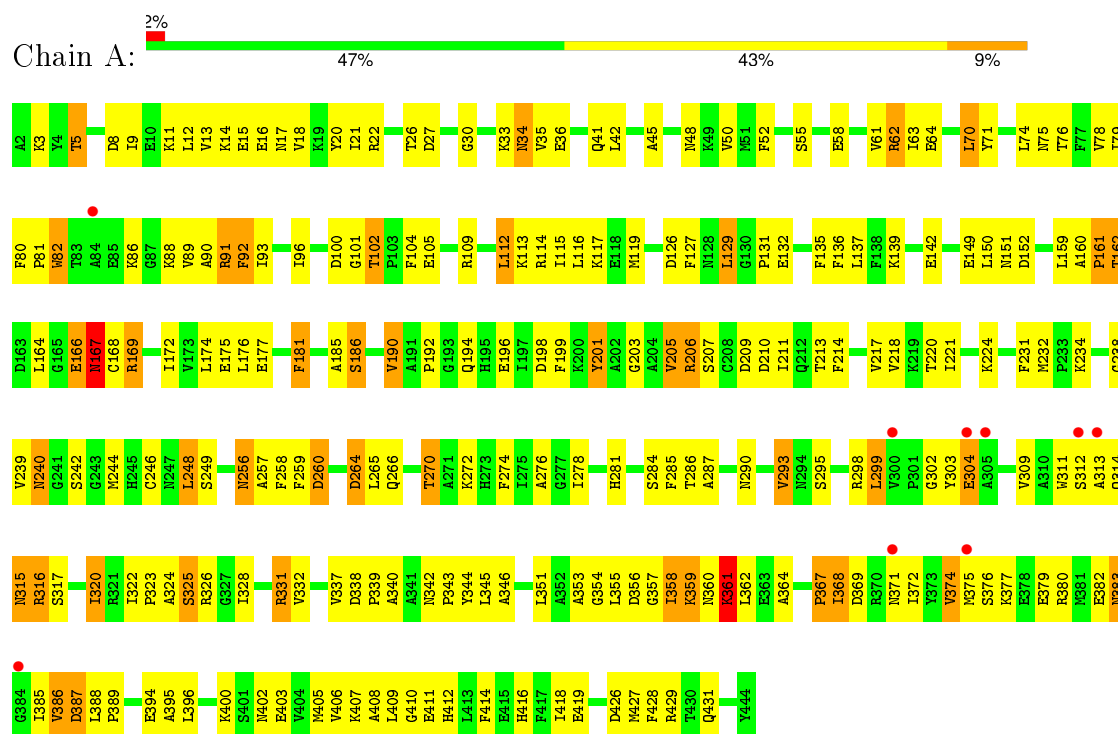
- Molecule 6 is water.

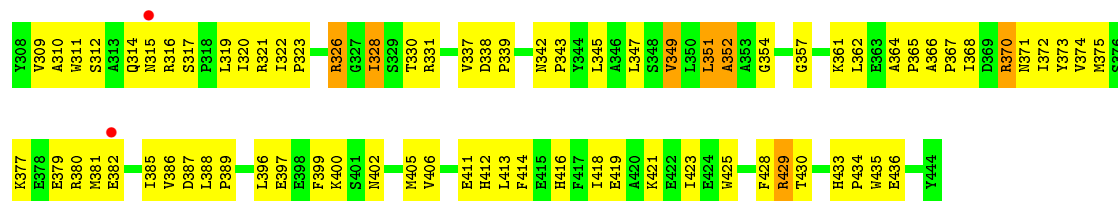
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	12	Total	O		0	0
			12	12			
6	B	7	Total	O		0	0
			7	7			
6	C	6	Total	O		0	0
			6	6			
6	D	10	Total	O		0	0
			10	10			
6	E	11	Total	O		0	0
			11	11			
6	F	11	Total	O		0	0
			11	11			

### 3 Residue-property plots

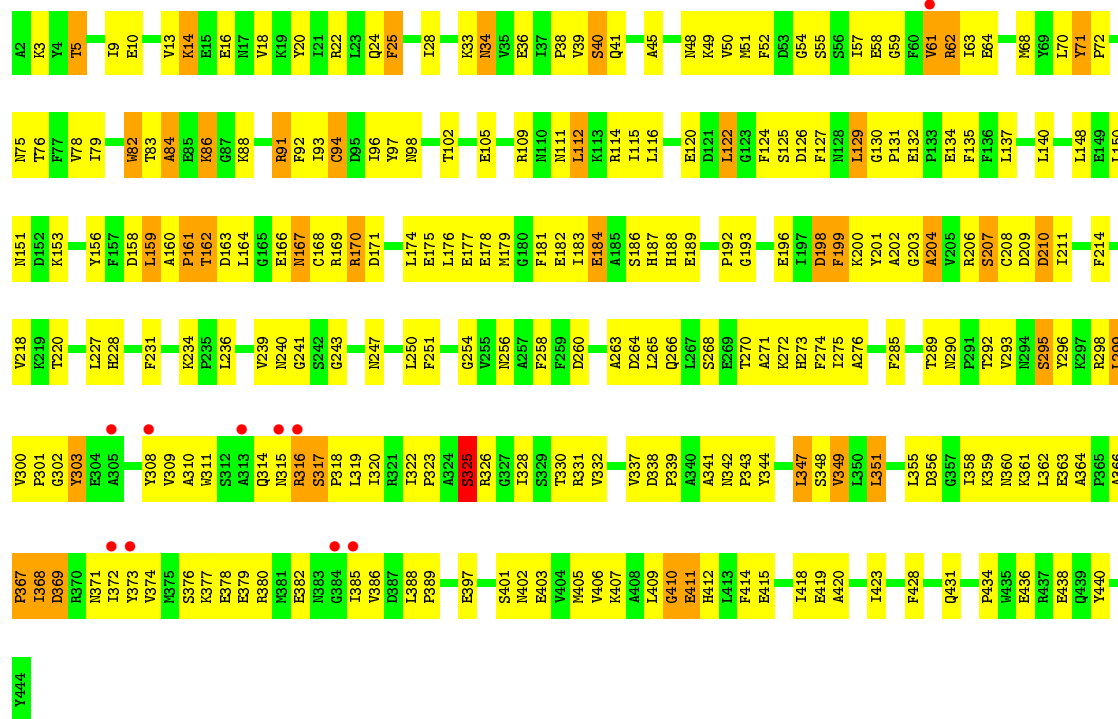
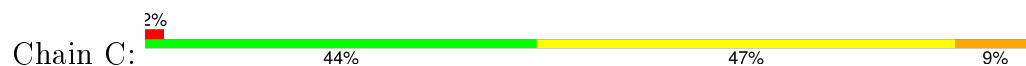
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Glutamine synthetase

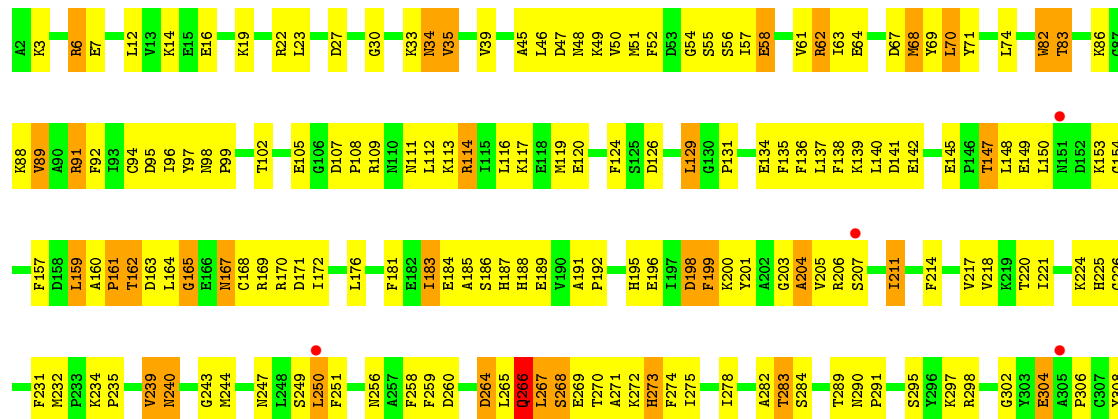


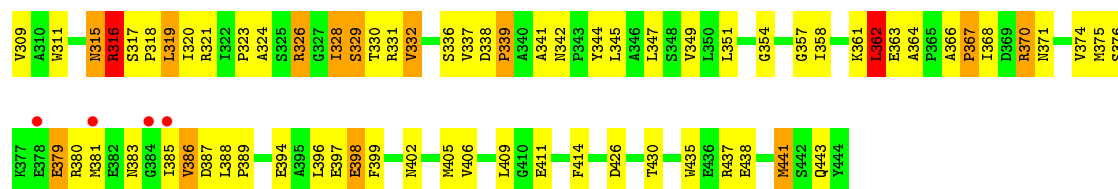


• Molecule 1: Glutamine synthetase

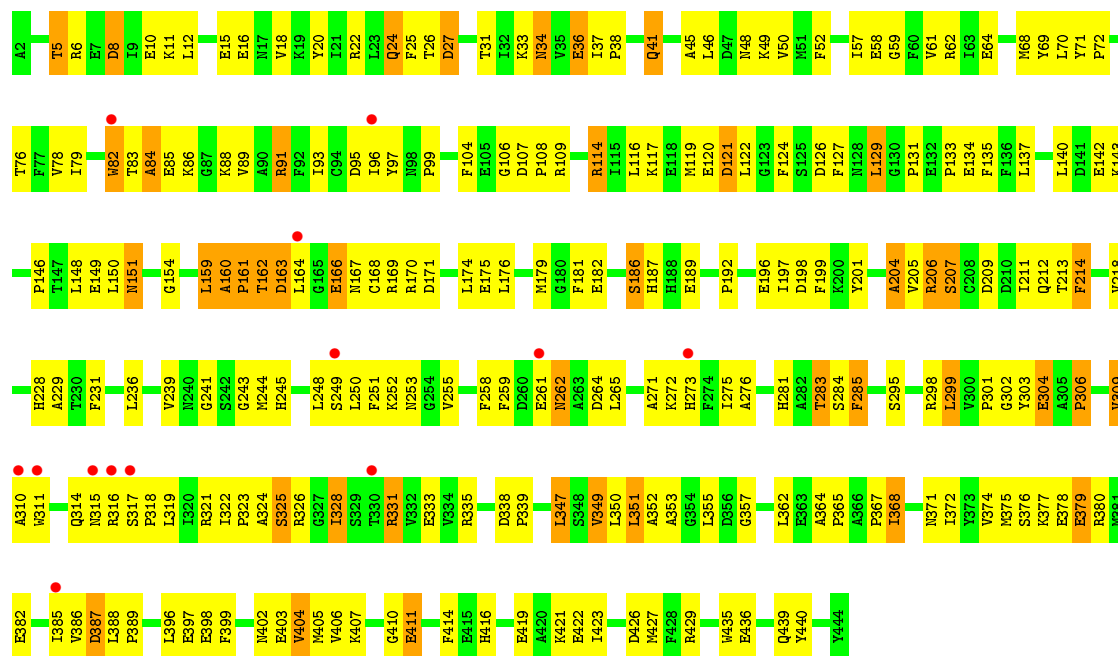


• Molecule 1: Glutamine synthetase

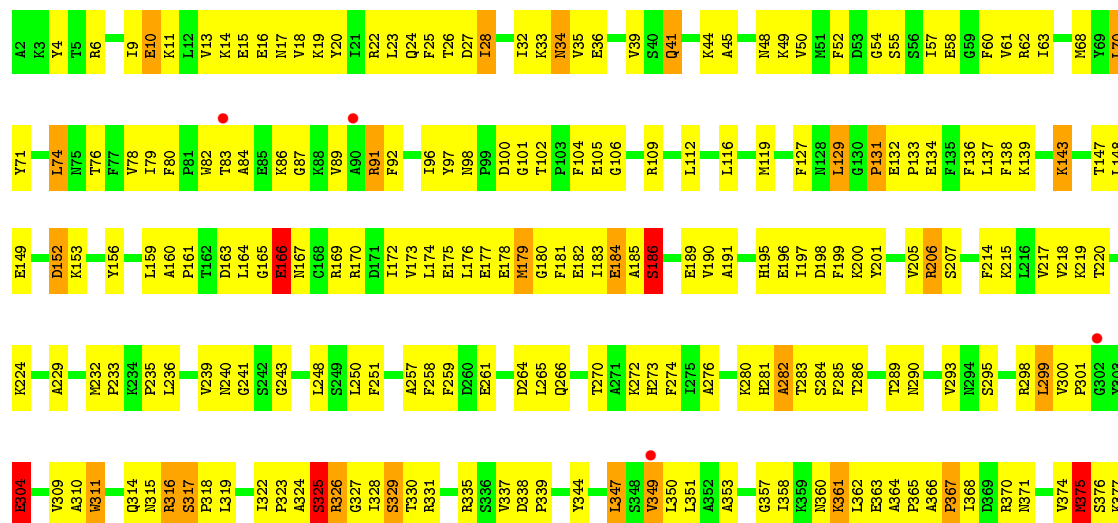




• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase



E378	E379	M381	N383	G384	V386	D387	L388	P389	L396	F399	K400	S401	N402	E403	V404	M405	V406	K407	A408	L409	G410	E411	H412	L413	F414	E419	A420	K421	E422	I423	E424	W425	D426	M427	F428	Q431	P434	W435	E436	R437	E438	Q439	Y440	M441	Y444
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.50Å 240.86Å 207.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	120.06 – 2.87 120.07 – 2.87	Depositor EDS
% Data completeness (in resolution range)	91.8 (120.06-2.87) 91.5 (120.07-2.87)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.195 , 0.236 0.194 , 0.214	Depositor DCC
$R_{free}$ test set	9598 reflections (15.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.7	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.2	EDS
Estimated twinning fraction	0.278 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.250 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.207 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
Reported twinning fraction	0.278 for -1/2*h+1/2*k,3/2*h+1/2*k,-l	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	2 of 72956 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	21514	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.84 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.5001e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, ADP

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	0.50	0/3618	0.64	0/4895
1	B	0.50	0/3618	0.64	0/4895
1	C	0.49	0/3618	0.64	0/4895
1	D	0.47	0/3618	0.64	0/4895
1	E	0.50	0/3618	0.64	1/4895 (0.0%)
1	F	0.50	0/3618	0.66	0/4895
All	All	0.49	0/21708	0.64	1/29370 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	160	ALA	C-N-CD	-5.41	108.69	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	160	ALA	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3535	0	3466	226	0
1	B	3535	0	3466	242	0
1	C	3535	0	3466	231	0
1	D	3535	0	3466	227	0
1	E	3535	0	3466	267	0
1	F	3535	0	3466	255	0
2	A	10	0	5	0	0
2	B	9	0	5	0	0
2	C	10	0	5	4	0
2	D	10	0	5	4	0
2	E	10	0	5	3	0
2	F	9	0	5	1	0
3	A	27	0	12	3	0
3	B	27	0	12	3	0
3	C	27	0	12	5	0
3	D	27	0	12	1	0
3	E	27	0	12	4	0
3	F	27	0	12	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	10	0	0	0	0
5	E	5	0	0	1	0
6	A	12	0	0	0	0
6	B	7	0	0	0	0
6	C	6	0	0	1	0
6	D	10	0	0	1	0
6	E	11	0	0	0	0
6	F	11	0	0	0	0
All	All	21514	0	20898	1379	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 33.

All (1379) 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:F:55:SER:HB2	1:F:62:ARG:HG3	1.32	1.10
1:C:182:GLU:HG3	1:C:200:LYS:HG3	1.32	1.08
1:C:162:THR:HG21	1:D:220:THR:OG1	1.54	1.07
1:D:328:ILE:HD13	1:D:328:ILE:H	1.14	1.05
1:B:231:PHE:HB3	1:B:339:PRO:HB2	1.40	1.03
1:A:27:ASP:HB3	1:A:33:LYS:HD2	1.38	1.02
1:C:160:ALA:CB	1:C:169:ARG:HH22	1.74	1.00
1:C:274:PHE:HB2	1:C:358:ILE:HD11	1.45	0.95
1:F:265:LEU:HD12	1:F:272:LYS:HE2	1.47	0.94
1:C:234:LYS:HE3	1:C:239:VAL:O	1.68	0.93
1:F:24:GLN:NE2	1:F:32:ILE:HD11	1.84	0.93
1:B:258:PHE:HA	1:B:271:ALA:HB2	1.47	0.93
1:F:74:LEU:HD22	1:F:74:LEU:H	1.33	0.91
1:D:57:ILE:HD11	1:D:96:ILE:HG12	1.53	0.91
1:C:160:ALA:HB3	1:C:169:ARG:HH12	1.37	0.90
1:E:380:ARG:O	1:E:385:ILE:HB	1.71	0.90
1:F:34:ASN:C	1:F:34:ASN:HD22	1.73	0.90
1:E:315:ASN:HB3	1:E:318:PRO:HB3	1.52	0.90
1:F:24:GLN:HE21	1:F:32:ILE:HD11	1.36	0.90
1:A:169:ARG:HG3	1:A:169:ARG:HH21	1.36	0.89
1:C:160:ALA:HB1	1:C:161:PRO:HD2	1.54	0.88
1:D:63:ILE:HG22	1:D:64:GLU:HG3	1.54	0.88
1:A:325:SER:O	1:A:326:ARG:HD3	1.74	0.88
1:D:318:PRO:HG2	1:D:321:ARG:HB2	1.53	0.88
1:B:13:VAL:HG13	1:B:18:VAL:HB	1.55	0.87
1:E:12:LEU:O	1:E:16:GLU:HB2	1.73	0.87
1:C:160:ALA:HB2	1:C:169:ARG:HH22	1.36	0.87
1:A:13:VAL:HG13	1:A:18:VAL:HB	1.58	0.85
1:B:160:ALA:CB	1:B:169:ARG:HH12	1.89	0.85
1:A:176:LEU:O	1:A:181:PHE:HB2	1.76	0.85
1:A:105:GLU:HG2	1:A:412:HIS:HB2	1.58	0.84
1:F:379:GLU:OE1	1:F:379:GLU:HA	1.76	0.84
1:B:160:ALA:HB3	1:B:169:ARG:HH12	1.42	0.83
1:E:83:THR:HG22	1:E:88:LYS:HG2	1.60	0.83
1:A:9:ILE:HD12	1:A:74:LEU:HG	1.58	0.83
1:C:130:GLY:HA3	3:C:502:ADP:O2'	1.79	0.83
1:B:164:LEU:HD12	1:C:220:THR:HG22	1.59	0.82
1:C:131:PRO:HG3	1:C:211:ILE:HD11	1.59	0.82
1:A:114:ARG:HH12	1:A:115:ILE:HD11	1.44	0.82
1:C:52:PHE:CD1	1:C:70:LEU:HD22	2.16	0.81
3:C:502:ADP:O2B	1:D:51:MET:HG3	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LEU:HD13	1:B:192:PRO:HB2	1.63	0.81
1:A:127:PHE:CD2	1:A:351:LEU:HD13	2.15	0.81
1:F:176:LEU:O	1:F:181:PHE:HB2	1.79	0.81
1:B:178:GLU:OE2	1:C:86:LYS:HD2	1.81	0.81
1:B:27:ASP:HB3	1:B:33:LYS:HE3	1.63	0.80
1:B:264:ASP:HB3	1:B:272:LYS:NZ	1.96	0.80
1:C:111:ASN:O	1:C:115:ILE:HD13	1.81	0.80
1:D:164:LEU:HD23	1:E:82:TRP:HB3	1.64	0.80
1:E:131:PRO:HD2	1:E:199:PHE:HB2	1.63	0.80
1:B:80:PHE:HB3	1:B:82:TRP:CE3	2.17	0.80
1:E:121:ASP:O	1:E:122:LEU:HD23	1.82	0.80
1:F:325:SER:HB2	1:F:331:ARG:HH22	1.47	0.80
1:F:58:GLU:O	1:F:61:VAL:HG22	1.82	0.79
1:D:51:MET:HE1	1:D:67:ASP:HB3	1.63	0.79
1:F:272:LYS:O	1:F:364:ALA:HB2	1.82	0.79
1:D:243:GLY:HA3	1:D:298:ARG:NH1	1.98	0.79
1:D:54:GLY:HA3	1:D:68:MET:HG3	1.64	0.79
1:F:368:ILE:HG12	1:F:385:ILE:HD11	1.63	0.79
1:E:206:ARG:HD3	1:E:206:ARG:O	1.81	0.79
1:F:329:SER:HB3	3:F:502:ADP:O1B	1.83	0.79
1:E:58:GLU:HG2	1:E:416:HIS:CD2	2.18	0.79
1:C:371:ASN:HB3	1:C:374:VAL:HG22	1.62	0.79
1:A:162:THR:HG21	1:B:220:THR:OG1	1.83	0.78
1:A:406:VAL:HG22	1:A:414:PHE:CE1	2.19	0.78
1:C:236:LEU:O	1:C:239:VAL:HG22	1.84	0.78
1:A:311:TRP:HB3	1:A:320:ILE:HB	1.64	0.78
1:E:243:GLY:HA2	1:E:298:ARG:NH1	1.97	0.78
1:D:406:VAL:HG22	1:D:414:PHE:CE1	2.20	0.77
1:B:131:PRO:HG3	1:B:211:ILE:HD11	1.65	0.77
1:C:52:PHE:HE1	1:C:70:LEU:HD13	1.48	0.77
1:C:236:LEU:HB2	1:C:239:VAL:CG2	2.14	0.77
1:E:167:ASN:HB3	1:E:170:ARG:HB3	1.66	0.77
1:D:55:SER:O	1:D:62:ARG:HB3	1.84	0.76
1:C:406:VAL:HG22	1:C:414:PHE:CE1	2.20	0.76
1:A:293:VAL:HG11	1:A:428:PHE:CD1	2.21	0.76
1:A:115:ILE:HG22	1:A:351:LEU:HD23	1.67	0.76
1:B:372:ILE:HD13	1:B:385:ILE:HD13	1.68	0.76
1:A:206:ARG:HH11	1:A:206:ARG:CG	1.98	0.76
1:B:258:PHE:CA	1:B:271:ALA:HB2	2.16	0.75
1:C:93:ILE:HD12	1:C:209:ASP:HB3	1.66	0.75
1:F:357:GLY:HA2	1:F:362:LEU:HD22	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:PRO:O	1:C:369:ASP:N	2.19	0.75
1:C:91:ARG:HD2	1:C:92:PHE:N	2.01	0.75
1:F:11:LYS:O	1:F:15:GLU:HG3	1.86	0.75
1:E:272:LYS:HA	1:E:275:ILE:HD12	1.67	0.75
1:F:184:GLU:HG2	1:F:200:LYS:HE3	1.66	0.75
1:F:377:LYS:HG3	1:F:380:ARG:HH21	1.50	0.75
1:D:160:ALA:HB1	1:D:161:PRO:CD	2.16	0.75
3:B:502:ADP:O3B	1:C:51:MET:HG3	1.85	0.75
1:E:375:MET:HG3	1:E:380:ARG:HG2	1.67	0.75
1:A:131:PRO:HD2	1:A:199:PHE:HB2	1.67	0.75
1:A:150:LEU:HD13	1:A:192:PRO:O	1.86	0.75
1:C:150:LEU:HD13	1:C:192:PRO:O	1.86	0.75
1:D:134:GLU:OE1	2:D:501:GLU:N	2.20	0.75
1:A:309:VAL:HG23	1:A:386:VAL:O	1.87	0.75
1:D:406:VAL:HG22	1:D:414:PHE:HE1	1.51	0.75
1:E:20:TYR:HB3	1:E:89:VAL:HG22	1.69	0.75
1:B:80:PHE:CD2	1:B:82:TRP:HZ3	2.04	0.75
1:C:411:GLU:HG3	1:C:415:GLU:OE1	1.87	0.75
1:F:34:ASN:ND2	1:F:34:ASN:C	2.41	0.74
1:A:357:GLY:HA2	1:A:362:LEU:HD22	1.67	0.74
1:C:182:GLU:HG3	1:C:200:LYS:CG	2.13	0.74
1:B:116:LEU:HD23	1:B:351:LEU:HD11	1.67	0.74
1:F:13:VAL:HG13	1:F:18:VAL:HB	1.69	0.74
1:F:405:MET:O	1:F:408:ALA:HB3	1.88	0.74
1:D:290:ASN:HB3	1:D:295:SER:HB3	1.70	0.74
1:B:22:ARG:HG2	1:B:34:ASN:OD1	1.88	0.74
1:C:52:PHE:CE1	1:C:70:LEU:HD13	2.22	0.73
1:E:161:PRO:HG2	1:E:167:ASN:CG	2.07	0.73
1:A:26:THR:HG22	1:A:27:ASP:O	1.88	0.73
1:B:97:TYR:CE2	1:B:103:PRO:HG3	2.24	0.73
1:F:374:VAL:HG23	1:F:375:MET:H	1.54	0.73
1:C:271:ALA:O	1:C:275:ILE:HG12	1.87	0.73
1:C:295:SER:O	1:C:299:LEU:HD23	1.89	0.73
1:D:167:ASN:ND2	1:E:22:ARG:HH22	1.86	0.73
1:B:223:ARG:HH11	1:B:223:ARG:HG3	1.54	0.72
1:E:303:TYR:O	1:E:304:GLU:HG3	1.89	0.72
1:A:287:ALA:HB2	1:A:395:ALA:O	1.88	0.72
1:E:116:LEU:O	1:E:119:MET:HB3	1.90	0.72
1:A:164:LEU:HD13	1:B:82:TRP:HB3	1.72	0.72
1:D:278:ILE:HG22	1:D:320:ILE:HD11	1.70	0.72
1:D:207:SER:O	1:D:211:ILE:HG12	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6:ARG:O	1:F:10:GLU:HB2	1.89	0.71
1:E:243:GLY:CA	1:E:298:ARG:NH1	2.53	0.71
1:F:183:ILE:HG23	1:F:198:ASP:O	1.90	0.71
1:F:129:LEU:HG	1:F:347:LEU:HD21	1.73	0.71
1:C:13:VAL:HG13	1:C:18:VAL:HB	1.71	0.71
1:A:55:SER:O	1:A:62:ARG:HB3	1.90	0.71
1:D:169:ARG:HH22	1:D:188:HIS:HB2	1.55	0.71
1:D:302:GLY:N	1:D:316:ARG:HH22	1.88	0.71
1:E:315:ASN:HB3	1:E:318:PRO:CB	2.20	0.71
1:C:236:LEU:HB2	1:C:239:VAL:HG21	1.73	0.70
1:E:243:GLY:CA	1:E:298:ARG:HH12	2.03	0.70
1:B:290:ASN:ND2	1:B:299:LEU:HD21	2.06	0.70
1:B:5:THR:HG23	1:B:8:ASP:CG	2.11	0.70
1:A:160:ALA:HB1	1:A:161:PRO:HD2	1.72	0.70
1:C:71:TYR:CE1	1:C:97:TYR:HB2	2.25	0.70
1:E:186:SER:O	1:F:36:GLU:HG2	1.91	0.70
1:F:160:ALA:O	1:F:169:ARG:NH2	2.25	0.70
1:A:160:ALA:CB	1:A:169:ARG:HH12	2.04	0.70
1:E:25:PHE:CE1	1:E:57:ILE:HD11	2.27	0.70
1:A:176:LEU:HD11	1:A:214:PHE:HD1	1.57	0.69
1:D:375:MET:HB3	1:D:379:GLU:HB3	1.74	0.69
1:A:377:LYS:HD3	1:A:380:ARG:HH12	1.57	0.69
1:C:52:PHE:HD1	1:C:70:LEU:HD22	1.57	0.69
1:B:264:ASP:HB3	1:B:272:LYS:HZ2	1.58	0.69
1:E:58:GLU:O	1:E:61:VAL:HG22	1.92	0.69
1:B:115:ILE:HG22	1:B:351:LEU:HD13	1.75	0.69
1:B:52:PHE:CD1	1:B:70:LEU:HD22	2.27	0.69
1:F:57:ILE:HD11	1:F:96:ILE:HG13	1.75	0.69
1:B:160:ALA:HB1	1:B:161:PRO:CD	2.23	0.69
1:F:58:GLU:HB3	1:F:61:VAL:HG23	1.75	0.69
1:E:27:ASP:OD1	1:E:33:LYS:HE3	1.93	0.69
1:E:27:ASP:HB3	1:E:33:LYS:HE3	1.75	0.69
1:C:300:VAL:HG13	1:C:301:PRO:HD2	1.73	0.69
1:D:274:PHE:HB2	1:D:358:ILE:HD11	1.75	0.69
1:D:6:ARG:HH11	1:D:6:ARG:HG3	1.58	0.69
1:B:347:LEU:O	1:B:351:LEU:HB2	1.92	0.69
1:D:176:LEU:O	1:D:181:PHE:HB2	1.94	0.68
1:E:161:PRO:HD3	1:E:169:ARG:NH1	2.09	0.68
1:D:129:LEU:HD12	1:D:347:LEU:HD11	1.74	0.68
1:C:160:ALA:CB	1:C:169:ARG:NH2	2.52	0.68
1:A:127:PHE:HZ	1:A:248:LEU:HD22	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASN:O	1:B:115:ILE:HD13	1.93	0.68
1:B:143:LYS:HB3	1:B:143:LYS:NZ	2.08	0.68
1:B:20:TYR:HB3	1:B:89:VAL:HG13	1.76	0.68
1:C:356:ASP:O	1:C:360:ASN:HB2	1.94	0.68
1:A:160:ALA:O	1:A:161:PRO:C	2.32	0.68
1:A:114:ARG:NH1	1:A:115:ILE:HD11	2.09	0.68
1:A:100:ASP:O	1:A:102:THR:N	2.27	0.68
1:B:77:PHE:CZ	1:B:79:ILE:HD11	2.29	0.67
1:B:77:PHE:HZ	1:B:79:ILE:HD11	1.58	0.67
1:C:207:SER:O	1:C:211:ILE:HG12	1.94	0.67
1:B:80:PHE:HB3	1:B:82:TRP:HE3	1.60	0.67
1:F:328:ILE:N	1:F:328:ILE:HD13	2.09	0.67
1:C:403:GLU:O	1:C:407:LYS:HG3	1.95	0.67
1:A:388:LEU:HB3	1:A:389:PRO:HD2	1.75	0.67
1:C:5:THR:O	1:C:9:ILE:HG12	1.94	0.67
1:D:83:THR:HG22	1:D:88:LYS:HG2	1.77	0.67
1:A:224:LYS:HB2	1:F:164:LEU:HD21	1.75	0.67
1:C:54:GLY:HA3	1:C:68:MET:HE3	1.76	0.67
1:F:241:GLY:HA3	1:F:298:ARG:HG2	1.77	0.67
1:E:140:LEU:HD21	1:E:228:HIS:HB2	1.76	0.67
1:E:331:ARG:HH11	3:E:502:ADP:H5'1	1.58	0.67
1:F:406:VAL:HG22	1:F:414:PHE:CE1	2.30	0.67
1:E:159:LEU:HD13	1:F:22:ARG:HH11	1.59	0.67
1:D:231:PHE:HB3	1:D:339:PRO:HB2	1.77	0.67
1:B:260:ASP:O	1:B:266:GLN:HA	1.95	0.66
1:E:351:LEU:CD2	1:E:355:LEU:HG	2.26	0.66
1:A:13:VAL:CG1	1:A:18:VAL:HB	2.25	0.66
1:B:10:GLU:O	1:B:14:LYS:HG2	1.94	0.66
1:A:376:SER:O	1:A:380:ARG:N	2.29	0.66
1:E:248:LEU:O	1:E:331:ARG:HB2	1.96	0.66
1:E:323:PRO:HB2	1:E:331:ARG:HH12	1.60	0.66
1:B:371:ASN:O	1:B:374:VAL:HG22	1.95	0.66
1:C:309:VAL:HG23	1:C:386:VAL:O	1.96	0.66
1:D:167:ASN:HD21	1:E:22:ARG:HH22	1.44	0.66
1:A:234:LYS:HE3	1:A:239:VAL:O	1.95	0.66
1:F:178:GLU:C	1:F:180:GLY:H	1.96	0.66
1:A:214:PHE:O	1:A:218:VAL:HG23	1.95	0.66
1:F:132:GLU:HB3	1:F:196:GLU:OE1	1.96	0.66
1:A:206:ARG:HH11	1:A:206:ARG:HG2	1.60	0.66
1:F:374:VAL:HG23	1:F:375:MET:N	2.10	0.66
1:D:83:THR:CG2	1:D:88:LYS:HG2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:322:ILE:HG23	1:F:331:ARG:O	1.96	0.66
1:A:177:GLU:OE1	1:B:38:PRO:HG2	1.96	0.65
1:C:175:GLU:O	1:C:179:MET:HB2	1.95	0.65
1:B:131:PRO:HD2	1:B:199:PHE:HB2	1.77	0.65
1:E:5:THR:HG23	1:E:8:ASP:OD1	1.96	0.65
1:A:30:GLY:HA2	1:A:342:ASN:OD1	1.97	0.65
1:B:181:PHE:HE2	1:B:199:PHE:HE2	1.43	0.65
1:F:27:ASP:HB3	1:F:33:LYS:HE3	1.77	0.65
1:D:315:ASN:HB3	1:D:318:PRO:HG3	1.78	0.65
1:B:140:LEU:HD23	1:B:146:PRO:HA	1.79	0.65
1:B:309:VAL:HA	1:B:319:LEU:HD23	1.79	0.65
1:A:270:THR:HG22	1:A:358:ILE:HD12	1.78	0.65
1:E:68:MET:HG2	1:E:96:ILE:HG22	1.77	0.65
1:E:380:ARG:HB3	1:E:385:ILE:HG21	1.79	0.64
1:F:371:ASN:O	1:F:374:VAL:HG22	1.98	0.64
1:B:71:TYR:CD2	1:B:97:TYR:CE1	2.84	0.64
1:A:45:ALA:HA	1:A:50:VAL:HG23	1.79	0.64
1:B:411:GLU:OE2	1:B:411:GLU:HA	1.96	0.64
1:B:323:PRO:HG2	1:B:331:ARG:HG3	1.79	0.64
1:B:187:HIS:HE1	1:B:196:GLU:OE1	1.80	0.64
1:E:231:PHE:HB3	1:E:339:PRO:HB2	1.80	0.64
1:E:315:ASN:CB	1:E:318:PRO:HB3	2.28	0.64
1:D:183:ILE:HA	1:D:199:PHE:HA	1.79	0.64
1:D:48:ASN:HB3	1:D:71:TYR:CE1	2.33	0.64
1:E:378:GLU:O	1:E:382:GLU:HG2	1.97	0.64
1:E:162:THR:HG23	1:F:220:THR:HG23	1.80	0.64
1:B:293:VAL:HG11	1:B:428:PHE:CD1	2.33	0.64
1:A:127:PHE:CZ	1:A:248:LEU:HD22	2.33	0.64
1:E:323:PRO:HD2	1:E:331:ARG:NH2	2.13	0.64
1:C:310:ALA:CB	1:C:368:ILE:HD13	2.28	0.64
1:B:78:VAL:HG11	1:B:179:MET:HE3	1.80	0.64
1:A:345:LEU:HD22	1:A:409:LEU:HD22	1.79	0.64
1:A:342:ASN:HD22	1:A:345:LEU:HG	1.63	0.64
1:C:160:ALA:HB3	1:C:169:ARG:NH1	2.10	0.64
1:F:74:LEU:H	1:F:74:LEU:CD2	2.08	0.64
1:D:328:ILE:H	1:D:328:ILE:CD1	1.93	0.64
1:C:311:TRP:CH2	1:C:367:PRO:HB3	2.33	0.64
1:E:371:ASN:O	1:E:374:VAL:HG22	1.98	0.63
1:F:259:PHE:CD2	1:F:327:GLY:HA2	2.33	0.63
1:C:135:PHE:HB3	1:C:231:PHE:CE1	2.33	0.63
1:D:224:LYS:HE2	1:D:225:HIS:CE1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:GLU:C	1:E:122:LEU:H	2.02	0.63
1:F:377:LYS:HG3	1:F:380:ARG:NH2	2.13	0.63
1:B:54:GLY:O	1:B:57:ILE:HG12	1.98	0.63
1:B:181:PHE:CE2	1:B:199:PHE:HE2	2.15	0.63
1:C:160:ALA:CB	1:C:188:HIS:HD2	2.11	0.63
1:E:406:VAL:HG13	1:E:414:PHE:CD1	2.32	0.63
1:A:224:LYS:HB2	1:F:164:LEU:CD2	2.29	0.63
1:D:311:TRP:CZ2	1:D:367:PRO:HD3	2.33	0.63
1:C:372:ILE:HD12	1:C:373:TYR:N	2.12	0.63
1:D:138:PHE:HA	1:D:149:GLU:O	1.99	0.63
1:F:368:ILE:HG12	1:F:385:ILE:CD1	2.29	0.63
1:F:273:HIS:O	1:F:276:ALA:HB3	1.99	0.63
1:D:370:ARG:HG3	1:D:371:ASN:N	2.13	0.63
1:F:91:ARG:HD2	1:F:91:ARG:C	2.18	0.63
1:A:169:ARG:HH21	1:A:169:ARG:CG	2.11	0.63
1:B:160:ALA:HB3	1:B:169:ARG:NH1	2.14	0.63
1:D:320:ILE:HG22	1:D:320:ILE:O	1.99	0.63
1:A:264:ASP:HB3	1:A:265:LEU:HD12	1.81	0.63
1:F:434:PRO:O	1:F:438:GLU:HG3	1.98	0.63
1:B:187:HIS:CE1	1:B:196:GLU:OE1	2.52	0.62
1:E:252:LYS:HG2	1:E:253:ASN:OD1	1.99	0.62
1:F:172:ILE:O	1:F:176:LEU:HG	1.98	0.62
1:E:131:PRO:CG	1:E:199:PHE:HD1	2.13	0.62
1:D:328:ILE:HD13	1:D:328:ILE:N	2.00	0.62
1:D:160:ALA:HB1	1:D:161:PRO:HD2	1.81	0.62
1:E:281:HIS:CE1	1:E:404:VAL:HG11	2.34	0.62
1:E:396:LEU:HD11	1:E:421:LYS:HB3	1.81	0.62
1:A:312:SER:OG	1:A:369:ASP:HA	1.99	0.62
1:F:11:LYS:HA	1:F:14:LYS:HE2	1.80	0.62
1:B:127:PHE:CE2	1:B:351:LEU:HG	2.34	0.62
1:D:91:ARG:HD2	1:D:92:PHE:N	2.14	0.62
1:D:375:MET:HB2	1:D:380:ARG:HG2	1.81	0.62
1:E:310:ALA:CB	1:E:368:ILE:HD12	2.29	0.62
1:A:176:LEU:HD11	1:A:214:PHE:CD1	2.34	0.62
1:E:241:GLY:HA3	1:E:298:ARG:HG3	1.82	0.62
1:D:105:GLU:CD	1:D:105:GLU:H	2.03	0.62
1:E:204:ALA:HB1	1:E:347:LEU:HD13	1.79	0.62
1:F:76:THR:O	1:F:78:VAL:HG23	2.00	0.62
1:E:306:PRO:HA	1:E:317:SER:HB3	1.80	0.62
1:E:371:ASN:HB3	1:E:374:VAL:HG13	1.80	0.62
1:A:127:PHE:CE2	1:A:351:LEU:HD13	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:THR:CG2	1:F:220:THR:HG23	2.30	0.62
1:F:322:ILE:N	1:F:322:ILE:HD12	2.15	0.61
1:C:323:PRO:HG2	1:C:331:ARG:CZ	2.30	0.61
1:E:206:ARG:HD3	1:E:206:ARG:C	2.20	0.61
1:E:351:LEU:HD23	1:E:355:LEU:HG	1.81	0.61
1:E:48:ASN:HB3	1:E:71:TYR:CD1	2.35	0.61
1:E:159:LEU:HD13	1:F:22:ARG:NH1	2.16	0.61
1:E:283:THR:HB	1:E:398:GLU:OE1	2.00	0.61
1:C:57:ILE:HG13	1:C:96:ILE:HD13	1.80	0.61
1:F:137:LEU:HD12	1:F:195:HIS:CD2	2.35	0.61
1:F:133:PRO:HD2	1:F:197:ILE:O	2.01	0.61
1:F:435:TRP:O	1:F:439:GLN:HG2	2.00	0.61
1:C:236:LEU:HB2	1:C:239:VAL:HG22	1.83	0.61
1:F:26:THR:HG22	1:F:27:ASP:O	2.00	0.61
1:E:406:VAL:HG22	1:E:414:PHE:CE1	2.35	0.61
1:B:153:LYS:HA	1:B:192:PRO:HB3	1.81	0.61
1:E:68:MET:HG2	1:E:96:ILE:CG2	2.31	0.61
1:A:377:LYS:CD	1:A:380:ARG:HH12	2.13	0.61
1:B:309:VAL:HG23	1:B:386:VAL:O	2.00	0.61
1:B:175:GLU:OE1	1:C:86:LYS:HE3	2.00	0.61
1:F:381:MET:HA	1:F:385:ILE:O	2.01	0.61
1:C:315:ASN:ND2	1:C:371:ASN:HA	2.15	0.61
1:D:399:PHE:HE1	1:D:405:MET:HB3	1.65	0.61
1:C:351:LEU:O	1:C:355:LEU:HG	2.00	0.61
1:F:384:GLY:O	1:F:385:ILE:HG13	2.00	0.61
1:D:71:TYR:CD2	1:D:97:TYR:CD1	2.89	0.61
1:A:160:ALA:HB3	1:A:169:ARG:NH1	2.16	0.61
1:B:167:ASN:HD22	1:B:170:ARG:H	1.47	0.61
1:D:185:ALA:HB2	1:E:37:ILE:HG22	1.83	0.61
1:D:51:MET:CE	1:D:67:ASP:HB3	2.30	0.60
1:C:310:ALA:HB1	1:C:368:ILE:HD13	1.82	0.60
1:F:104:PHE:HZ	1:F:412:HIS:CE1	2.19	0.60
1:F:423:ILE:C	1:F:423:ILE:HD12	2.21	0.60
1:F:91:ARG:HD2	1:F:92:PHE:N	2.17	0.60
1:A:119:MET:CE	1:A:127:PHE:HB2	2.31	0.60
1:C:93:ILE:CD1	1:C:209:ASP:HB3	2.31	0.60
1:D:243:GLY:HA3	1:D:298:ARG:HH12	1.65	0.60
1:E:273:HIS:O	1:E:276:ALA:HB3	2.01	0.60
1:E:154:GLY:O	1:E:192:PRO:HA	2.01	0.60
1:F:274:PHE:HB2	1:F:358:ILE:HD11	1.83	0.60
1:E:377:LYS:HE2	1:E:387:ASP:OD2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ALA:HB3	1:A:169:ARG:HH12	1.65	0.60
1:A:160:ALA:HB1	1:A:161:PRO:CD	2.31	0.60
1:B:27:ASP:CB	1:B:33:LYS:HE3	2.29	0.60
1:C:231:PHE:HB3	1:C:339:PRO:HB2	1.83	0.60
1:D:217:VAL:O	1:D:221:ILE:HD13	2.01	0.60
1:B:145:GLU:HA	1:B:145:GLU:OE1	2.02	0.60
1:A:105:GLU:HG2	1:A:412:HIS:CB	2.29	0.60
1:E:315:ASN:C	1:E:318:PRO:HD3	2.22	0.60
1:C:290:ASN:O	1:C:296:TYR:HE1	1.84	0.60
1:D:23:LEU:HB2	1:D:35:VAL:HG13	1.83	0.60
1:A:3:LYS:HB2	1:A:75:ASN:CG	2.22	0.60
1:A:136:PHE:CE2	1:A:194:GLN:HB2	2.36	0.60
1:E:380:ARG:HB3	1:E:385:ILE:CG2	2.31	0.60
1:F:261:GLU:HA	1:F:266:GLN:HG2	1.84	0.60
1:F:175:GLU:O	1:F:179:MET:HG3	2.02	0.60
1:F:104:PHE:CZ	1:F:412:HIS:CE1	2.90	0.59
1:B:396:LEU:O	1:B:400:LYS:HB2	2.01	0.59
1:D:426:ASP:O	1:D:430:THR:HG23	2.02	0.59
1:B:372:ILE:HD11	1:B:385:ILE:HG21	1.83	0.59
1:C:61:VAL:HB	1:C:419:GLU:OE1	2.01	0.59
1:F:55:SER:CB	1:F:62:ARG:HG3	2.21	0.59
1:B:80:PHE:CD2	1:B:82:TRP:CZ3	2.89	0.59
1:C:316:ARG:HD3	1:C:317:SER:OG	2.02	0.59
1:E:124:PHE:CD2	1:E:250:LEU:HD13	2.37	0.59
1:E:403:GLU:OE2	1:E:407:LYS:HE3	2.02	0.59
1:D:131:PRO:HG3	1:D:211:ILE:HD11	1.84	0.59
1:F:250:LEU:O	1:F:257:ALA:HB3	2.02	0.59
1:B:141:ASP:OD2	1:B:145:GLU:HB2	2.02	0.59
1:A:290:ASN:HB3	1:A:295:SER:HB3	1.82	0.59
1:B:217:VAL:O	1:B:221:ILE:HG12	2.03	0.59
1:C:371:ASN:HB3	1:C:374:VAL:CG2	2.30	0.59
1:B:164:LEU:HB2	1:C:220:THR:CG2	2.32	0.59
1:D:381:MET:HA	1:D:385:ILE:O	2.02	0.59
1:C:310:ALA:HB1	1:C:368:ILE:HB	1.85	0.59
1:C:160:ALA:HB2	1:C:169:ARG:NH2	2.13	0.59
1:B:131:PRO:CG	1:B:211:ILE:HD11	2.31	0.59
1:F:136:PHE:CD1	1:F:235:PRO:HG2	2.36	0.59
1:A:161:PRO:O	1:A:167:ASN:ND2	2.36	0.59
1:B:168:CYS:SG	1:B:222:ALA:HA	2.42	0.59
1:B:414:PHE:O	1:B:418:ILE:HG12	2.03	0.59
1:A:338:ASP:HB2	1:A:339:PRO:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PHE:CD1	1:A:70:LEU:HD13	2.38	0.59
1:C:174:LEU:HD13	1:D:86:LYS:HB2	1.83	0.59
1:E:315:ASN:O	1:E:318:PRO:HD3	2.03	0.58
1:D:186:SER:HB2	1:D:196:GLU:O	2.02	0.58
1:C:292:THR:OG1	1:C:295:SER:HB2	2.03	0.58
1:E:161:PRO:HD3	1:E:169:ARG:HH11	1.66	0.58
1:C:167:ASN:HD21	1:D:22:ARG:HH22	1.51	0.58
1:E:161:PRO:HG2	1:E:167:ASN:ND2	2.17	0.58
1:F:250:LEU:HB2	1:F:258:PHE:CZ	2.39	0.58
1:C:137:LEU:HD13	1:C:227:LEU:HD13	1.86	0.58
1:D:264:ASP:O	1:D:265:LEU:HB2	2.03	0.58
1:B:176:LEU:O	1:B:181:PHE:HB2	2.04	0.58
1:E:272:LYS:CA	1:E:275:ILE:HD12	2.32	0.58
1:E:388:LEU:HB3	1:E:389:PRO:HD2	1.84	0.58
1:C:167:ASN:HD21	1:D:22:ARG:NH2	2.01	0.58
1:B:264:ASP:HB3	1:B:272:LYS:HZ1	1.67	0.58
1:E:375:MET:HB2	1:E:379:GLU:HB3	1.85	0.58
1:A:63:ILE:HD12	1:F:316:ARG:NH2	2.19	0.58
1:D:278:ILE:CG2	1:D:320:ILE:HD11	2.34	0.58
1:C:164:LEU:HD12	1:D:220:THR:HG22	1.86	0.58
1:A:169:ARG:HG3	1:A:169:ARG:NH2	2.14	0.58
1:A:325:SER:O	1:A:326:ARG:CD	2.49	0.58
1:E:134:GLU:OE2	2:E:501:GLU:HG2	2.04	0.58
1:F:240:ASN:HD21	2:F:501:GLU:HB2	1.68	0.58
1:E:148:LEU:HD12	1:E:236:LEU:HD21	1.86	0.57
1:F:131:PRO:O	1:F:133:PRO:HD3	2.03	0.57
1:E:310:ALA:HB2	1:E:368:ILE:HD12	1.85	0.57
1:C:315:ASN:HB3	1:C:318:PRO:HD3	1.85	0.57
1:A:86:LYS:HD2	1:F:178:GLU:OE1	2.05	0.57
1:B:160:ALA:CB	1:B:169:ARG:HH22	2.17	0.57
1:F:28:ILE:HB	1:F:57:ILE:O	2.04	0.57
1:D:244:MET:HE2	1:D:339:PRO:HA	1.85	0.57
1:C:28:ILE:HD11	1:C:58:GLU:OE2	2.03	0.57
1:C:206:ARG:HG3	1:C:206:ARG:HH11	1.69	0.57
1:F:152:ASP:C	1:F:153:LYS:HD2	2.25	0.57
1:D:402:ASN:O	1:D:406:VAL:HG23	2.05	0.57
1:D:320:ILE:HG23	1:D:332:VAL:HG23	1.87	0.57
1:C:366:ALA:O	1:C:368:ILE:N	2.37	0.57
1:E:124:PHE:CE2	1:E:250:LEU:HD13	2.39	0.57
1:B:406:VAL:HG12	1:B:406:VAL:O	2.04	0.57
1:B:425:TRP:O	1:B:429:ARG:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:LEU:HB3	1:D:271:ALA:HB3	1.87	0.57
1:A:354:GLY:O	1:A:358:ILE:HG12	2.04	0.57
1:C:115:ILE:HG22	1:C:351:LEU:HD13	1.85	0.57
1:A:402:ASN:O	1:A:406:VAL:HG23	2.05	0.57
1:D:167:ASN:ND2	1:E:22:ARG:NH2	2.52	0.57
1:E:323:PRO:HG2	1:E:331:ARG:NH1	2.20	0.57
1:A:372:ILE:HA	1:A:375:MET:SD	2.45	0.57
1:A:135:PHE:HB3	1:A:231:PHE:CE1	2.39	0.57
1:F:309:VAL:HG13	1:F:319:LEU:HD23	1.87	0.57
1:D:159:LEU:CD1	1:E:22:ARG:HH11	2.17	0.57
1:E:350:LEU:O	1:E:353:ALA:HB3	2.04	0.57
1:E:315:ASN:OD1	1:E:371:ASN:HA	2.05	0.56
1:E:199:PHE:HZ	1:E:214:PHE:HB2	1.70	0.56
1:D:112:LEU:HD23	1:D:116:LEU:HG	1.87	0.56
1:C:130:GLY:CA	3:C:502:ADP:O2'	2.52	0.56
1:B:244:MET:H	1:B:338:ASP:HA	1.70	0.56
1:C:270:THR:CG2	1:C:358:ILE:HD12	2.35	0.56
1:C:129:LEU:O	1:C:201:TYR:HA	2.06	0.56
1:B:47:ASP:O	1:B:48:ASN:HB2	2.06	0.56
1:E:204:ALA:HB1	1:E:347:LEU:CD1	2.34	0.56
1:F:191:ALA:HB1	1:F:239:VAL:CG2	2.35	0.56
1:B:181:PHE:HE2	1:B:199:PHE:CE2	2.23	0.56
1:E:399:PHE:HE1	1:E:405:MET:HB3	1.69	0.56
1:A:11:LYS:HE2	1:A:15:GLU:OE2	2.05	0.56
1:E:265:LEU:HD13	1:E:272:LYS:NZ	2.20	0.56
1:F:20:TYR:HB3	1:F:89:VAL:HG22	1.87	0.56
1:E:27:ASP:CB	1:E:33:LYS:HE3	2.35	0.56
1:B:160:ALA:HB2	1:B:188:HIS:HD2	1.69	0.56
1:C:202:ALA:HB1	1:C:206:ARG:HD3	1.88	0.56
1:A:388:LEU:HB3	1:A:389:PRO:CD	2.35	0.56
1:B:402:ASN:O	1:B:406:VAL:HG23	2.05	0.56
1:F:293:VAL:HG11	1:F:428:PHE:CG	2.40	0.56
1:D:247:ASN:HB3	1:D:331:ARG:HD2	1.87	0.56
1:C:207:SER:HA	1:C:210:ASP:HB2	1.88	0.56
1:D:283:THR:HB	1:D:398:GLU:OE1	2.05	0.56
1:B:143:LYS:HB3	1:B:143:LYS:HZ3	1.71	0.56
1:A:396:LEU:O	1:A:400:LYS:HG3	2.05	0.56
1:B:271:ALA:O	1:B:275:ILE:HG12	2.06	0.56
1:B:91:ARG:HD2	1:B:92:PHE:N	2.21	0.56
1:C:273:HIS:HA	1:C:362:LEU:O	2.05	0.56
1:C:160:ALA:CB	1:C:169:ARG:HH12	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:LYS:HD3	1:A:380:ARG:NH1	2.20	0.56
1:A:64:GLU:OE2	1:F:371:ASN:OD1	2.24	0.55
1:D:357:GLY:HA2	1:D:362:LEU:HD22	1.87	0.55
1:B:5:THR:HG23	1:B:8:ASP:OD2	2.07	0.55
1:B:52:PHE:HD1	1:B:70:LEU:HD22	1.71	0.55
1:D:138:PHE:CD2	1:D:148:LEU:HA	2.42	0.55
1:B:249:SER:HA	1:B:258:PHE:CE1	2.41	0.55
1:A:86:LYS:HG3	1:F:174:LEU:HB3	1.88	0.55
1:C:28:ILE:HG13	1:C:57:ILE:O	2.05	0.55
1:F:317:SER:HB3	1:F:335:ARG:HH22	1.70	0.55
1:D:316:ARG:HG2	1:D:317:SER:N	2.20	0.55
1:F:178:GLU:C	1:F:180:GLY:N	2.60	0.55
1:A:338:ASP:OD2	1:A:340:ALA:HB3	2.06	0.55
1:B:137:LEU:HD13	1:B:227:LEU:HD13	1.89	0.55
1:F:24:GLN:OE1	1:F:91:ARG:HD3	2.07	0.55
1:B:160:ALA:HB2	1:B:169:ARG:HH12	1.69	0.55
1:A:116:LEU:HD23	1:A:351:LEU:CD2	2.37	0.55
1:B:265:LEU:O	1:B:266:GLN:HB2	2.06	0.55
1:D:111:ASN:OD1	1:D:114:ARG:NH1	2.39	0.55
1:B:419:GLU:O	1:B:423:ILE:HG12	2.06	0.55
1:E:302:GLY:H	1:E:316:ARG:NH1	2.05	0.55
1:A:79:ILE:HD13	1:A:90:ALA:HB2	1.88	0.55
1:A:351:LEU:O	1:A:355:LEU:HG	2.06	0.55
1:F:325:SER:HB2	1:F:331:ARG:NH2	2.21	0.55
1:B:71:TYR:CD2	1:B:97:TYR:CD1	2.95	0.55
1:E:27:ASP:C	1:E:27:ASP:OD2	2.44	0.55
1:D:45:ALA:HA	1:D:50:VAL:HG23	1.89	0.55
1:E:25:PHE:CD1	1:E:57:ILE:HD11	2.41	0.55
1:C:39:VAL:C	1:C:41:GLN:H	2.09	0.55
1:B:119:MET:HE3	1:B:120:GLU:HG3	1.89	0.55
1:A:164:LEU:HD22	1:B:82:TRP:CD1	2.41	0.55
1:D:298:ARG:NH1	2:D:501:GLU:O	2.40	0.55
1:D:159:LEU:CD1	1:E:22:ARG:NH1	2.70	0.55
1:E:20:TYR:OH	1:E:36:GLU:HG3	2.07	0.55
1:E:163:ASP:OD2	1:F:89:VAL:HG11	2.07	0.55
1:C:308:TYR:HE2	1:C:380:ARG:NH1	2.05	0.55
1:A:302:GLY:H	1:A:316:ARG:NH2	2.05	0.55
1:F:311:TRP:CZ2	1:F:367:PRO:HD3	2.42	0.55
1:E:419:GLU:O	1:E:423:ILE:HG12	2.07	0.55
1:E:83:THR:HB	5:E:505:SO4:O4	2.07	0.55
1:A:356:ASP:HA	1:A:359:LYS:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:VAL:HG23	1:D:240:ASN:N	2.20	0.55
1:C:160:ALA:O	1:C:161:PRO:C	2.45	0.54
1:F:9:ILE:CD1	1:F:74:LEU:HB3	2.37	0.54
3:A:502:ADP:O1A	1:B:44:LYS:NZ	2.40	0.54
1:D:394:GLU:O	1:D:398:GLU:HB2	2.07	0.54
1:F:161:PRO:HG2	1:F:166:GLU:OE1	2.07	0.54
1:F:236:LEU:HB2	1:F:239:VAL:CG1	2.37	0.54
1:A:5:THR:HG23	1:A:8:ASP:CG	2.27	0.54
1:B:244:MET:CB	1:B:339:PRO:HD3	2.37	0.54
1:E:379:GLU:HA	1:E:382:GLU:HG3	1.90	0.54
1:B:371:ASN:OD1	1:B:374:VAL:HG13	2.07	0.54
1:C:293:VAL:HG11	1:C:428:PHE:CG	2.43	0.54
1:C:126:ASP:HB2	1:C:251:PHE:HB2	1.88	0.54
1:D:109:ARG:HG3	1:D:344:TYR:CE2	2.42	0.54
1:C:178:GLU:HG3	1:C:178:GLU:O	2.07	0.54
1:E:131:PRO:C	1:E:133:PRO:HD3	2.28	0.54
1:B:52:PHE:CE1	1:B:70:LEU:HD13	2.43	0.54
1:D:311:TRP:CE3	1:D:367:PRO:HB3	2.43	0.54
1:E:27:ASP:OD1	1:E:31:THR:HB	2.07	0.54
1:E:131:PRO:HG3	1:E:199:PHE:HD1	1.73	0.54
1:C:311:TRP:HB3	1:C:320:ILE:HB	1.90	0.54
1:F:138:PHE:HB3	1:F:147:THR:O	2.07	0.54
1:C:301:PRO:HA	1:C:316:ARG:HH22	1.73	0.54
1:D:69:TYR:HD1	1:D:99:PRO:HA	1.71	0.54
1:F:236:LEU:HB2	1:F:239:VAL:HG12	1.89	0.54
1:B:244:MET:HB2	1:B:339:PRO:HD3	1.90	0.54
1:C:402:ASN:O	1:C:406:VAL:HG23	2.08	0.54
1:E:386:VAL:HG23	1:E:386:VAL:O	2.08	0.54
1:A:142:GLU:CD	1:A:142:GLU:H	2.11	0.54
1:B:304:GLU:HA	1:B:317:SER:OG	2.07	0.54
1:A:274:PHE:O	1:A:278:ILE:HG12	2.08	0.54
1:F:68:MET:HG2	1:F:97:TYR:O	2.07	0.54
1:A:403:GLU:O	1:A:407:LYS:HG3	2.08	0.54
1:C:25:PHE:CD2	1:C:25:PHE:N	2.76	0.53
1:B:223:ARG:NH1	1:B:223:ARG:HG3	2.21	0.53
1:A:270:THR:HG22	1:A:358:ILE:CD1	2.38	0.53
1:C:25:PHE:CE1	1:C:33:LYS:HB2	2.43	0.53
1:E:243:GLY:HA3	1:E:298:ARG:HH12	1.71	0.53
1:D:136:PHE:CD1	1:D:235:PRO:HG2	2.43	0.53
1:A:323:PRO:HB2	1:A:331:ARG:NH1	2.23	0.53
1:F:233:PRO:O	1:F:298:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:GLU:OE2	1:C:58:GLU:HA	2.08	0.53
1:F:215:LYS:O	1:F:219:LYS:HG3	2.08	0.53
1:E:322:ILE:HD12	1:E:322:ILE:H	1.73	0.53
1:A:160:ALA:HB2	1:A:169:ARG:HH12	1.72	0.53
1:D:332:VAL:HG22	1:D:332:VAL:O	2.08	0.53
1:A:238:GLY:HA2	1:A:303:TYR:CZ	2.43	0.53
1:B:164:LEU:HB2	1:C:220:THR:HG22	1.91	0.53
1:F:57:ILE:CD1	1:F:96:ILE:HG13	2.38	0.53
1:D:271:ALA:O	1:D:275:ILE:HG13	2.09	0.53
1:C:78:VAL:HG12	1:C:79:ILE:N	2.23	0.53
1:C:260:ASP:OD1	1:C:263:ALA:HB2	2.09	0.53
1:E:175:GLU:O	1:E:179:MET:HG3	2.09	0.53
1:A:41:GLN:HE22	1:F:200:LYS:HD2	1.74	0.53
1:D:34:ASN:C	1:D:34:ASN:ND2	2.60	0.53
1:D:160:ALA:HB3	1:D:169:ARG:NH1	2.22	0.53
1:B:129:LEU:O	1:B:201:TYR:HA	2.09	0.53
1:D:304:GLU:HB3	2:D:501:GLU:HB3	1.90	0.53
1:F:127:PHE:CD1	1:F:351:LEU:HD12	2.44	0.53
1:B:375:MET:HB3	1:B:379:GLU:HG3	1.91	0.53
1:F:338:ASP:HB2	1:F:339:PRO:HD2	1.91	0.53
1:A:418:ILE:O	1:A:419:GLU:C	2.47	0.53
1:F:17:ASN:O	1:F:19:LYS:HG2	2.08	0.53
1:C:379:GLU:HA	1:C:382:GLU:HB2	1.91	0.53
1:D:159:LEU:HD11	1:E:22:ARG:HH11	1.73	0.52
1:B:127:PHE:CD2	1:B:351:LEU:HG	2.43	0.52
1:A:356:ASP:O	1:A:360:ASN:HB2	2.09	0.52
1:D:124:PHE:HB3	1:D:251:PHE:O	2.09	0.52
1:C:420:ALA:O	1:C:423:ILE:HB	2.10	0.52
1:E:376:SER:O	1:E:380:ARG:HG3	2.10	0.52
1:B:266:GLN:HB3	1:B:326:ARG:HG2	1.90	0.52
1:C:111:ASN:HD21	1:C:409:LEU:HD23	1.75	0.52
1:E:57:ILE:HG13	1:E:96:ILE:HD13	1.90	0.52
1:E:252:LYS:O	1:E:255:VAL:HG22	2.09	0.52
1:E:45:ALA:HA	1:E:50:VAL:HG23	1.91	0.52
1:F:295:SER:O	1:F:299:LEU:HD22	2.08	0.52
1:E:85:GLU:HG3	1:E:86:LYS:HG2	1.92	0.52
1:C:160:ALA:HB1	1:C:161:PRO:CD	2.32	0.52
1:F:281:HIS:CE1	1:F:404:VAL:HG11	2.44	0.52
1:F:290:ASN:ND2	1:F:299:LEU:HD21	2.25	0.52
1:F:315:ASN:O	1:F:318:PRO:HD3	2.09	0.52
1:D:142:GLU:CD	1:D:142:GLU:H	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:372:ILE:HG23	1:E:385:ILE:HD13	1.91	0.52
1:F:281:HIS:CD2	1:F:353:ALA:HB1	2.45	0.52
1:E:164:LEU:HD21	1:F:224:LYS:HB2	1.92	0.52
1:A:389:PRO:HB3	1:A:394:GLU:HB3	1.91	0.52
1:E:402:ASN:O	1:E:406:VAL:HG23	2.10	0.52
1:D:184:GLU:HG3	1:D:200:LYS:HG2	1.91	0.52
1:A:80:PHE:CZ	1:A:91:ARG:HG2	2.44	0.52
1:F:264:ASP:O	1:F:265:LEU:HB2	2.10	0.52
1:B:323:PRO:O	1:B:326:ARG:NH2	2.43	0.52
1:F:378:GLU:C	1:F:380:ARG:H	2.11	0.52
1:D:160:ALA:HB2	1:D:188:HIS:HB2	1.91	0.52
1:E:25:PHE:CE1	1:E:57:ILE:CD1	2.93	0.52
1:C:338:ASP:HB2	1:C:339:PRO:HD2	1.91	0.52
1:A:3:LYS:HB2	1:A:75:ASN:ND2	2.25	0.52
1:A:96:ILE:HG22	1:A:104:PHE:CB	2.40	0.52
1:D:19:LYS:HA	1:D:39:VAL:HG11	1.91	0.52
1:A:9:ILE:O	1:A:13:VAL:HG23	2.09	0.52
1:D:243:GLY:CA	1:D:298:ARG:NH1	2.72	0.52
1:E:243:GLY:HA2	1:E:298:ARG:HH12	1.62	0.52
1:F:281:HIS:O	1:F:284:SER:N	2.26	0.52
1:B:52:PHE:CE2	1:B:54:GLY:HA2	2.44	0.52
1:B:414:PHE:CE1	1:B:418:ILE:HD11	2.44	0.52
1:E:423:ILE:O	1:E:427:MET:HG3	2.10	0.52
1:C:285:PHE:HB2	1:C:349:VAL:HG13	1.90	0.52
1:C:160:ALA:HB2	1:C:188:HIS:HD2	1.74	0.52
1:B:349:VAL:O	1:B:352:ALA:HB3	2.10	0.52
1:D:68:MET:CE	1:D:98:ASN:HA	2.40	0.52
1:E:170:ARG:NH1	1:F:84:ALA:HB2	2.25	0.52
1:E:435:TRP:O	1:E:439:GLN:HB2	2.10	0.52
1:E:212:GLN:HA	1:E:212:GLN:OE1	2.10	0.52
1:E:161:PRO:HG2	1:E:167:ASN:OD1	2.09	0.51
1:E:176:LEU:O	1:E:181:PHE:HB2	2.10	0.51
1:F:329:SER:CB	3:F:502:ADP:O1B	2.54	0.51
1:F:282:ALA:HA	1:F:285:PHE:CZ	2.45	0.51
1:A:177:GLU:HA	1:A:177:GLU:OE2	2.10	0.51
1:A:270:THR:CG2	1:A:358:ILE:HD12	2.41	0.51
1:B:136:PHE:CE2	1:B:194:GLN:HB2	2.45	0.51
1:B:97:TYR:HE2	1:B:103:PRO:HG3	1.75	0.51
1:A:5:THR:O	1:A:8:ASP:HB2	2.11	0.51
1:E:309:VAL:HG23	1:E:386:VAL:O	2.10	0.51
1:E:259:PHE:CZ	1:E:261:GLU:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ASP:HB2	1:D:82:TRP:HE3	1.75	0.51
1:A:185:ALA:O	1:A:186:SER:HB3	2.10	0.51
1:E:34:ASN:O	1:E:34:ASN:ND2	2.43	0.51
1:E:6:ARG:O	1:E:10:GLU:HG3	2.09	0.51
1:B:117:LYS:HG2	1:B:118:GLU:N	2.25	0.51
1:D:139:LYS:O	1:D:147:THR:HG23	2.10	0.51
1:A:21:ILE:HD13	1:A:42:LEU:HD13	1.92	0.51
1:A:314:GLN:O	1:A:315:ASN:ND2	2.26	0.51
1:E:12:LEU:O	1:E:16:GLU:CB	2.55	0.51
1:F:323:PRO:O	1:F:326:ARG:NH2	2.42	0.51
1:D:48:ASN:HB3	1:D:71:TYR:CD1	2.46	0.51
1:C:322:ILE:HG23	1:C:331:ARG:O	2.10	0.51
1:F:54:GLY:HA3	1:F:68:MET:CE	2.41	0.51
1:C:260:ASP:HB3	1:C:263:ALA:HB3	1.93	0.51
1:B:234:LYS:HE3	1:B:239:VAL:O	2.11	0.51
1:F:106:GLY:HA2	1:F:413:LEU:HG	1.93	0.51
1:E:196:GLU:OE1	1:E:198:ASP:OD1	2.27	0.51
1:B:372:ILE:CD1	1:B:385:ILE:HD13	2.38	0.51
1:A:265:LEU:O	1:A:266:GLN:HB2	2.11	0.51
1:E:281:HIS:HE1	1:E:404:VAL:HG11	1.75	0.51
1:F:317:SER:HB3	1:F:335:ARG:NH2	2.26	0.51
1:F:402:ASN:OD1	1:F:404:VAL:HG12	2.11	0.51
1:B:96:ILE:HD12	1:B:96:ILE:N	2.26	0.51
1:A:137:LEU:HB2	1:A:151:ASN:OD1	2.11	0.51
1:C:160:ALA:HB2	1:C:188:HIS:CD2	2.46	0.51
1:D:159:LEU:HD13	1:E:34:ASN:ND2	2.25	0.51
1:F:285:PHE:HB2	1:F:349:VAL:HG13	1.91	0.51
1:C:302:GLY:H	1:C:316:ARG:HH21	1.58	0.51
1:C:112:LEU:HA	1:C:348:SER:OG	2.11	0.51
1:E:379:GLU:HA	1:E:382:GLU:CG	2.41	0.50
1:E:189:GLU:OE1	1:E:196:GLU:OE2	2.30	0.50
1:C:91:ARG:C	1:C:91:ARG:HD2	2.30	0.50
1:F:402:ASN:HB3	1:F:405:MET:CG	2.41	0.50
1:D:95:ASP:OD1	1:D:113:LYS:NZ	2.38	0.50
1:B:286:THR:O	1:B:288:VAL:N	2.44	0.50
1:D:170:ARG:HH11	1:E:84:ALA:HB2	1.75	0.50
1:F:375:MET:HB2	1:F:380:ARG:HG2	1.92	0.50
1:A:91:ARG:CD	1:A:91:ARG:C	2.80	0.50
1:D:19:LYS:HA	1:D:39:VAL:CG1	2.41	0.50
1:C:3:LYS:HB3	1:C:75:ASN:OD1	2.11	0.50
1:F:23:LEU:HD23	1:F:92:PHE:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:HG13	1:A:18:VAL:CB	2.37	0.50
1:D:338:ASP:HB2	1:D:339:PRO:HD2	1.93	0.50
1:D:331:ARG:NH1	3:D:502:ADP:O2A	2.43	0.50
1:C:202:ALA:HB3	1:C:207:SER:HB2	1.94	0.50
1:D:71:TYR:CE2	1:D:97:TYR:CG	3.00	0.50
1:E:52:PHE:CE1	1:E:70:LEU:HD13	2.46	0.50
1:F:45:ALA:HA	1:F:50:VAL:HG23	1.94	0.50
1:B:274:PHE:CE1	1:B:354:GLY:HA3	2.47	0.50
1:A:26:THR:HG21	1:A:342:ASN:OD1	2.11	0.50
1:A:152:ASP:OD1	1:A:161:PRO:HD3	2.11	0.50
1:E:48:ASN:OD1	1:E:72:PRO:HD2	2.12	0.50
1:E:159:LEU:CD1	1:F:22:ARG:NH1	2.75	0.50
1:B:396:LEU:HD11	1:B:421:LYS:HB3	1.93	0.50
1:A:91:ARG:NH2	1:A:213:THR:OG1	2.45	0.50
1:B:21:ILE:HG21	1:B:37:ILE:HD11	1.93	0.50
1:F:251:PHE:N	1:F:251:PHE:HD1	2.10	0.50
1:B:258:PHE:O	1:B:267:LEU:HA	2.12	0.50
1:E:322:ILE:HD12	1:E:322:ILE:N	2.26	0.50
1:B:110:ASN:O	1:B:113:LYS:N	2.45	0.50
1:D:119:MET:SD	1:D:250:LEU:HD21	2.52	0.50
1:C:290:ASN:ND2	1:C:299:LEU:HD21	2.27	0.50
1:A:287:ALA:HB2	1:A:395:ALA:C	2.31	0.50
1:C:71:TYR:CD1	1:C:97:TYR:CD1	3.00	0.50
1:F:251:PHE:N	1:F:251:PHE:CD1	2.79	0.50
1:F:265:LEU:HD12	1:F:272:LYS:CE	2.31	0.50
1:C:177:GLU:C	1:C:179:MET:H	2.15	0.50
1:E:236:LEU:HB2	1:E:239:VAL:CG2	2.42	0.50
1:E:164:LEU:HD23	1:E:164:LEU:O	2.12	0.50
1:A:58:GLU:O	1:A:61:VAL:HG22	2.11	0.50
1:D:315:ASN:HB3	1:D:318:PRO:CG	2.43	0.49
1:C:300:VAL:CG1	1:C:301:PRO:HD2	2.42	0.49
1:C:372:ILE:HD12	1:C:373:TYR:H	1.75	0.49
1:D:282:ALA:O	1:D:283:THR:C	2.49	0.49
1:F:80:PHE:HB3	1:F:82:TRP:CE3	2.47	0.49
1:D:96:ILE:N	1:D:96:ILE:HD12	2.27	0.49
1:F:322:ILE:H	1:F:322:ILE:HD12	1.77	0.49
1:D:47:ASP:O	1:D:49:LYS:HD2	2.12	0.49
1:C:25:PHE:CD1	1:C:33:LYS:HB2	2.47	0.49
1:D:58:GLU:O	1:D:61:VAL:HG22	2.12	0.49
1:A:16:GLU:HG3	1:A:88:LYS:NZ	2.27	0.49
1:D:249:SER:HA	1:D:258:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:318:PRO:HD2	1:E:335:ARG:NH2	2.27	0.49
1:A:160:ALA:O	1:A:161:PRO:O	2.30	0.49
1:B:169:ARG:HD3	1:B:195:HIS:HB3	1.94	0.49
1:B:131:PRO:CB	1:B:211:ILE:HD11	2.42	0.49
1:D:159:LEU:HD11	1:E:22:ARG:NH1	2.27	0.49
1:D:52:PHE:CE1	1:D:70:LEU:HD13	2.47	0.49
1:A:244:MET:O	1:A:337:VAL:HB	2.12	0.49
1:E:93:ILE:HD12	1:E:209:ASP:HB3	1.93	0.49
1:D:98:ASN:HB2	1:D:102:THR:O	2.12	0.49
1:D:47:ASP:O	1:D:48:ASN:HB2	2.12	0.49
1:B:155:GLY:O	1:B:158:ASP:HB2	2.12	0.49
1:C:111:ASN:ND2	1:C:409:LEU:HD23	2.28	0.49
1:D:187:HIS:NE2	1:D:196:GLU:OE1	2.45	0.49
1:D:54:GLY:CA	1:D:68:MET:HG3	2.40	0.49
1:F:191:ALA:HB1	1:F:239:VAL:HG22	1.93	0.49
1:D:203:GLY:O	1:D:205:VAL:N	2.46	0.49
1:F:48:ASN:ND2	1:F:71:TYR:CD2	2.81	0.49
1:C:127:PHE:HE2	1:C:347:LEU:HD12	1.78	0.49
1:F:325:SER:CB	1:F:331:ARG:HH22	2.21	0.49
1:F:285:PHE:HB3	1:F:405:MET:SD	2.52	0.49
1:A:58:GLU:OE2	1:A:416:HIS:CD2	2.66	0.49
1:A:249:SER:OG	3:A:502:ADP:N1	2.40	0.49
1:B:368:ILE:N	1:B:368:ILE:HD12	2.27	0.49
1:E:323:PRO:HD2	1:E:331:ARG:HH22	1.77	0.49
1:D:394:GLU:OE1	6:D:601:HOH:O	2.20	0.49
1:B:321:ARG:C	1:B:322:ILE:HD12	2.32	0.49
1:B:244:MET:O	1:B:244:MET:HG2	2.12	0.49
1:E:120:GLU:C	1:E:122:LEU:N	2.65	0.49
1:B:291:PRO:HB2	1:B:421:LYS:NZ	2.28	0.49
1:E:285:PHE:C	1:E:285:PHE:CD1	2.86	0.49
1:F:19:LYS:HD2	1:F:39:VAL:HG11	1.94	0.49
1:A:256:ASN:ND2	1:A:328:ILE:O	2.36	0.49
1:B:160:ALA:HB1	1:B:161:PRO:HD2	1.95	0.49
1:A:78:VAL:HG13	1:A:91:ARG:HG3	1.93	0.49
1:D:291:PRO:HG3	1:D:341:ALA:HA	1.95	0.49
1:A:217:VAL:O	1:A:221:ILE:HG12	2.12	0.49
1:F:134:GLU:HG2	1:F:189:GLU:HG3	1.94	0.49
1:E:371:ASN:HB3	1:E:374:VAL:CG1	2.42	0.49
1:A:172:ILE:CD1	1:A:218:VAL:HA	2.42	0.49
1:F:402:ASN:O	1:F:406:VAL:HG23	2.12	0.49
1:E:159:LEU:CD1	1:F:22:ARG:HH11	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:CYS:O	1:B:172:ILE:HG13	2.13	0.49
1:C:378:GLU:N	1:C:378:GLU:OE2	2.44	0.48
1:F:165:GLY:O	1:F:166:GLU:C	2.52	0.48
1:D:203:GLY:O	1:D:204:ALA:C	2.52	0.48
1:A:304:GLU:HG3	1:A:304:GLU:O	2.13	0.48
1:E:69:TYR:CE1	1:E:99:PRO:HA	2.48	0.48
1:D:46:LEU:HD23	1:D:74:LEU:HD21	1.94	0.48
1:B:21:ILE:O	1:B:21:ILE:HG22	2.13	0.48
1:C:16:GLU:O	1:C:88:LYS:HD2	2.13	0.48
1:D:51:MET:HE2	1:D:51:MET:HB3	1.68	0.48
1:A:119:MET:HE1	1:A:127:PHE:HB2	1.94	0.48
1:C:414:PHE:O	1:C:418:ILE:HG12	2.14	0.48
1:F:78:VAL:HB	1:F:91:ARG:HG3	1.95	0.48
1:A:127:PHE:CZ	1:A:248:LEU:CD2	2.96	0.48
1:F:205:VAL:C	1:F:207:SER:N	2.63	0.48
1:A:383:ASN:OD1	1:A:383:ASN:N	2.47	0.48
1:C:270:THR:HG22	1:C:358:ILE:HD12	1.94	0.48
1:E:323:PRO:HG2	1:E:331:ARG:CZ	2.43	0.48
1:B:78:VAL:HG11	1:B:179:MET:CE	2.43	0.48
1:C:58:GLU:O	1:C:61:VAL:HG22	2.14	0.48
1:A:76:THR:O	1:A:91:ARG:NH1	2.46	0.48
1:C:285:PHE:HB3	1:C:405:MET:SD	2.54	0.48
1:D:170:ARG:HH11	1:E:84:ALA:CB	2.27	0.48
1:B:58:GLU:O	1:B:61:VAL:HG22	2.13	0.48
1:A:181:PHE:HZ	1:A:210:ASP:HA	1.78	0.48
1:A:207:SER:O	1:A:211:ILE:HG13	2.13	0.48
1:A:311:TRP:CB	1:A:320:ILE:HB	2.39	0.48
1:C:290:ASN:O	1:C:296:TYR:CE1	2.65	0.48
1:B:319:LEU:HD12	1:B:319:LEU:O	2.14	0.48
1:F:259:PHE:CG	1:F:327:GLY:HA2	2.49	0.48
1:B:311:TRP:HB3	1:B:320:ILE:HB	1.96	0.48
1:F:388:LEU:HB3	1:F:389:PRO:CD	2.44	0.48
1:E:211:ILE:O	1:E:211:ILE:HG22	2.13	0.48
1:E:187:HIS:CE1	1:E:196:GLU:CD	2.86	0.48
1:D:302:GLY:HA2	1:D:316:ARG:HH12	1.78	0.48
1:F:131:PRO:HG2	1:F:199:PHE:HD1	1.79	0.48
1:F:139:LYS:N	1:F:149:GLU:O	2.46	0.48
1:E:104:PHE:CZ	1:E:106:GLY:HA3	2.49	0.48
1:C:10:GLU:O	1:C:14:LYS:HD3	2.14	0.48
1:C:22:ARG:HB3	1:C:34:ASN:HD22	1.79	0.48
1:C:169:ARG:HH21	1:C:188:HIS:HA	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:PHE:CZ	1:F:248:LEU:HD22	2.49	0.48
1:D:266:GLN:O	1:D:267:LEU:HD13	2.13	0.48
1:D:328:ILE:C	1:D:330:THR:H	2.18	0.48
1:F:265:LEU:CD1	1:F:272:LYS:HE2	2.30	0.48
1:A:324:ALA:O	1:A:325:SER:O	2.32	0.48
1:E:68:MET:HG3	1:E:97:TYR:O	2.13	0.48
1:C:285:PHE:HB2	1:C:349:VAL:CG1	2.43	0.48
1:E:131:PRO:HG2	1:E:199:PHE:CD1	2.49	0.47
1:D:134:GLU:HG2	1:D:196:GLU:HB2	1.95	0.47
1:E:251:PHE:HE1	3:E:502:ADP:HN62	1.60	0.47
1:B:285:PHE:HB2	1:B:349:VAL:CG1	2.43	0.47
1:C:240:ASN:HD21	2:C:501:GLU:HA	1.78	0.47
1:B:27:ASP:CG	1:B:33:LYS:HE3	2.35	0.47
1:E:243:GLY:HA3	2:E:501:GLU:HB3	1.96	0.47
1:F:284:SER:O	1:F:399:PHE:HB2	2.14	0.47
1:F:351:LEU:C	1:F:351:LEU:HD23	2.34	0.47
1:F:98:ASN:OD1	1:F:104:PHE:HA	2.14	0.47
1:F:274:PHE:C	1:F:274:PHE:CD2	2.87	0.47
1:E:174:LEU:HD13	1:F:86:LYS:HB2	1.95	0.47
1:A:376:SER:H	1:A:379:GLU:HB3	1.79	0.47
1:F:52:PHE:CZ	1:F:96:ILE:HD12	2.50	0.47
1:F:311:TRP:HD1	1:F:311:TRP:H	1.60	0.47
1:F:100:ASP:O	1:F:102:THR:N	2.47	0.47
1:C:161:PRO:HB2	1:C:167:ASN:HA	1.97	0.47
1:D:117:LYS:HA	1:D:120:GLU:HB2	1.96	0.47
1:E:285:PHE:HB3	1:E:405:MET:SD	2.55	0.47
1:A:256:ASN:OD1	1:A:258:PHE:HB2	2.14	0.47
1:F:205:VAL:HG13	1:F:206:ARG:N	2.28	0.47
1:E:175:GLU:OE1	1:F:86:LYS:HE3	2.14	0.47
1:B:34:ASN:ND2	1:B:34:ASN:C	2.67	0.47
1:F:191:ALA:CB	1:F:239:VAL:HG22	2.44	0.47
1:C:214:PHE:O	1:C:218:VAL:HG23	2.14	0.47
1:E:11:LYS:O	1:E:15:GLU:HG2	2.13	0.47
1:C:187:HIS:CE1	1:C:196:GLU:OE1	2.68	0.47
1:F:78:VAL:HG21	1:F:91:ARG:NH2	2.30	0.47
1:A:172:ILE:HD13	1:A:218:VAL:HA	1.95	0.47
1:C:129:LEU:HD22	1:C:131:PRO:N	2.29	0.47
1:D:396:LEU:O	1:D:399:PHE:N	2.48	0.47
1:F:316:ARG:HD2	1:F:371:ASN:ND2	2.29	0.47
1:A:286:THR:OG1	1:A:388:LEU:HD22	2.15	0.47
1:D:135:PHE:HB3	1:D:231:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:ASN:HB3	1:C:331:ARG:HD2	1.97	0.47
1:F:250:LEU:HB2	1:F:258:PHE:CE2	2.49	0.47
1:C:25:PHE:CE1	1:C:33:LYS:CB	2.98	0.47
1:B:379:GLU:HA	1:B:382:GLU:HG3	1.96	0.47
1:A:190:VAL:HG21	1:A:304:GLU:OE1	2.14	0.47
1:D:150:LEU:HD13	1:D:192:PRO:HB2	1.97	0.47
1:A:129:LEU:O	1:A:201:TYR:HA	2.15	0.47
1:D:221:ILE:O	1:D:225:HIS:ND1	2.48	0.47
1:B:429:ARG:HD3	1:B:430:THR:HG23	1.97	0.47
1:C:164:LEU:HD23	1:C:164:LEU:HA	1.74	0.47
1:E:315:ASN:ND2	1:E:372:ILE:HD12	2.30	0.47
1:B:160:ALA:O	1:B:161:PRO:C	2.53	0.47
1:B:342:ASN:OD1	1:B:343:PRO:HD2	2.15	0.47
1:F:60:PHE:CE1	1:F:423:ILE:HD11	2.50	0.47
1:F:134:GLU:HB2	1:F:243:GLY:H	1.80	0.47
1:D:388:LEU:HB3	1:D:389:PRO:HD2	1.97	0.47
1:E:137:LEU:HD23	1:E:229:ALA:HA	1.97	0.47
1:B:160:ALA:CB	1:B:188:HIS:HD2	2.28	0.47
1:D:376:SER:OG	1:D:379:GLU:HB2	2.15	0.47
1:D:49:LYS:HA	1:D:69:TYR:CE2	2.49	0.47
1:C:372:ILE:HG22	1:C:385:ILE:HD13	1.97	0.47
1:B:118:GLU:O	1:B:121:ASP:HB2	2.15	0.47
1:A:139:LYS:HB2	1:A:149:GLU:HB2	1.96	0.47
1:A:17:ASN:OD1	1:A:17:ASN:O	2.33	0.47
1:E:24:GLN:HB2	1:E:24:GLN:HE21	1.47	0.47
1:B:315:ASN:HD21	1:B:372:ILE:H	1.63	0.46
1:D:58:GLU:HB3	1:D:61:VAL:HG23	1.98	0.46
1:D:309:VAL:HG23	1:D:386:VAL:HB	1.97	0.46
1:E:357:GLY:HA2	1:E:362:LEU:HD12	1.96	0.46
1:C:314:GLN:HE21	1:D:64:GLU:HB2	1.79	0.46
1:A:116:LEU:HD23	1:A:351:LEU:HD22	1.96	0.46
1:B:315:ASN:ND2	1:B:372:ILE:HG22	2.30	0.46
1:A:206:ARG:HH11	1:A:206:ARG:HG3	1.79	0.46
1:F:375:MET:HB2	1:F:380:ARG:CG	2.45	0.46
1:B:184:GLU:HG3	3:B:502:ADP:H3'	1.98	0.46
1:F:399:PHE:CE1	1:F:405:MET:HB3	2.49	0.46
1:F:402:ASN:HB3	1:F:405:MET:HG3	1.98	0.46
1:D:131:PRO:HG2	1:D:199:PHE:CD1	2.51	0.46
1:E:124:PHE:CD1	1:E:124:PHE:N	2.83	0.46
1:E:124:PHE:H	1:E:124:PHE:HD1	1.61	0.46
1:B:164:LEU:HD11	1:C:82:TRP:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:ARG:HD3	1:F:326:ARG:HA	1.64	0.46
1:B:176:LEU:HD13	1:B:183:ILE:HD11	1.98	0.46
1:B:48:ASN:HB3	1:B:71:TYR:CD1	2.50	0.46
1:E:303:TYR:C	1:E:304:GLU:HG3	2.35	0.46
1:D:211:ILE:O	1:D:214:PHE:N	2.47	0.46
1:A:80:PHE:C	1:A:82:TRP:H	2.18	0.46
1:A:91:ARG:C	1:A:92:PHE:CD1	2.88	0.46
1:B:286:THR:C	1:B:288:VAL:H	2.19	0.46
1:F:289:THR:HB	1:F:337:VAL:HG22	1.98	0.46
1:C:131:PRO:HG2	1:C:199:PHE:CE1	2.50	0.46
1:D:383:ASN:C	1:D:385:ILE:H	2.19	0.46
1:A:379:GLU:O	1:A:382:GLU:HG2	2.15	0.46
1:C:260:ASP:HB2	1:C:268:SER:HB3	1.98	0.46
1:F:300:VAL:CG1	1:F:301:PRO:HD2	2.45	0.46
1:A:374:VAL:O	1:A:374:VAL:HG23	2.14	0.46
1:E:131:PRO:CG	1:E:199:PHE:CD1	2.96	0.46
1:A:164:LEU:HD12	1:A:164:LEU:HA	1.76	0.46
1:F:323:PRO:HD2	1:F:331:ARG:O	2.15	0.46
1:A:64:GLU:OE1	1:F:314:GLN:OE1	2.34	0.46
1:D:160:ALA:HB1	1:D:161:PRO:HD3	1.96	0.46
1:D:160:ALA:O	1:D:161:PRO:C	2.54	0.46
1:D:311:TRP:CZ3	1:D:367:PRO:HB3	2.50	0.46
1:D:323:PRO:HG3	1:D:331:ARG:NE	2.30	0.46
1:D:239:VAL:CG2	1:D:240:ASN:N	2.78	0.46
1:F:189:GLU:OE2	1:F:190:VAL:HG23	2.16	0.46
1:E:315:ASN:HB3	1:E:318:PRO:CG	2.45	0.46
1:E:71:TYR:CD2	1:E:97:TYR:CD1	3.03	0.46
1:E:71:TYR:CD2	1:E:97:TYR:CE1	3.03	0.46
1:F:259:PHE:HB2	1:F:330:THR:OG1	2.15	0.46
1:F:19:LYS:HB2	1:F:87:GLY:HA3	1.97	0.46
1:F:48:ASN:ND2	1:F:71:TYR:CG	2.83	0.46
1:A:132:GLU:HB3	1:A:196:GLU:OE2	2.15	0.46
1:A:345:LEU:HD22	1:A:409:LEU:CD2	2.44	0.46
1:E:120:GLU:O	1:E:122:LEU:N	2.48	0.46
1:E:134:GLU:CD	2:E:501:GLU:HG2	2.36	0.46
1:E:57:ILE:HG13	1:E:96:ILE:CD1	2.45	0.46
1:D:185:ALA:CB	1:E:37:ILE:HG22	2.44	0.46
1:C:125:SER:O	1:C:126:ASP:OD1	2.34	0.46
1:B:121:ASP:O	1:B:122:LEU:HD23	2.16	0.46
1:D:318:PRO:CG	1:D:321:ARG:HB2	2.36	0.46
1:C:410:GLY:O	1:C:411:GLU:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:GLU:O	1:C:415:GLU:HG3	2.15	0.46
1:A:45:ALA:HA	1:A:50:VAL:CG2	2.44	0.46
1:B:399:PHE:CE1	1:B:405:MET:HB3	2.51	0.46
1:A:427:MET:O	1:A:431:GLN:HG2	2.16	0.46
1:A:109:ARG:HG3	1:A:344:TYR:CE2	2.51	0.46
1:B:433:HIS:HB3	1:B:434:PRO:HD2	1.98	0.46
1:A:112:LEU:HD13	1:A:205:VAL:HG12	1.98	0.46
1:C:241:GLY:HA3	1:C:298:ARG:HG3	1.98	0.46
1:A:34:ASN:CG	1:F:159:LEU:HG	2.36	0.46
1:F:381:MET:HE2	1:F:381:MET:HB2	1.82	0.46
1:C:48:ASN:OD1	1:C:72:PRO:HD2	2.16	0.46
1:E:129:LEU:HD12	1:E:207:SER:HB3	1.97	0.46
1:D:161:PRO:HB2	1:D:167:ASN:H	1.81	0.46
1:B:397:GLU:OE1	1:B:400:LYS:HE3	2.16	0.46
1:C:132:GLU:HB3	1:C:198:ASP:OD1	2.16	0.46
1:D:256:ASN:ND2	1:D:330:THR:O	2.50	0.45
1:A:207:SER:O	1:A:210:ASP:HB2	2.16	0.45
1:A:114:ARG:NH1	1:A:115:ILE:CD1	2.78	0.45
1:A:164:LEU:HB2	1:B:220:THR:HG23	1.97	0.45
1:A:220:THR:HG23	1:F:164:LEU:HB3	1.97	0.45
1:D:112:LEU:HD23	1:D:112:LEU:O	2.17	0.45
1:F:80:PHE:C	1:F:82:TRP:H	2.19	0.45
1:C:22:ARG:HB3	1:C:34:ASN:ND2	2.31	0.45
1:A:20:TYR:HB3	1:A:89:VAL:HG22	1.98	0.45
1:C:98:ASN:OD1	1:C:102:THR:HG23	2.16	0.45
1:C:164:LEU:HB2	1:D:220:THR:HG23	1.98	0.45
1:B:164:LEU:CD1	1:C:220:THR:HG22	2.39	0.45
1:E:48:ASN:HB3	1:E:71:TYR:CE1	2.50	0.45
1:F:309:VAL:HG23	1:F:386:VAL:O	2.16	0.45
1:B:128:ASN:HB3	1:B:201:TYR:HD1	1.80	0.45
1:B:370:ARG:NH2	1:B:379:GLU:OE1	2.49	0.45
1:A:12:LEU:O	1:A:16:GLU:HB2	2.16	0.45
1:D:137:LEU:HD12	1:D:195:HIS:NE2	2.31	0.45
1:F:285:PHE:HB2	1:F:349:VAL:CG1	2.46	0.45
1:E:338:ASP:HB2	1:E:339:PRO:HD2	1.98	0.45
1:E:85:GLU:OE1	1:E:86:LYS:HE2	2.16	0.45
1:C:256:ASN:OD1	1:C:258:PHE:HB2	2.16	0.45
1:A:160:ALA:CB	1:A:169:ARG:NH1	2.72	0.45
1:B:161:PRO:O	1:B:167:ASN:OD1	2.35	0.45
1:E:5:THR:H	1:E:8:ASP:HB2	1.82	0.45
1:D:138:PHE:HB3	1:D:147:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:LEU:O	1:E:239:VAL:HG22	2.15	0.45
1:C:38:PRO:O	1:C:41:GLN:HB2	2.16	0.45
1:D:232:MET:O	1:D:235:PRO:HD3	2.17	0.45
1:A:96:ILE:HG22	1:A:104:PHE:HB3	1.97	0.45
1:E:95:ASP:OD1	1:E:109:ARG:HG2	2.17	0.45
1:B:204:ALA:O	1:B:207:SER:N	2.50	0.45
1:A:405:MET:O	1:A:408:ALA:HB3	2.17	0.45
1:B:162:THR:HG21	1:C:220:THR:OG1	2.16	0.45
1:F:127:PHE:CG	1:F:351:LEU:HD12	2.52	0.45
1:E:249:SER:OG	3:E:502:ADP:N1	2.43	0.45
1:F:27:ASP:CB	1:F:33:LYS:HE3	2.46	0.45
1:C:122:LEU:HD11	1:C:359:LYS:HB2	1.99	0.45
1:C:388:LEU:HB3	1:C:389:PRO:HD2	1.97	0.45
1:E:310:ALA:HB1	1:E:368:ILE:HD12	1.98	0.45
1:A:105:GLU:O	1:A:105:GLU:HG3	2.16	0.45
1:B:309:VAL:O	1:B:310:ALA:HB2	2.17	0.45
1:D:147:THR:OG1	1:D:149:GLU:HB2	2.16	0.45
1:D:361:LYS:O	1:D:362:LEU:O	2.34	0.45
1:B:285:PHE:HB3	1:B:405:MET:SD	2.57	0.45
1:A:315:ASN:OD1	1:A:371:ASN:HA	2.16	0.45
1:B:388:LEU:HB3	1:B:389:PRO:HD2	1.99	0.45
1:B:214:PHE:O	1:B:216:LEU:N	2.49	0.45
1:C:160:ALA:O	1:C:161:PRO:O	2.35	0.45
1:C:351:LEU:HD22	1:C:355:LEU:HG	1.98	0.45
1:E:271:ALA:O	1:E:275:ILE:HD12	2.16	0.45
1:E:5:THR:N	1:E:8:ASP:HB2	2.32	0.45
1:D:69:TYR:CD1	1:D:99:PRO:HA	2.50	0.45
1:C:368:ILE:O	1:C:368:ILE:HG22	2.16	0.45
1:E:285:PHE:HB2	1:E:349:VAL:HG13	1.98	0.45
1:F:311:TRP:CE2	1:F:367:PRO:HB3	2.52	0.45
1:B:282:ALA:HA	1:B:285:PHE:CE2	2.52	0.45
1:D:150:LEU:HD13	1:D:192:PRO:O	2.16	0.45
1:C:120:GLU:HA	1:C:124:PHE:O	2.17	0.45
1:E:59:GLY:O	1:E:62:ARG:HG3	2.17	0.45
1:F:421:LYS:O	1:F:424:GLU:HB3	2.16	0.45
1:F:370:ARG:HH21	1:F:375:MET:HG2	1.82	0.45
1:E:135:PHE:HB3	1:E:231:PHE:CE1	2.52	0.45
1:C:293:VAL:HG11	1:C:428:PHE:CD1	2.52	0.45
1:B:136:PHE:CD1	1:B:235:PRO:HG2	2.52	0.45
1:B:311:TRP:CE2	1:B:367:PRO:HB3	2.51	0.45
1:C:276:ALA:HB2	1:C:364:ALA:CA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:LYS:O	1:D:364:ALA:HB2	2.17	0.45
1:A:206:ARG:NH1	1:A:206:ARG:CG	2.67	0.45
1:F:116:LEU:O	1:F:119:MET:HB3	2.17	0.45
1:E:249:SER:HA	1:E:258:PHE:CE1	2.52	0.45
1:E:331:ARG:HD2	3:E:502:ADP:C4	2.52	0.45
1:A:264:ASP:C	1:A:265:LEU:HD12	2.38	0.45
1:E:37:ILE:HD12	1:E:41:GLN:HB2	1.99	0.45
1:A:92:PHE:CD1	1:A:92:PHE:N	2.85	0.45
1:E:310:ALA:CB	1:E:372:ILE:HD11	2.47	0.45
1:B:368:ILE:HG12	1:B:385:ILE:HD11	1.99	0.45
1:C:410:GLY:O	1:C:412:HIS:N	2.50	0.45
1:B:20:TYR:HE2	1:B:22:ARG:NH1	2.14	0.45
1:D:171:ASP:OD1	1:D:225:HIS:NE2	2.40	0.45
1:B:21:ILE:CG2	1:B:37:ILE:HD11	2.46	0.45
1:B:106:GLY:HA2	1:B:413:LEU:HG	1.99	0.45
1:A:259:PHE:O	1:A:260:ASP:HB2	2.17	0.45
1:F:214:PHE:O	1:F:218:VAL:HG23	2.17	0.45
1:D:30:GLY:N	1:D:342:ASN:ND2	2.64	0.45
1:E:301:PRO:HA	1:E:316:ARG:HH12	1.82	0.44
1:F:41:GLN:HE22	1:F:44:LYS:HD3	1.82	0.44
1:D:172:ILE:HG21	1:D:218:VAL:HG22	1.98	0.44
1:C:176:LEU:O	1:C:181:PHE:HB2	2.17	0.44
1:C:181:PHE:HB3	1:C:183:ILE:HG13	1.98	0.44
1:F:9:ILE:HD11	1:F:74:LEU:HB3	1.98	0.44
1:E:379:GLU:OE1	1:E:382:GLU:HG3	2.18	0.44
1:B:160:ALA:CB	1:B:169:ARG:NH1	2.68	0.44
1:A:105:GLU:O	1:A:105:GLU:CG	2.65	0.44
1:E:170:ARG:NH1	1:E:171:ASP:OD2	2.50	0.44
1:F:374:VAL:CG2	1:F:375:MET:H	2.27	0.44
1:F:20:TYR:CZ	1:F:36:GLU:HB2	2.52	0.44
1:B:142:GLU:OE2	1:B:143:LYS:HG3	2.18	0.44
1:E:285:PHE:HB2	1:E:349:VAL:CG1	2.48	0.44
1:E:164:LEU:CD2	1:F:224:LYS:HB2	2.46	0.44
1:C:289:THR:O	1:C:341:ALA:HB2	2.17	0.44
1:E:372:ILE:HA	1:E:375:MET:CE	2.47	0.44
1:F:52:PHE:HZ	1:F:96:ILE:HD12	1.81	0.44
1:E:231:PHE:CD1	1:E:339:PRO:HB3	2.52	0.44
1:D:141:ASP:HB3	1:D:147:THR:CG2	2.48	0.44
1:F:137:LEU:HD23	1:F:229:ALA:HA	1.98	0.44
1:B:213:THR:O	1:B:217:VAL:HG23	2.17	0.44
1:A:281:HIS:HD2	1:A:353:ALA:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LEU:HD22	1:B:74:LEU:HD21	1.98	0.44
1:F:9:ILE:O	1:F:13:VAL:HG23	2.18	0.44
1:E:306:PRO:HB3	1:E:319:LEU:HA	1.99	0.44
1:A:325:SER:OG	1:B:51:MET:CE	2.65	0.44
1:D:164:LEU:O	1:D:165:GLY:O	2.34	0.44
1:E:197:ILE:HD12	1:E:214:PHE:HE1	1.82	0.44
1:B:372:ILE:CD1	1:B:385:ILE:HG21	2.48	0.44
1:A:131:PRO:HD2	1:A:199:PHE:CB	2.44	0.44
1:A:274:PHE:CE1	1:A:354:GLY:HA3	2.52	0.44
1:D:371:ASN:O	1:D:374:VAL:HG22	2.17	0.44
1:E:37:ILE:HB	1:E:38:PRO:HD2	2.00	0.44
1:F:423:ILE:HA	1:F:426:ASP:HB2	1.99	0.44
1:D:326:ARG:HD3	1:D:326:ARG:HA	1.68	0.44
1:F:134:GLU:OE2	1:F:189:GLU:OE1	2.35	0.44
1:C:243:GLY:HA3	2:C:501:GLU:OXT	2.18	0.44
1:B:280:LYS:HD2	1:B:362:LEU:HD21	1.98	0.44
1:F:4:TYR:HB3	1:F:9:ILE:HD11	1.98	0.44
1:E:25:PHE:HE1	1:E:57:ILE:CD1	2.30	0.44
1:E:364:ALA:HA	1:E:365:PRO:HD3	1.79	0.44
1:C:182:GLU:HA	1:C:182:GLU:OE2	2.17	0.44
1:B:167:ASN:ND2	1:B:170:ARG:H	2.13	0.44
1:F:370:ARG:NH2	1:F:375:MET:HG2	2.33	0.44
1:D:188:HIS:HE1	1:D:191:ALA:O	2.01	0.44
1:E:140:LEU:CD2	1:E:228:HIS:HB2	2.46	0.44
1:F:419:GLU:O	1:F:423:ILE:HG23	2.18	0.44
1:E:150:LEU:HD13	1:E:192:PRO:HG2	1.99	0.44
1:B:425:TRP:NE1	1:B:429:ARG:HG2	2.33	0.44
1:B:433:HIS:HB3	1:B:434:PRO:CD	2.47	0.44
1:D:268:SER:O	1:D:272:LYS:HG2	2.17	0.44
1:C:170:ARG:O	1:C:171:ASP:C	2.56	0.44
1:E:306:PRO:HG2	1:E:335:ARG:C	2.37	0.44
1:B:162:THR:HG22	1:B:163:ASP:H	1.83	0.44
1:E:119:MET:HA	1:E:355:LEU:HD11	2.00	0.44
1:E:68:MET:CG	1:E:96:ILE:HG22	2.45	0.44
1:F:131:PRO:HG2	1:F:199:PHE:CD1	2.53	0.44
1:A:96:ILE:HG21	1:A:104:PHE:HD2	1.83	0.44
1:D:269:GLU:O	1:D:273:HIS:CG	2.70	0.44
1:D:289:THR:HB	1:D:337:VAL:HG22	2.00	0.44
1:F:379:GLU:OE1	1:F:379:GLU:CA	2.57	0.44
1:A:119:MET:HE3	1:A:127:PHE:HB2	2.00	0.44
1:C:311:TRP:CE2	1:C:367:PRO:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:LEU:HD22	1:C:193:GLY:HA3	1.99	0.44
1:A:276:ALA:HB1	1:A:362:LEU:HB3	2.00	0.44
1:B:48:ASN:HB3	1:B:71:TYR:CE1	2.53	0.44
1:E:406:VAL:HG22	1:E:414:PHE:CD1	2.52	0.44
1:C:308:TYR:CD1	1:C:372:ILE:HD13	2.53	0.44
1:E:76:THR:HG21	1:E:93:ILE:HB	1.99	0.44
1:A:22:ARG:NH2	1:F:163:ASP:OD1	2.39	0.44
1:B:249:SER:HA	1:B:258:PHE:HE1	1.83	0.44
1:A:325:SER:HB2	1:A:331:ARG:HH11	1.83	0.44
1:E:16:GLU:HB3	1:E:18:VAL:HG23	2.00	0.44
1:D:154:GLY:HA3	1:D:188:HIS:NE2	2.33	0.44
1:F:205:VAL:O	1:F:207:SER:N	2.51	0.44
1:C:124:PHE:CD2	1:C:250:LEU:HD22	2.53	0.44
1:E:321:ARG:HD3	1:E:335:ARG:HD2	1.99	0.43
1:A:331:ARG:NH2	3:A:502:ADP:O4'	2.51	0.43
1:F:182:GLU:HB2	1:F:200:LYS:HG3	2.00	0.43
1:B:116:LEU:CD2	1:B:351:LEU:HD11	2.45	0.43
1:A:376:SER:O	1:A:379:GLU:N	2.51	0.43
1:E:159:LEU:HD12	1:E:159:LEU:C	2.38	0.43
1:C:14:LYS:N	1:C:14:LYS:HD2	2.33	0.43
1:E:426:ASP:HA	1:E:429:ARG:HG2	1.99	0.43
1:C:270:THR:HG23	1:C:358:ILE:HD12	1.98	0.43
1:B:135:PHE:CE1	1:B:195:HIS:HB2	2.53	0.43
1:D:134:GLU:HG2	1:D:189:GLU:HG3	2.00	0.43
1:F:399:PHE:HE1	1:F:405:MET:HB3	1.81	0.43
1:D:183:ILE:HG22	1:D:198:ASP:O	2.17	0.43
1:F:52:PHE:CD1	1:F:70:LEU:HD22	2.52	0.43
1:D:49:LYS:HA	1:D:69:TYR:HE2	1.84	0.43
1:C:376:SER:OG	1:C:378:GLU:CD	2.56	0.43
1:E:284:SER:HA	1:E:398:GLU:HB3	1.99	0.43
1:E:347:LEU:HD23	1:E:347:LEU:HA	1.55	0.43
1:D:269:GLU:OE1	1:D:272:LYS:HG3	2.18	0.43
1:C:264:ASP:HB3	1:C:272:LYS:HZ1	1.82	0.43
1:E:161:PRO:O	1:E:162:THR:C	2.56	0.43
1:B:112:LEU:O	1:B:116:LEU:HB2	2.17	0.43
1:E:406:VAL:O	1:E:410:GLY:N	2.48	0.43
1:B:23:LEU:HD23	1:B:92:PHE:HB2	2.01	0.43
1:D:354:GLY:O	1:D:357:GLY:N	2.51	0.43
1:F:185:ALA:O	1:F:186:SER:CB	2.65	0.43
1:C:436:GLU:O	1:C:440:TYR:CD2	2.71	0.43
1:D:27:ASP:OD1	1:D:33:LYS:CE	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:435:TRP:O	1:D:438:GLU:HG2	2.17	0.43
1:A:342:ASN:ND2	1:A:345:LEU:HG	2.31	0.43
1:B:130:GLY:HA3	3:B:502:ADP:O2'	2.18	0.43
1:D:320:ILE:CG2	1:D:332:VAL:HG23	2.47	0.43
1:B:288:VAL:HG11	1:B:345:LEU:O	2.19	0.43
1:E:325:SER:O	1:E:326:ARG:NE	2.51	0.43
1:E:142:GLU:H	1:E:142:GLU:CD	2.20	0.43
1:E:16:GLU:O	1:E:88:LYS:HD2	2.17	0.43
1:F:261:GLU:HA	1:F:266:GLN:CG	2.49	0.43
1:D:266:GLN:HG2	1:D:326:ARG:HG3	2.00	0.43
1:A:246:CYS:SG	1:A:337:VAL:HG21	2.58	0.43
1:A:48:ASN:OD1	1:A:71:TYR:HA	2.18	0.43
1:C:434:PRO:O	1:C:438:GLU:HG3	2.18	0.43
1:A:27:ASP:HB3	1:A:33:LYS:CD	2.27	0.43
1:F:384:GLY:C	1:F:385:ILE:HG13	2.39	0.43
1:E:170:ARG:O	1:E:174:LEU:HG	2.18	0.43
1:A:426:ASP:HA	1:A:429:ARG:HG2	2.00	0.43
1:B:164:LEU:HA	1:B:164:LEU:HD23	1.86	0.43
1:B:131:PRO:C	1:B:133:PRO:HD3	2.38	0.43
1:B:343:PRO:O	1:B:347:LEU:HD23	2.18	0.43
1:E:414:PHE:C	1:E:414:PHE:CD2	2.91	0.43
1:D:27:ASP:OD2	1:D:27:ASP:C	2.57	0.43
1:A:175:GLU:OE2	1:B:86:LYS:HE3	2.19	0.43
1:C:265:LEU:O	1:C:266:GLN:HB2	2.19	0.43
1:F:404:VAL:HG13	1:F:405:MET:HE2	2.01	0.43
1:A:295:SER:O	1:A:299:LEU:HD23	2.19	0.43
1:A:298:ARG:HH21	1:A:338:ASP:HB3	1.84	0.43
1:F:309:VAL:O	1:F:310:ALA:HB2	2.19	0.43
1:E:181:PHE:HZ	1:E:213:THR:HB	1.84	0.43
1:A:368:ILE:HG13	1:A:385:ILE:HD11	2.01	0.43
1:C:20:TYR:CE2	1:C:36:GLU:HB3	2.54	0.43
1:A:387:ASP:OD2	1:A:387:ASP:N	2.43	0.43
1:F:304:GLU:HG2	1:F:304:GLU:H	1.39	0.43
1:A:33:LYS:HE2	1:F:156:TYR:O	2.18	0.43
1:C:161:PRO:O	1:C:167:ASN:ND2	2.52	0.43
1:F:374:VAL:CG2	1:F:375:MET:N	2.80	0.43
1:D:282:ALA:O	1:D:284:SER:N	2.52	0.43
1:A:360:ASN:O	1:A:361:LYS:C	2.57	0.43
1:D:153:LYS:HA	1:D:192:PRO:HB3	2.00	0.43
1:D:168:CYS:O	1:D:172:ILE:HG13	2.18	0.43
1:F:364:ALA:HA	1:F:365:PRO:HD2	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:GLU:H	1:C:199:PHE:HA	1.83	0.43
1:D:406:VAL:HA	1:D:414:PHE:CD1	2.53	0.43
1:E:272:LYS:HA	1:E:275:ILE:CD1	2.43	0.43
1:E:281:HIS:O	1:E:284:SER:N	2.52	0.43
1:A:164:LEU:CB	1:B:220:THR:HG23	2.49	0.42
1:B:48:ASN:ND2	1:B:71:TYR:CG	2.86	0.42
1:B:10:GLU:HG2	1:B:42:LEU:HD21	2.01	0.42
1:A:239:VAL:O	1:A:240:ASN:C	2.57	0.42
1:F:178:GLU:O	1:F:180:GLY:N	2.52	0.42
1:D:141:ASP:OD1	1:D:145:GLU:HB2	2.20	0.42
1:F:366:ALA:HA	1:F:367:PRO:HD2	1.78	0.42
1:A:314:GLN:C	1:A:315:ASN:HD22	2.17	0.42
1:F:205:VAL:C	1:F:207:SER:H	2.22	0.42
1:C:134:GLU:HG2	1:C:189:GLU:HG3	2.00	0.42
1:E:436:GLU:O	1:E:440:TYR:HB2	2.19	0.42
1:B:377:LYS:NZ	1:B:380:ARG:HH12	2.17	0.42
1:D:406:VAL:HG13	1:D:414:PHE:CE1	2.54	0.42
1:F:41:GLN:NE2	1:F:44:LYS:HD3	2.33	0.42
1:B:31:THR:HG22	1:B:32:ILE:N	2.34	0.42
1:D:345:LEU:O	1:D:349:VAL:HG22	2.19	0.42
1:A:169:ARG:NH2	1:A:169:ARG:CG	2.73	0.42
1:F:376:SER:O	1:F:378:GLU:N	2.52	0.42
1:B:301:PRO:HA	1:B:307:CYS:SG	2.59	0.42
1:D:258:PHE:HB2	1:D:330:THR:HG22	2.02	0.42
1:C:325:SER:HB2	3:C:502:ADP:O3B	2.19	0.42
1:F:385:ILE:HG22	1:F:385:ILE:O	2.19	0.42
1:A:311:TRP:CZ2	1:A:367:PRO:HD3	2.55	0.42
1:C:72:PRO:HA	1:C:94:CYS:HB3	2.01	0.42
1:D:6:ARG:NH1	1:D:6:ARG:HG3	2.29	0.42
1:C:114:ARG:NH2	1:C:407:LYS:O	2.53	0.42
1:D:366:ALA:HA	1:D:367:PRO:HD2	1.86	0.42
1:C:39:VAL:HG22	1:C:39:VAL:O	2.19	0.42
1:A:34:ASN:O	1:A:34:ASN:ND2	2.52	0.42
1:D:107:ASP:HA	1:D:108:PRO:HD3	1.88	0.42
1:C:83:THR:C	1:C:84:ALA:O	2.58	0.42
1:E:78:VAL:CG1	1:E:79:ILE:N	2.82	0.42
1:B:116:LEU:HD23	1:B:116:LEU:HA	1.80	0.42
1:B:140:LEU:HD23	1:B:146:PRO:CA	2.47	0.42
1:E:41:GLN:HB3	1:E:41:GLN:HE21	1.63	0.42
1:B:328:ILE:C	1:B:330:THR:H	2.22	0.42
1:E:244:MET:O	1:E:244:MET:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:377:LYS:HD3	1:F:387:ASP:OD2	2.20	0.42
1:F:360:ASN:O	1:F:361:LYS:O	2.38	0.42
1:D:266:GLN:HB3	1:D:326:ARG:HH11	1.85	0.42
1:D:234:LYS:HG2	1:D:297:LYS:O	2.19	0.42
1:C:129:LEU:HD22	1:C:131:PRO:CD	2.49	0.42
1:D:304:GLU:CG	2:D:501:GLU:HG2	2.50	0.42
1:E:187:HIS:HE1	1:E:196:GLU:CD	2.23	0.42
1:A:274:PHE:CE2	1:A:278:ILE:HD11	2.54	0.42
1:D:71:TYR:CD2	1:D:97:TYR:CG	3.08	0.42
1:F:273:HIS:CD2	1:F:361:LYS:HG2	2.55	0.42
1:D:324:ALA:O	1:D:326:ARG:NE	2.52	0.42
1:A:93:ILE:HD12	1:A:209:ASP:CG	2.40	0.42
1:A:9:ILE:CD1	1:A:74:LEU:HG	2.41	0.42
1:B:160:ALA:HB2	1:B:188:HIS:CD2	2.51	0.42
1:C:55:SER:O	1:C:62:ARG:HB3	2.20	0.42
1:B:16:GLU:O	1:B:17:ASN:HB3	2.20	0.42
1:D:140:LEU:HD12	1:D:226:GLY:C	2.40	0.42
1:F:280:LYS:HB2	1:F:280:LYS:HE3	1.66	0.42
1:E:134:GLU:OE2	1:E:196:GLU:OE2	2.37	0.42
1:B:372:ILE:HD12	1:B:372:ILE:O	2.20	0.42
1:D:131:PRO:HG2	1:D:199:PHE:HD1	1.84	0.42
1:E:109:ARG:NH1	1:E:209:ASP:OD1	2.53	0.42
1:D:349:VAL:HG13	1:D:409:LEU:HD21	2.02	0.42
1:B:298:ARG:C	1:B:300:VAL:H	2.23	0.42
1:E:127:PHE:CE2	1:E:351:LEU:HG	2.54	0.42
1:B:386:VAL:HG22	1:B:387:ASP:O	2.19	0.42
1:A:312:SER:OG	1:A:313:ALA:N	2.52	0.42
1:F:131:PRO:C	1:F:133:PRO:HD3	2.40	0.42
1:E:399:PHE:CE1	1:E:405:MET:HB3	2.53	0.42
1:F:54:GLY:HA3	1:F:68:MET:HE1	2.01	0.42
1:B:285:PHE:HB2	1:B:349:VAL:HG11	2.00	0.42
1:A:113:LYS:O	1:A:117:LYS:HG3	2.20	0.42
1:E:321:ARG:HG2	1:E:321:ARG:O	2.19	0.41
1:A:311:TRP:O	1:A:311:TRP:CD2	2.73	0.41
1:D:380:ARG:HB3	1:D:385:ILE:HG21	2.02	0.41
1:E:146:PRO:HB3	1:E:228:HIS:CG	2.55	0.41
1:C:163:ASP:HB2	1:D:82:TRP:CE3	2.54	0.41
1:B:412:HIS:CD2	1:B:416:HIS:CD2	3.08	0.41
1:F:109:ARG:HG3	1:F:344:TYR:CE2	2.55	0.41
1:B:18:VAL:CG2	1:B:79:ILE:HD12	2.51	0.41
1:B:160:ALA:HB1	1:B:161:PRO:HD3	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ASP:HB2	1:B:268:SER:HB3	2.01	0.41
1:A:311:TRP:O	1:A:311:TRP:CG	2.73	0.41
1:C:414:PHE:C	1:C:414:PHE:CD2	2.93	0.41
1:F:119:MET:SD	1:F:127:PHE:HB2	2.61	0.41
1:B:42:LEU:O	1:B:45:ALA:HB3	2.20	0.41
1:E:387:ASP:N	1:E:387:ASP:OD2	2.49	0.41
1:E:6:ARG:NE	1:E:46:LEU:HD13	2.35	0.41
1:D:309:VAL:HG23	1:D:386:VAL:O	2.20	0.41
1:C:326:ARG:HD3	1:C:330:THR:OG1	2.20	0.41
1:B:16:GLU:O	1:B:17:ASN:CB	2.68	0.41
1:E:321:ARG:O	1:E:333:GLU:HB3	2.20	0.41
1:D:55:SER:O	1:D:62:ARG:CB	2.61	0.41
1:F:176:LEU:HD23	1:F:217:VAL:HG11	2.00	0.41
1:A:164:LEU:HD13	1:B:82:TRP:CB	2.47	0.41
1:A:174:LEU:O	1:A:177:GLU:HB2	2.20	0.41
1:B:173:VAL:HG22	1:B:197:ILE:HD13	2.01	0.41
1:C:342:ASN:HA	1:C:343:PRO:HD2	1.94	0.41
1:E:328:ILE:H	1:E:328:ILE:HG12	1.44	0.41
1:C:160:ALA:HB1	1:C:169:ARG:HH22	1.71	0.41
1:F:399:PHE:HZ	1:F:409:LEU:HD12	1.86	0.41
1:F:259:PHE:CE2	1:F:327:GLY:HA2	2.54	0.41
1:C:135:PHE:HB3	1:C:231:PHE:CD1	2.55	0.41
1:E:285:PHE:C	1:E:285:PHE:HD1	2.23	0.41
1:F:290:ASN:HB3	1:F:295:SER:HB3	2.01	0.41
1:D:52:PHE:CD1	1:D:70:LEU:HD13	2.55	0.41
1:E:24:GLN:OE1	1:E:91:ARG:HD3	2.21	0.41
1:C:140:LEU:HD21	1:C:228:HIS:HB2	2.01	0.41
1:A:272:LYS:O	1:A:364:ALA:HB2	2.21	0.41
1:B:167:ASN:ND2	1:B:170:ARG:HB2	2.35	0.41
1:C:206:ARG:NH1	1:C:206:ARG:HG3	2.35	0.41
1:C:131:PRO:CG	1:C:211:ILE:HD11	2.41	0.41
1:E:27:ASP:HB3	1:E:33:LYS:HG3	2.01	0.41
1:F:293:VAL:HG11	1:F:428:PHE:CD2	2.55	0.41
1:B:239:VAL:HG23	1:B:240:ASN:O	2.20	0.41
1:A:196:GLU:OE2	1:A:198:ASP:OD1	2.38	0.41
1:C:45:ALA:HA	1:C:50:VAL:HG23	2.03	0.41
1:F:351:LEU:O	1:F:351:LEU:HG	2.21	0.41
1:C:377:LYS:HA	1:C:380:ARG:HG3	2.01	0.41
1:E:236:LEU:HB2	1:E:239:VAL:HG21	2.02	0.41
1:F:161:PRO:CG	1:F:166:GLU:OE1	2.69	0.41
1:B:56:SER:C	1:B:58:GLU:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:TYR:HA	1:D:386:VAL:O	2.20	0.41
1:F:143:LYS:H	1:F:143:LYS:HG2	1.55	0.41
1:A:284:SER:CB	1:A:402:ASN:HD22	2.34	0.41
1:A:311:TRP:HE3	1:A:322:ILE:HD11	1.85	0.41
1:B:131:PRO:HG2	1:B:199:PHE:CD1	2.56	0.41
1:C:71:TYR:C	1:C:94:CYS:HB3	2.41	0.41
1:B:304:GLU:OE1	1:C:63:ILE:O	2.39	0.41
1:B:113:LYS:O	1:B:117:LYS:N	2.51	0.41
1:E:137:LEU:CD2	1:E:229:ALA:HB2	2.50	0.41
1:C:303:TYR:HB2	6:C:605:HOH:O	2.19	0.41
1:B:232:MET:HA	1:B:233:PRO:HD3	1.93	0.41
1:B:244:MET:O	1:B:337:VAL:HB	2.21	0.41
1:B:268:SER:O	1:B:272:LYS:HB2	2.21	0.41
1:C:351:LEU:CD2	1:C:355:LEU:HG	2.51	0.41
1:C:376:SER:O	1:C:380:ARG:HG3	2.21	0.41
1:D:82:TRP:O	1:D:89:VAL:HG23	2.21	0.41
1:B:435:TRP:O	1:B:436:GLU:C	2.59	0.41
1:B:53:ASP:OD2	1:B:53:ASP:C	2.59	0.41
1:C:169:ARG:HD3	1:C:186:SER:HB2	2.03	0.41
1:C:187:HIS:CD2	1:C:187:HIS:C	2.94	0.41
1:C:187:HIS:HD2	1:C:188:HIS:O	2.04	0.41
1:F:375:MET:HG3	1:F:375:MET:H	1.53	0.41
1:F:281:HIS:O	1:F:282:ALA:C	2.58	0.41
1:E:71:TYR:HA	1:E:72:PRO:HD2	1.89	0.41
1:F:232:MET:HA	1:F:233:PRO:HD2	1.92	0.41
1:E:126:ASP:HB2	1:E:251:PHE:HB2	2.03	0.41
1:C:308:TYR:HE2	1:C:380:ARG:CZ	2.33	0.41
1:B:285:PHE:C	1:B:285:PHE:CD1	2.94	0.41
1:A:186:SER:O	1:B:36:GLU:HG2	2.20	0.41
1:B:366:ALA:HA	1:B:367:PRO:HD2	1.93	0.41
1:F:286:THR:HG21	1:F:389:PRO:HD2	2.03	0.41
1:C:134:GLU:OE2	2:C:501:GLU:OE2	2.39	0.41
1:A:20:TYR:CZ	1:F:170:ARG:HG3	2.56	0.41
1:B:280:LYS:HD3	1:B:281:HIS:CE1	2.56	0.41
1:F:396:LEU:O	1:F:400:LYS:HB2	2.21	0.41
1:A:410:GLY:O	1:A:411:GLU:C	2.59	0.41
1:C:203:GLY:O	1:C:204:ALA:C	2.59	0.41
1:E:295:SER:O	1:E:299:LEU:HD22	2.21	0.41
1:F:16:GLU:HG2	1:F:79:ILE:HD13	2.03	0.41
1:B:132:GLU:HB3	1:B:198:ASP:OD1	2.21	0.41
1:C:109:ARG:HG3	1:C:344:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:ARG:HG2	1:F:63:ILE:N	2.35	0.41
1:D:62:ARG:O	1:D:63:ILE:HD13	2.21	0.41
1:A:116:LEU:HD23	1:A:351:LEU:HD21	2.03	0.41
1:B:312:SER:CB	1:B:315:ASN:HB2	2.51	0.41
1:D:6:ARG:O	1:D:6:ARG:HD3	2.20	0.41
1:C:260:ASP:CG	1:C:263:ALA:HB2	2.41	0.41
1:A:34:ASN:C	1:A:34:ASN:ND2	2.74	0.41
1:E:151:ASN:ND2	1:E:166:GLU:OE2	2.54	0.41
1:D:259:PHE:N	1:D:330:THR:HG21	2.36	0.40
1:D:54:GLY:C	1:D:56:SER:N	2.74	0.40
1:F:347:LEU:HA	1:F:347:LEU:HD13	1.69	0.40
1:D:380:ARG:O	1:D:385:ILE:HB	2.21	0.40
1:E:236:LEU:HB2	1:E:239:VAL:HG22	2.03	0.40
1:B:399:PHE:HE1	1:B:405:MET:HB3	1.85	0.40
1:F:170:ARG:O	1:F:173:VAL:HB	2.20	0.40
1:C:258:PHE:CE1	1:C:332:VAL:HG12	2.56	0.40
1:C:116:LEU:O	1:C:120:GLU:HG2	2.21	0.40
1:C:289:THR:HB	1:C:337:VAL:HG22	2.04	0.40
1:E:311:TRP:CZ2	1:E:367:PRO:HD3	2.56	0.40
1:F:436:GLU:O	1:F:440:TYR:HD2	2.03	0.40
1:B:364:ALA:HA	1:B:365:PRO:HD2	1.77	0.40
1:E:245:HIS:CD2	1:E:245:HIS:H	2.38	0.40
1:D:396:LEU:O	1:D:397:GLU:C	2.59	0.40
1:E:250:LEU:HD23	1:E:250:LEU:HA	1.84	0.40
1:C:76:THR:O	1:C:78:VAL:HG23	2.21	0.40
1:A:201:TYR:HD2	1:A:201:TYR:H	1.69	0.40
1:D:437:ARG:O	1:D:441:MET:N	2.47	0.40
1:C:319:LEU:HG	1:C:319:LEU:O	2.21	0.40
1:E:114:ARG:HG3	1:E:114:ARG:O	2.22	0.40
1:A:285:PHE:CD1	1:A:285:PHE:C	2.95	0.40
1:B:265:LEU:HA	1:B:265:LEU:HD13	1.84	0.40
1:C:315:ASN:HB3	1:C:318:PRO:HG3	2.03	0.40
1:E:406:VAL:HG13	1:E:414:PHE:CG	2.57	0.40
1:E:410:GLY:O	1:E:411:GLU:C	2.60	0.40
1:A:104:PHE:C	1:A:104:PHE:CD1	2.93	0.40
1:E:69:TYR:HE1	1:E:99:PRO:HA	1.87	0.40
1:C:265:LEU:O	1:C:326:ARG:NH1	2.54	0.40
1:B:273:HIS:ND1	1:B:361:LYS:HA	2.37	0.40
1:D:328:ILE:HG12	1:D:329:SER:N	2.37	0.40
1:C:325:SER:CB	3:C:502:ADP:O3B	2.69	0.40
1:D:402:ASN:OD1	1:D:405:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:LEU:HD11	1:E:22:ARG:HD3	2.03	0.40
1:F:248:LEU:HD11	1:F:350:LEU:HD13	2.04	0.40
1:F:127:PHE:HE2	1:F:347:LEU:CD1	2.34	0.40
1:C:240:ASN:ND2	2:C:501:GLU:HA	2.37	0.40
1:D:12:LEU:O	1:D:16:GLU:HB2	2.22	0.40
1:E:26:THR:HG22	1:E:26:THR:O	2.21	0.40
1:F:25:PHE:CD2	1:F:25:PHE:N	2.89	0.40
1:B:373:TYR:C	1:B:373:TYR:CD1	2.95	0.40
1:C:129:LEU:HD22	1:C:131:PRO:HD3	2.03	0.40
1:E:264:ASP:O	1:E:265:LEU:HB2	2.21	0.40
1:A:64:GLU:HG2	1:F:316:ARG:HA	2.03	0.40
1:D:161:PRO:O	1:D:162:THR:C	2.60	0.40
1:D:169:ARG:NH2	1:D:188:HIS:CA	2.84	0.40
1:A:379:GLU:C	1:A:382:GLU:HG2	2.42	0.40
1:D:270:THR:HG23	1:D:358:ILE:HD12	2.02	0.40
1:C:57:ILE:C	1:C:59:GLY:H	2.25	0.40
1:F:250:LEU:HD12	1:F:274:PHE:CD1	2.56	0.40
1:E:302:GLY:N	1:E:316:ARG:NH1	2.69	0.40
1:B:128:ASN:HB3	1:B:201:TYR:CD1	2.56	0.40
1:A:78:VAL:CG1	1:A:91:ARG:HG3	2.51	0.40
1:A:258:PHE:CE1	1:A:332:VAL:HG23	2.57	0.40
1:D:319:LEU:HD11	1:D:388:LEU:HD11	2.03	0.40
1:B:357:GLY:HA2	1:B:362:LEU:HD13	2.04	0.40
1:D:27:ASP:OD1	1:D:33:LYS:HE3	2.22	0.40
1:B:412:HIS:O	1:B:416:HIS:HD2	2.03	0.40
1:E:107:ASP:OD1	1:E:108:PRO:HD2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/443 (100%)	362 (82%)	57 (13%)	22 (5%)	3	8
1	B	441/443 (100%)	348 (79%)	76 (17%)	17 (4%)	4	14
1	C	441/443 (100%)	359 (81%)	60 (14%)	22 (5%)	3	8
1	D	441/443 (100%)	360 (82%)	59 (13%)	22 (5%)	3	8
1	E	441/443 (100%)	364 (82%)	61 (14%)	16 (4%)	4	16
1	F	441/443 (100%)	369 (84%)	55 (12%)	17 (4%)	4	14
All	All	2646/2658 (100%)	2162 (82%)	368 (14%)	116 (4%)	3	11

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLY
1	A	190	VAL
1	A	325	SER
1	B	316	ARG
1	C	84	ALA
1	C	86	LYS
1	C	184	GLU
1	C	368	ILE
1	D	165	GLY
1	D	204	ALA
1	D	362	LEU
1	D	368	ILE
1	E	161	PRO
1	F	282	ALA
1	F	316	ARG
1	F	361	LYS
1	F	411	GLU
1	A	260	ASP
1	A	304	GLU
1	B	100	ASP
1	B	162	THR
1	B	214	PHE
1	B	215	LYS
1	C	159	LEU
1	C	161	PRO
1	C	166	GLU
1	C	170	ARG
1	C	325	SER
1	C	369	ASP
1	C	410	GLY

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Mol	Chain	Res	Type
1	C	411	GLU
1	D	157	PHE
1	D	162	THR
1	D	167	ASN
1	D	260	ASP
1	E	121	ASP
1	E	166	GLU
1	E	204	ALA
1	E	324	ALA
1	E	325	SER
1	E	411	GLU
1	F	167	ASN
1	F	186	SER
1	F	304	GLU
1	A	167	ASN
1	A	186	SER
1	A	203	GLY
1	A	256	ASN
1	A	317	SER
1	A	368	ILE
1	B	101	GLY
1	B	287	ALA
1	B	314	GLN
1	C	158	ASP
1	C	167	ASN
1	D	240	ASN
1	D	266	GLN
1	D	268	SER
1	D	315	ASN
1	D	411	GLU
1	E	186	SER
1	E	262	ASN
1	E	352	ALA
1	F	101	GLY
1	F	166	GLU
1	F	179	MET
1	F	324	ALA
1	F	325	SER
1	F	412	HIS
1	A	166	GLU
1	A	240	ASN
1	A	361	LYS

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Mol	Chain	Res	Type
1	B	17	ASN
1	B	263	ALA
1	C	204	ALA
1	C	367	PRO
1	D	283	THR
1	D	306	PRO
1	D	329	SER
1	E	306	PRO
1	E	368	ILE
1	A	161	PRO
1	A	346	ALA
1	A	367	PRO
1	B	166	GLU
1	B	245	HIS
1	B	284	SER
1	B	352	ALA
1	C	40	SER
1	C	303	TYR
1	C	361	LYS
1	D	161	PRO
1	D	316	ARG
1	E	309	VAL
1	F	375	MET
1	A	257	ALA
1	A	358	ILE
1	B	34	ASN
1	D	3	LYS
1	E	84	ALA
1	E	214	PHE
1	F	383	ASN
1	C	317	SER
1	D	211	ILE
1	D	367	PRO
1	A	343	PRO
1	C	254	GLY
1	F	367	PRO
1	A	374	VAL
1	B	275	ILE
1	B	57	ILE
1	C	61	VAL
1	D	339	PRO
1	A	81	PRO

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Mol	Chain	Res	Type
1	E	218	VAL
1	F	131	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/382 (100%)	342 (90%)	40 (10%)	8	23
1	B	382/382 (100%)	349 (91%)	33 (9%)	13	35
1	C	382/382 (100%)	341 (89%)	41 (11%)	8	22
1	D	382/382 (100%)	334 (87%)	48 (13%)	5	15
1	E	382/382 (100%)	340 (89%)	42 (11%)	8	21
1	F	382/382 (100%)	342 (90%)	40 (10%)	8	23
All	All	2292/2292 (100%)	2048 (89%)	244 (11%)	8	23

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	14	LYS
1	A	34	ASN
1	A	35	VAL
1	A	36	GLU
1	A	62	ARG
1	A	70	LEU
1	A	82	TRP
1	A	91	ARG
1	A	92	PHE
1	A	102	THR
1	A	112	LEU
1	A	126	ASP
1	A	129	LEU
1	A	159	LEU
1	A	162	THR

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Mol	Chain	Res	Type
1	A	166	GLU
1	A	167	ASN
1	A	168	CYS
1	A	169	ARG
1	A	181	PHE
1	A	201	TYR
1	A	205	VAL
1	A	206	ARG
1	A	232	MET
1	A	242	SER
1	A	248	LEU
1	A	264	ASP
1	A	270	THR
1	A	293	VAL
1	A	299	LEU
1	A	315	ASN
1	A	316	ARG
1	A	320	ILE
1	A	331	ARG
1	A	359	LYS
1	A	361	LYS
1	A	383	ASN
1	A	386	VAL
1	A	387	ASP
1	B	3	LYS
1	B	5	THR
1	B	12	LEU
1	B	34	ASN
1	B	35	VAL
1	B	37	ILE
1	B	58	GLU
1	B	62	ARG
1	B	70	LEU
1	B	82	TRP
1	B	83	THR
1	B	91	ARG
1	B	92	PHE
1	B	102	THR
1	B	105	GLU
1	B	117	LYS
1	B	129	LEU
1	B	142	GLU

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Mol	Chain	Res	Type
1	B	153	LYS
1	B	159	LEU
1	B	162	THR
1	B	167	ASN
1	B	181	PHE
1	B	265	LEU
1	B	272	LYS
1	B	304	GLU
1	B	326	ARG
1	B	328	ILE
1	B	349	VAL
1	B	351	LEU
1	B	370	ARG
1	B	381	MET
1	B	429	ARG
1	C	5	THR
1	C	14	LYS
1	C	24	GLN
1	C	25	PHE
1	C	34	ASN
1	C	40	SER
1	C	49	LYS
1	C	62	ARG
1	C	64	GLU
1	C	71	TYR
1	C	82	TRP
1	C	91	ARG
1	C	94	CYS
1	C	105	GLU
1	C	112	LEU
1	C	122	LEU
1	C	129	LEU
1	C	148	LEU
1	C	151	ASN
1	C	153	LYS
1	C	156	TYR
1	C	159	LEU
1	C	162	THR
1	C	168	CYS
1	C	198	ASP
1	C	199	PHE
1	C	207	SER

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Mol	Chain	Res	Type
1	C	208	CYS
1	C	210	ASP
1	C	295	SER
1	C	299	LEU
1	C	316	ARG
1	C	325	SER
1	C	328	ILE
1	C	347	LEU
1	C	349	VAL
1	C	351	LEU
1	C	363	GLU
1	C	397	GLU
1	C	401	SER
1	C	431	GLN
1	D	6	ARG
1	D	7	GLU
1	D	14	LYS
1	D	34	ASN
1	D	35	VAL
1	D	58	GLU
1	D	62	ARG
1	D	68	MET
1	D	70	LEU
1	D	82	TRP
1	D	83	THR
1	D	89	VAL
1	D	91	ARG
1	D	94	CYS
1	D	114	ARG
1	D	126	ASP
1	D	129	LEU
1	D	147	THR
1	D	159	LEU
1	D	163	ASP
1	D	183	ILE
1	D	198	ASP
1	D	199	PHE
1	D	201	TYR
1	D	206	ARG
1	D	239	VAL
1	D	250	LEU
1	D	264	ASP

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Mol	Chain	Res	Type
1	D	266	GLN
1	D	267	LEU
1	D	273	HIS
1	D	304	GLU
1	D	316	ARG
1	D	319	LEU
1	D	326	ARG
1	D	328	ILE
1	D	332	VAL
1	D	336	SER
1	D	351	LEU
1	D	362	LEU
1	D	363	GLU
1	D	370	ARG
1	D	379	GLU
1	D	386	VAL
1	D	387	ASP
1	D	398	GLU
1	D	441	MET
1	D	443	GLN
1	E	5	THR
1	E	8	ASP
1	E	24	GLN
1	E	27	ASP
1	E	34	ASN
1	E	36	GLU
1	E	41	GLN
1	E	49	LYS
1	E	64	GLU
1	E	82	TRP
1	E	91	ARG
1	E	114	ARG
1	E	117	LYS
1	E	129	LEU
1	E	143	LYS
1	E	149	GLU
1	E	151	ASN
1	E	159	LEU
1	E	162	THR
1	E	163	ASP
1	E	168	CYS
1	E	182	GLU

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Mol	Chain	Res	Type
1	E	201	TYR
1	E	205	VAL
1	E	206	ARG
1	E	207	SER
1	E	262	ASN
1	E	283	THR
1	E	285	PHE
1	E	299	LEU
1	E	304	GLU
1	E	314	GLN
1	E	328	ILE
1	E	331	ARG
1	E	347	LEU
1	E	349	VAL
1	E	351	LEU
1	E	379	GLU
1	E	387	ASP
1	E	397	GLU
1	E	404	VAL
1	E	422	GLU
1	F	10	GLU
1	F	28	ILE
1	F	34	ASN
1	F	35	VAL
1	F	41	GLN
1	F	49	LYS
1	F	70	LEU
1	F	74	LEU
1	F	83	THR
1	F	91	ARG
1	F	105	GLU
1	F	112	LEU
1	F	129	LEU
1	F	143	LYS
1	F	148	LEU
1	F	152	ASP
1	F	166	GLU
1	F	177	GLU
1	F	184	GLU
1	F	186	SER
1	F	201	TYR
1	F	206	ARG

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Mol	Chain	Res	Type
1	F	270	THR
1	F	283	THR
1	F	299	LEU
1	F	304	GLU
1	F	311	TRP
1	F	317	SER
1	F	325	SER
1	F	326	ARG
1	F	329	SER
1	F	347	LEU
1	F	349	VAL
1	F	363	GLU
1	F	375	MET
1	F	379	GLU
1	F	382	GLU
1	F	423	ILE
1	F	431	GLN
1	F	441	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	41	GLN
1	A	245	HIS
1	A	443	GLN
1	B	187	HIS
1	B	315	ASN
1	C	110	ASN
1	C	167	ASN
1	D	342	ASN
1	E	41	GLN
1	E	98	ASN
1	E	314	GLN
1	E	416	HIS
1	F	194	GLN
1	F	240	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 12 are monoatomic - leaving 15 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	$\# Z  > 2$
2	GLU	A	501	4	3,9,9	0.40	0	2,11,11	0.11	0
3	ADP	A	502	-	22,29,29	1.25	3 (13%)	27,45,45	1.68	4 (14%)
5	SO4	A	505	-	4,4,4	0.10	0	6,6,6	0.16	0
5	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.25	0
2	GLU	B	501	4	4,8,9	0.65	0	3,9,11	0.83	0
3	ADP	B	502	-	22,29,29	1.10	2 (9%)	27,45,45	1.69	3 (11%)
2	GLU	C	501	4	3,9,9	0.34	0	2,11,11	0.16	0
3	ADP	C	502	-	22,29,29	1.10	2 (9%)	27,45,45	1.68	2 (7%)
2	GLU	D	501	4	3,9,9	0.42	0	2,11,11	0.16	0
3	ADP	D	502	-	22,29,29	1.27	2 (9%)	27,45,45	1.77	3 (11%)
2	GLU	E	501	4	3,9,9	0.38	0	2,11,11	0.20	0
3	ADP	E	502	-	22,29,29	1.06	1 (4%)	27,45,45	1.92	4 (14%)
5	SO4	E	505	-	4,4,4	0.21	0	6,6,6	0.14	0
2	GLU	F	501	-	4,8,9	0.85	0	3,9,11	1.17	1 (33%)
3	ADP	F	502	-	22,29,29	1.12	2 (9%)	27,45,45	1.84	4 (14%)

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
2	GLU	A	501	4	-	0/3/9/9	0/0/0/0
3	ADP	A	502	-	-	0/12/32/32	0/3/3/3
5	SO4	A	505	-	-	0/0/0/0	0/0/0/0
5	SO4	A	506	-	-	0/0/0/0	0/0/0/0
2	GLU	B	501	4	-	0/3/7/9	0/0/0/0
3	ADP	B	502	-	-	0/12/32/32	0/3/3/3
2	GLU	C	501	4	-	0/3/9/9	0/0/0/0
3	ADP	C	502	-	-	0/12/32/32	0/3/3/3
2	GLU	D	501	4	-	0/3/9/9	0/0/0/0
3	ADP	D	502	-	-	0/12/32/32	0/3/3/3
2	GLU	E	501	4	-	0/3/9/9	0/0/0/0
3	ADP	E	502	-	-	0/12/32/32	0/3/3/3
5	SO4	E	505	-	-	0/0/0/0	0/0/0/0
2	GLU	F	501	-	-	0/3/7/9	0/0/0/0
3	ADP	F	502	-	-	0/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	ADP	O4'-C1'	2.06	1.43	1.41
3	A	502	ADP	C2-N3	2.07	1.35	1.32
3	C	502	ADP	O4'-C1'	2.24	1.44	1.41
3	D	502	ADP	O4'-C1'	2.69	1.44	1.41
3	F	502	ADP	O4'-C1'	2.76	1.44	1.41
3	A	502	ADP	O4'-C1'	2.82	1.44	1.41
3	E	502	ADP	C5-C4	3.24	1.47	1.40
3	F	502	ADP	C5-C4	3.26	1.47	1.40
3	C	502	ADP	C5-C4	3.33	1.48	1.40
3	B	502	ADP	C5-C4	3.46	1.48	1.40
3	A	502	ADP	C5-C4	3.58	1.48	1.40
3	D	502	ADP	C5-C4	3.66	1.48	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	502	ADP	N3-C2-N1	-7.16	123.41	128.89
3	F	502	ADP	N3-C2-N1	-6.96	123.57	128.89
3	C	502	ADP	N3-C2-N1	-6.90	123.61	128.89
3	D	502	ADP	N3-C2-N1	-6.07	124.25	128.89
3	B	502	ADP	N3-C2-N1	-5.79	124.46	128.89
3	A	502	ADP	N3-C2-N1	-5.57	124.63	128.89
3	B	502	ADP	C4-C5-N7	-4.06	105.74	109.48
3	A	502	ADP	C4-C5-N7	-3.91	105.88	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	502	ADP	C4-C5-N7	-3.61	106.16	109.48
3	D	502	ADP	C4-C5-N7	-3.34	106.41	109.48
3	E	502	ADP	C1'-N9-C4	-3.27	122.00	126.94
3	F	502	ADP	C4-C5-N7	-3.01	106.71	109.48
3	F	502	ADP	PA-O3A-PB	-2.71	123.57	132.67
3	C	502	ADP	C4-C5-N7	-2.57	107.11	109.48
3	E	502	ADP	O3A-PA-O5'	-2.23	97.02	102.94
2	F	501	GLU	O-C-CA	-2.01	120.27	125.49
3	F	502	ADP	O3B-PB-O2B	2.01	115.05	107.38
3	B	502	ADP	C4'-O4'-C1'	2.22	112.16	109.72
3	A	502	ADP	O4'-C1'-N9	2.46	113.25	108.10
3	D	502	ADP	C4'-O4'-C1'	2.76	112.75	109.72
3	A	502	ADP	C4'-O4'-C1'	2.77	112.76	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	ADP	3	0
3	B	502	ADP	3	0
2	C	501	GLU	4	0
3	C	502	ADP	5	0
2	D	501	GLU	4	0
3	D	502	ADP	1	0
2	E	501	GLU	3	0
3	E	502	ADP	4	0
5	E	505	SO4	1	0
2	F	501	GLU	1	0
3	F	502	ADP	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	443/443 (100%)	0.32	9 (2%) 68 65	43, 61, 97, 127	1 (0%)
1	B	443/443 (100%)	0.31	7 (1%) 74 73	42, 62, 95, 118	1 (0%)
1	C	443/443 (100%)	0.33	10 (2%) 64 60	45, 63, 94, 120	1 (0%)
1	D	443/443 (100%)	0.30	8 (1%) 71 69	45, 63, 98, 128	0
1	E	443/443 (100%)	0.33	13 (2%) 55 50	44, 61, 96, 122	1 (0%)
1	F	443/443 (100%)	0.27	8 (1%) 71 69	45, 63, 96, 136	2 (0%)
All	All	2658/2658 (100%)	0.31	55 (2%) 67 63	42, 62, 97, 136	6 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	250	LEU	4.3
1	A	312	SER	4.2
1	D	381	MET	4.0
1	D	378	GLU	4.0
1	A	313	ALA	3.8
1	B	382	GLU	3.6
1	C	372	ILE	3.4
1	D	384	GLY	3.4
1	B	264	ASP	3.4
1	F	378	GLU	3.3
1	B	61	VAL	3.3
1	E	261	GLU	3.2
1	B	305	ALA	3.1
1	D	305	ALA	3.0
1	D	207	SER	3.0
1	A	371	ASN	3.0
1	E	311	TRP	2.8
1	E	317	SER	2.8
1	C	61	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	315	ASN	2.6
1	A	305	ALA	2.6
1	F	381	MET	2.6
1	A	384	GLY	2.6
1	C	316	ARG	2.6
1	B	307	CYS	2.6
1	E	310	ALA	2.5
1	C	308	TYR	2.5
1	E	82	TRP	2.5
1	E	164	LEU	2.4
1	B	306	PRO	2.4
1	C	313	ALA	2.4
1	E	249	SER	2.4
1	F	90	ALA	2.4
1	C	373	TYR	2.4
1	F	302	GLY	2.4
1	C	384	GLY	2.4
1	F	379	GLU	2.4
1	C	315	ASN	2.3
1	A	300	VAL	2.3
1	E	316	ARG	2.3
1	E	96	ILE	2.3
1	F	83	THR	2.3
1	D	385	ILE	2.2
1	D	151	ASN	2.2
1	C	385	ILE	2.2
1	E	385	ILE	2.2
1	A	304	GLU	2.2
1	B	315	ASN	2.2
1	A	375	MET	2.1
1	F	349	VAL	2.1
1	E	273	HIS	2.1
1	E	330	THR	2.1
1	C	305	ALA	2.1
1	A	84	ALA	2.1
1	F	384	GLY	2.0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GLU	F	501	9/10	0.67	0.55	6.56	55,68,71,72	0
3	ADP	A	502	27/27	0.66	0.42	4.72	83,106,152,159	0
4	MG	C	503	1/1	0.87	0.29	4.34	60,60,60,60	0
2	GLU	E	501	10/10	0.75	0.42	4.09	57,63,68,68	0
4	MG	D	503	1/1	0.89	0.26	3.78	49,49,49,49	0
2	GLU	C	501	10/10	0.80	0.44	3.62	57,62,68,68	0
5	SO4	A	506	5/5	0.84	0.28	3.56	73,74,82,90	0
2	GLU	B	501	9/10	0.79	0.47	3.22	65,71,75,76	0
4	MG	B	503	1/1	0.87	0.29	3.18	51,51,51,51	0
3	ADP	E	502	27/27	0.77	0.42	3.13	79,97,130,141	0
2	GLU	D	501	10/10	0.74	0.45	3.03	58,71,76,79	0
3	ADP	D	502	27/27	0.82	0.32	2.38	75,93,114,131	0
3	ADP	F	502	27/27	0.84	0.29	1.68	81,108,134,135	0
2	GLU	A	501	10/10	0.82	0.34	1.32	64,70,75,78	0
3	ADP	C	502	27/27	0.81	0.28	1.10	70,85,98,108	0
4	MG	F	503	1/1	0.96	0.23	1.09	59,59,59,59	0
4	MG	F	504	1/1	0.95	0.22	0.70	53,53,53,53	0
5	SO4	E	505	5/5	0.77	0.31	0.51	93,98,100,104	0
3	ADP	B	502	27/27	0.84	0.24	0.05	71,83,114,117	0
4	MG	E	504	1/1	0.92	0.17	-0.99	49,49,49,49	0
5	SO4	A	505	5/5	0.86	0.14	-1.24	90,93,99,108	0
4	MG	A	503	1/1	0.90	0.17	-1.76	64,64,64,64	0
4	MG	A	504	1/1	0.94	0.14	-2.74	50,50,50,50	0
4	MG	E	503	1/1	0.68	0.24	-	61,61,61,61	0
4	MG	C	504	1/1	0.85	0.38	-	51,51,51,51	0
4	MG	D	504	1/1	0.90	0.22	-	61,61,61,61	0
4	MG	B	504	1/1	0.92	0.22	-	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.