



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:43 PM GMT

PDB ID : 3MVQ  
Title : Bovine Glutamate dehydrogenase complexed with zinc  
Authors : Smith, T.J.; Li, M.  
Deposited on : 2010-05-04  
Resolution : 2.94 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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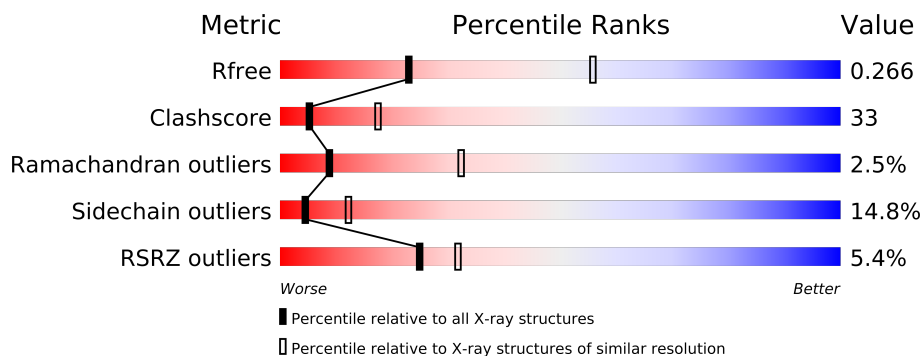
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.94 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))
$R_{free}$	66092	1424 (2.98-2.90)
Clashscore	79885	1761 (2.98-2.90)
Ramachandran outliers	78287	1708 (2.98-2.90)
Sidechain outliers	78261	1710 (2.98-2.90)
RSRZ outliers	66119	1425 (2.98-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	501	
1	B	501	
1	C	501	
1	D	501	
1	E	501	
1	F	501	

## 2 Entry composition i

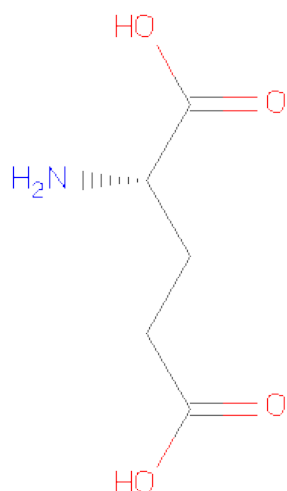
There are 5 unique types of molecules in this entry. The entry contains 23874 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Glutamate dehydrogenase 1, mitochondrial.

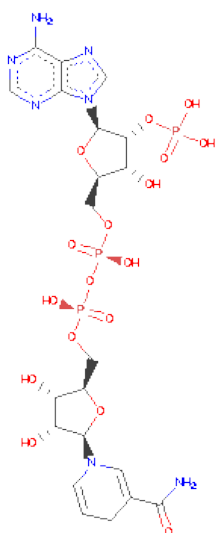
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	B	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	C	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	D	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	E	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	F	501	Total	C	N	O	S	0	0	0
			3922	2476	687	740	19			

- 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
			10	5	1	4		
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
			10	5	1	4		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



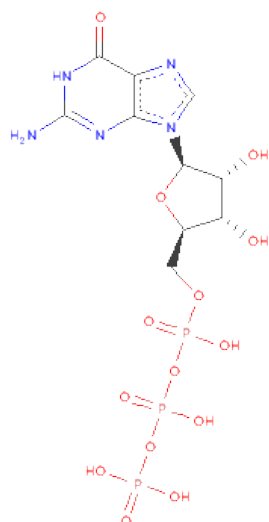
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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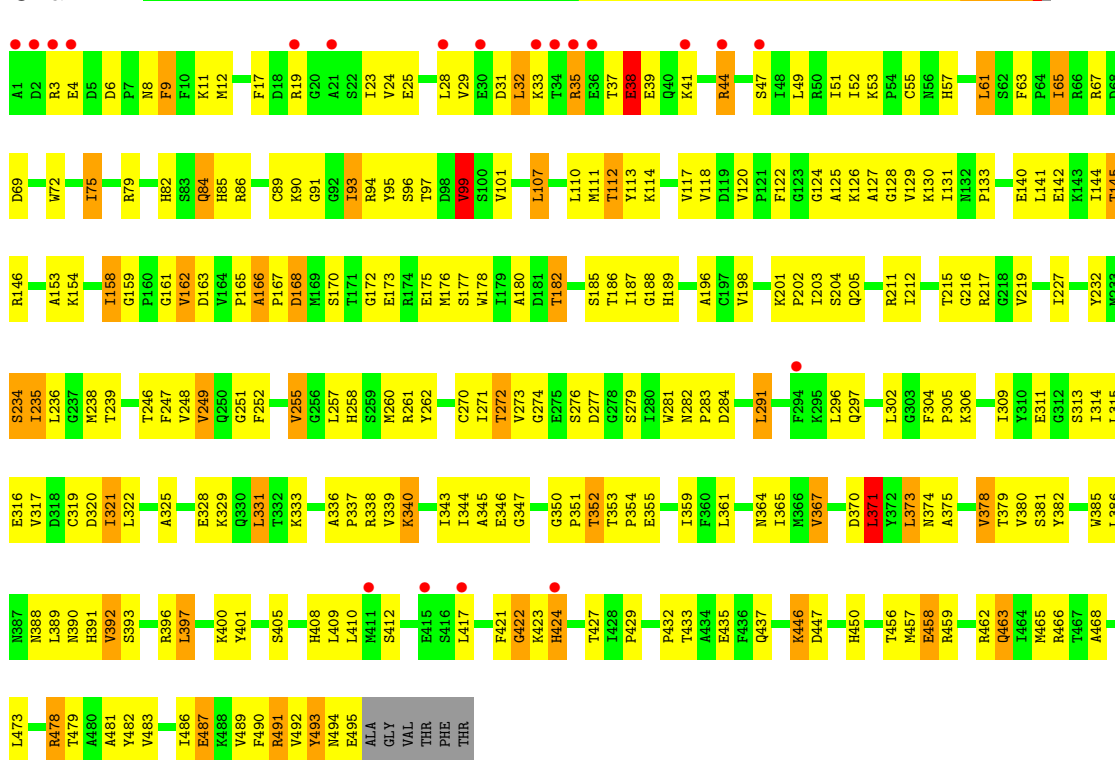
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Zn 2	0	0
5	C	3	Total 3	Zn 3	0	0
5	A	2	Total 2	Zn 2	0	0
5	F	1	Total 1	Zn 1	0	0

### 3 Residue-property plots

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

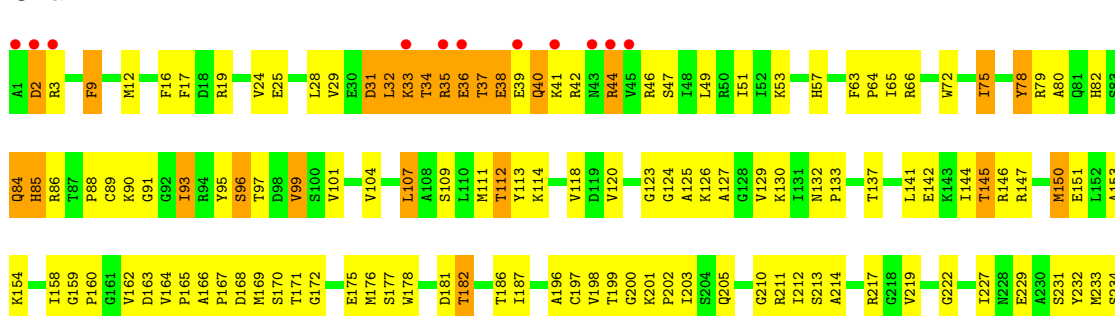
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

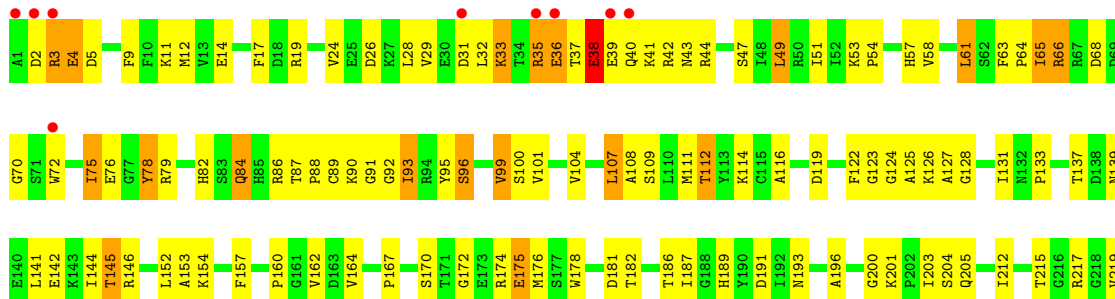
Chain A:

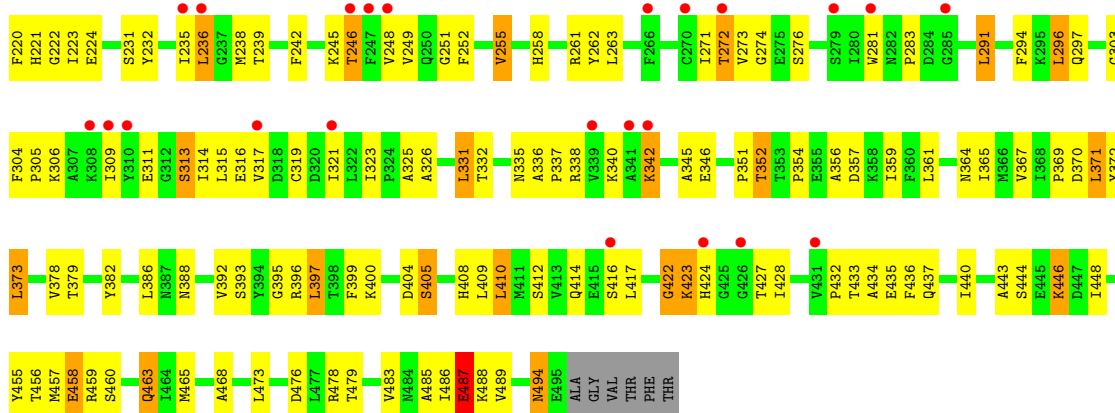


- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain B:

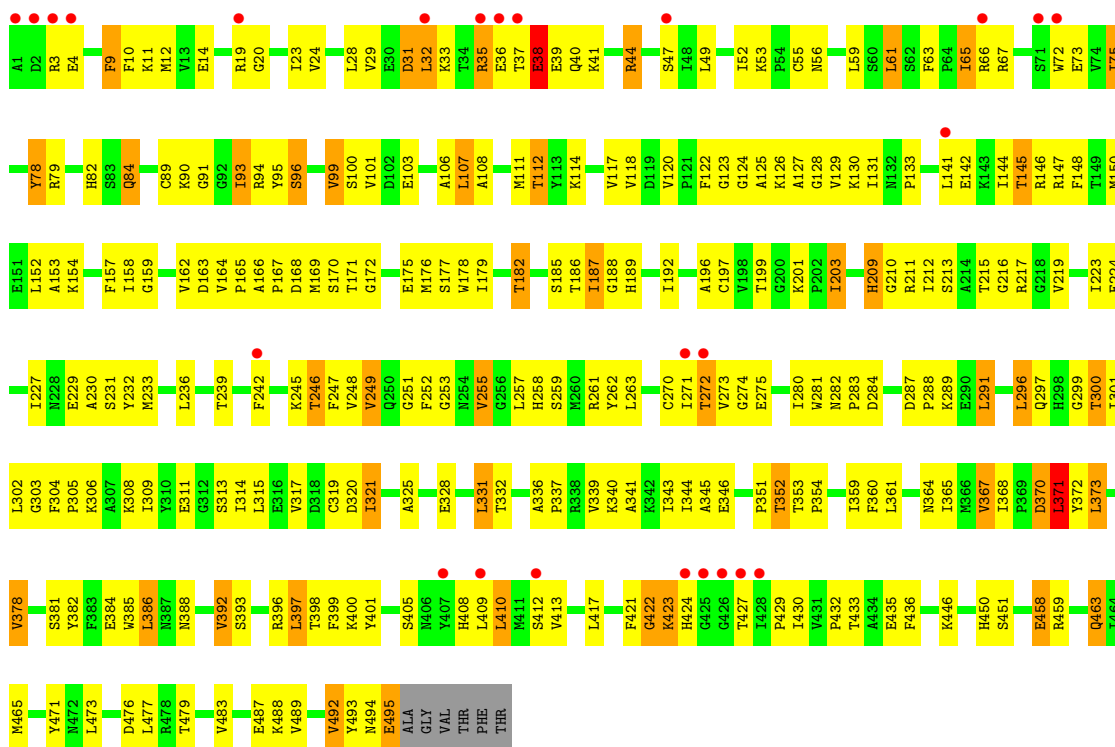






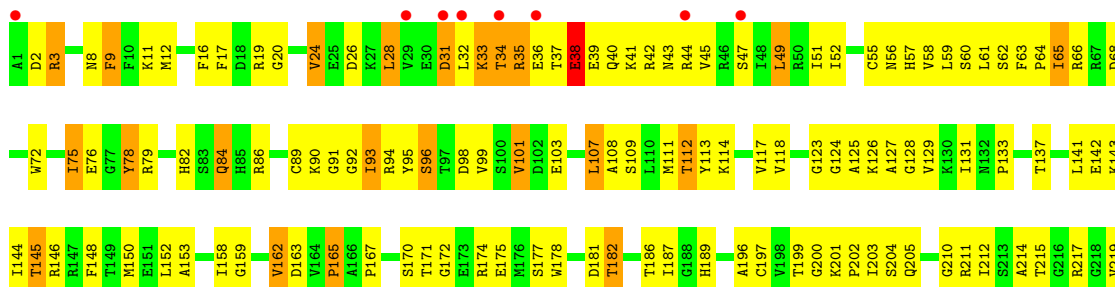
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

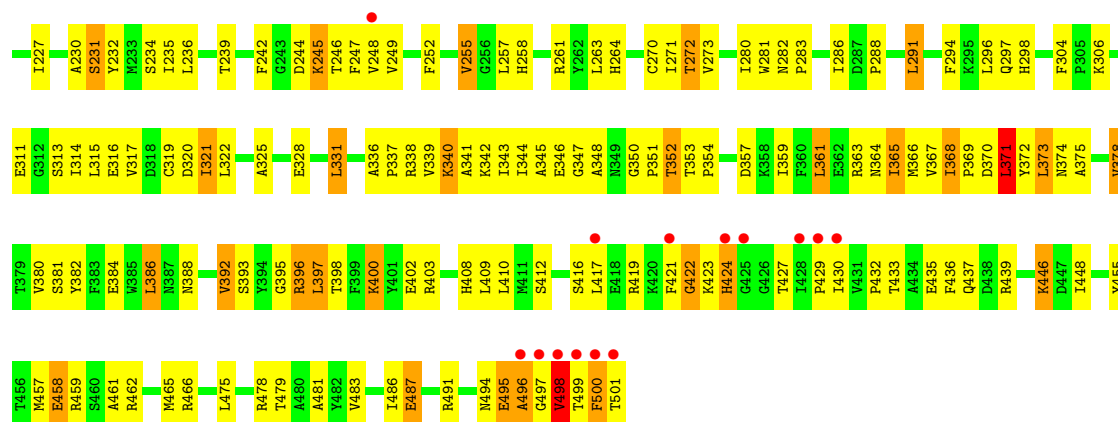
Chain E:



• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain F:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.11Å 98.76Å 165.64Å 90.00° 101.55° 90.00°	Depositor
Resolution (Å)	45.88 – 2.94 47.44 – 2.94	Depositor EDS
% Data completeness (in resolution range)	92.9 (45.88-2.94) 93.1 (47.44-2.94)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_353)	Depositor
R, $R_{free}$	0.223 , 0.262 0.206 , 0.266	Depositor DCC
$R_{free}$ test set	3821 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 10.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 75931 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	23874	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, NDP, ZN

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	0.46	0/3962	0.65	0/5348
1	B	0.46	0/3962	0.64	1/5348 (0.0%)
1	C	0.46	0/3962	0.63	0/5348
1	D	0.48	0/3962	0.63	0/5348
1	E	0.47	0/3962	0.63	0/5348
1	F	0.48	0/4005	0.65	0/5406
All	All	0.47	0/23815	0.64	1/32146 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	VAL	CB-CA-C	-5.01	101.88	111.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3880	0	3843	281	0
1	B	3880	0	3843	278	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3880	0	3843	292	0
1	D	3880	0	3843	237	0
1	E	3880	0	3843	274	0
1	F	3922	0	3883	282	0
2	A	10	0	5	3	0
2	B	10	0	5	3	0
2	C	10	0	5	5	0
2	D	10	0	5	1	0
2	E	10	0	5	3	0
2	F	10	0	5	2	0
3	A	48	0	26	4	0
3	B	48	0	26	7	0
3	C	48	0	26	5	0
3	D	48	0	26	3	0
3	E	48	0	26	5	0
3	F	48	0	26	5	0
4	A	32	0	12	1	0
4	B	32	0	12	0	0
4	C	32	0	12	1	0
4	D	32	0	12	0	0
4	E	32	0	12	1	0
4	F	32	0	12	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	3	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
All	All	23874	0	23356	1557	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

All (1557) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:93:ILE:HD11	1:F:95:TYR:CE1	1.78	1.18
1:C:38:GLU:HG2	1:C:39:GLU:N	1.58	1.13
1:D:392:VAL:HG11	1:D:397:LEU:HD11	1.27	1.12
1:F:38:GLU:HG2	1:F:39:GLU:H	1.00	1.09
1:E:38:GLU:HG2	1:E:39:GLU:H	0.96	1.09
1:B:82:HIS:HD2	1:B:112:THR:HG21	1.18	1.08
1:D:38:GLU:HG2	1:D:39:GLU:N	1.68	1.07

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:38:GLU:HG3	1:B:39:GLU:H	1.15	1.07
1:A:38:GLU:HG2	1:A:39:GLU:H	0.96	1.06
1:B:82:HIS:CD2	1:B:112:THR:HG21	1.91	1.05
1:D:82:HIS:HD2	1:D:112:THR:HG21	1.19	1.05
1:C:93:ILE:HD11	1:C:95:TYR:CE1	1.92	1.04
1:D:38:GLU:HG2	1:D:39:GLU:H	0.92	1.04
1:C:38:GLU:HG2	1:C:39:GLU:H	0.91	1.03
1:A:478:ARG:HG3	1:A:478:ARG:HH11	1.18	1.02
1:B:37:THR:O	1:B:38:GLU:HG2	1.59	1.02
1:E:38:GLU:HG2	1:E:39:GLU:N	1.71	1.01
1:A:38:GLU:HG2	1:A:39:GLU:N	1.63	1.01
1:C:82:HIS:HD2	1:C:112:THR:HG21	1.22	1.01
1:D:82:HIS:CD2	1:D:112:THR:HG21	1.96	1.00
1:A:107:LEU:HB3	1:A:126:LYS:HG2	1.41	1.00
1:F:82:HIS:CD2	1:F:112:THR:HG21	1.97	1.00
1:D:153:ALA:HB1	1:D:187:ILE:HG13	1.39	1.00
1:F:346:GLU:OE1	1:F:352:THR:HG23	1.61	0.99
1:E:107:LEU:HB3	1:E:126:LYS:HG2	1.44	0.99
1:F:38:GLU:HG2	1:F:39:GLU:N	1.74	0.98
1:A:112:THR:HG22	1:A:124:GLY:CA	1.93	0.98
1:A:141:LEU:O	1:A:145:THR:HG23	1.64	0.97
1:E:141:LEU:O	1:E:145:THR:HG23	1.64	0.97
1:B:93:ILE:HD11	1:B:95:TYR:CE1	2.01	0.95
1:D:35:ARG:HD3	1:D:35:ARG:H	1.29	0.95
1:D:93:ILE:HD11	1:D:95:TYR:CE1	2.02	0.95
1:C:337:PRO:HD3	1:C:359:ILE:HD13	1.47	0.95
1:C:82:HIS:CD2	1:C:112:THR:HG21	2.02	0.94
1:B:35:ARG:H	1:B:35:ARG:HD3	1.32	0.94
1:E:112:THR:HG22	1:E:124:GLY:H	1.32	0.94
1:C:3:ARG:H	1:C:3:ARG:HD3	1.33	0.93
1:A:93:ILE:HD11	1:A:95:TYR:HE1	1.31	0.92
1:E:35:ARG:HD3	1:E:35:ARG:H	1.34	0.92
1:A:112:THR:HG22	1:A:124:GLY:HA3	1.49	0.92
1:A:107:LEU:HG	1:A:126:LYS:HE3	1.49	0.92
1:F:82:HIS:HD2	1:F:112:THR:HG21	1.34	0.91
1:C:112:THR:HG22	1:C:124:GLY:H	1.34	0.91
1:A:82:HIS:CD2	1:A:112:THR:HG21	2.05	0.91
1:D:346:GLU:OE1	1:D:352:THR:HG23	1.69	0.91
1:A:82:HIS:HD2	1:A:112:THR:HG21	1.35	0.91
1:A:457:MET:HA	1:A:457:MET:HE2	1.53	0.90
1:C:35:ARG:HD3	1:C:35:ARG:H	1.34	0.90
1:C:93:ILE:HD11	1:C:95:TYR:HE1	1.33	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:417:LEU:HD21	1:C:417:LEU:HD13	1.53	0.90
2:B:502:GLU:HA	3:B:552:NDP:H41N	1.53	0.90
1:A:47:SER:HB3	1:D:72:TRP:HB2	1.54	0.88
1:C:112:THR:HG22	1:C:124:GLY:N	1.89	0.88
1:D:408:HIS:HB3	1:F:436:PHE:HB2	1.56	0.87
1:F:141:LEU:O	1:F:145:THR:HG23	1.74	0.87
1:D:38:GLU:CG	1:D:39:GLU:H	1.83	0.87
1:F:35:ARG:H	1:F:35:ARG:HD3	1.40	0.86
1:E:201:LYS:NZ	1:E:388:ASN:HD21	1.74	0.85
1:B:91:GLY:HA3	1:B:125:ALA:O	1.75	0.85
1:E:93:ILE:HD11	1:E:95:TYR:CE1	2.11	0.85
1:B:72:TRP:HB2	1:E:47:SER:HB3	1.58	0.85
1:A:478:ARG:HG3	1:A:478:ARG:NH1	1.90	0.85
1:C:112:THR:HG22	1:C:124:GLY:CA	2.06	0.85
1:F:258:HIS:HD2	1:F:261:ARG:HH11	1.25	0.85
1:A:112:THR:HG22	1:A:124:GLY:N	1.91	0.85
1:F:107:LEU:HB3	1:F:126:LYS:HG2	1.58	0.85
1:A:93:ILE:HD11	1:A:95:TYR:CE1	2.11	0.84
1:E:82:HIS:CD2	1:E:112:THR:HG21	2.12	0.84
1:E:38:GLU:CG	1:E:39:GLU:H	1.86	0.84
1:F:112:THR:HG22	1:F:124:GLY:HA3	1.58	0.84
1:E:112:THR:HG22	1:E:124:GLY:N	1.92	0.84
1:A:146:ARG:HE	1:A:182:THR:HG22	1.43	0.84
1:F:32:LEU:HD13	1:F:494:ASN:HD21	1.43	0.84
1:F:38:GLU:CG	1:F:39:GLU:H	1.89	0.83
1:A:112:THR:HG22	1:A:124:GLY:H	1.44	0.83
1:B:38:GLU:HG3	1:B:39:GLU:N	1.93	0.83
1:A:345:ALA:HB1	1:A:373:LEU:HD11	1.59	0.83
1:A:248:VAL:HB	1:A:272:THR:HG23	1.62	0.82
1:C:315:LEU:HD13	1:C:331:LEU:CD1	2.10	0.82
1:D:346:GLU:HG2	1:D:351:PRO:HG2	1.60	0.82
1:C:248:VAL:HG23	1:C:272:THR:O	1.80	0.82
1:A:35:ARG:H	1:A:35:ARG:HD3	1.45	0.82
1:E:153:ALA:HB1	1:E:187:ILE:HG13	1.62	0.81
1:C:38:GLU:CG	1:C:39:GLU:N	2.43	0.81
1:B:219:VAL:HG22	1:B:373:LEU:HD22	1.62	0.81
1:A:142:GLU:O	1:A:146:ARG:HG3	1.81	0.81
1:A:118:VAL:HG23	1:A:120:VAL:HG23	1.62	0.81
1:B:47:SER:HB3	1:E:72:TRP:HB2	1.62	0.80
1:B:248:VAL:HG12	1:B:319:CYS:SG	2.22	0.80
1:E:258:HIS:HD2	1:E:261:ARG:HH11	1.30	0.80
1:C:271:ILE:HD12	1:C:272:THR:HG22	1.64	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:458:GLU:HG3	1:E:459:ARG:N	1.98	0.79
1:D:271:ILE:HD12	1:D:272:THR:HG22	1.63	0.79
1:B:112:THR:HG22	1:B:124:GLY:HA3	1.65	0.79
1:F:458:GLU:HG3	1:F:459:ARG:N	1.98	0.79
1:E:258:HIS:CD2	1:E:261:ARG:HH11	2.00	0.79
1:A:281:TRP:CZ2	1:A:283:PRO:HG3	2.17	0.79
1:D:93:ILE:HD11	1:D:95:TYR:HE1	1.43	0.79
1:D:19:ARG:HG2	1:D:479:THR:HG21	1.63	0.78
1:E:201:LYS:HZ1	1:E:388:ASN:HD21	1.27	0.78
1:C:279:SER:OG	1:C:314:ILE:HB	1.83	0.78
1:A:38:GLU:CG	1:A:39:GLU:N	2.45	0.78
1:E:337:PRO:HD3	1:E:359:ILE:HD13	1.64	0.78
1:B:112:THR:HG22	1:B:124:GLY:CA	2.14	0.78
1:B:82:HIS:CD2	1:B:112:THR:CG2	2.67	0.78
1:A:346:GLU:OE1	1:A:352:THR:HG23	1.83	0.78
1:D:82:HIS:CD2	1:D:112:THR:CG2	2.67	0.77
1:F:336:ALA:N	1:F:337:PRO:HD2	1.98	0.77
1:A:248:VAL:HG12	1:A:319:CYS:SG	2.24	0.77
1:E:432:PRO:HB3	1:E:436:PHE:HD2	1.49	0.77
1:D:178:TRP:HE1	1:F:498:VAL:CG2	1.96	0.77
1:B:201:LYS:NZ	1:B:388:ASN:HD21	1.82	0.77
1:A:201:LYS:HZ1	1:A:388:ASN:HD21	1.32	0.77
1:F:93:ILE:CD1	1:F:95:TYR:CE1	2.66	0.77
1:B:107:LEU:HG	1:B:126:LYS:HE3	1.66	0.77
1:E:90:LYS:HD3	1:E:122:PHE:CE1	2.18	0.77
1:F:432:PRO:HB2	1:F:437:GLN:HG2	1.65	0.77
1:C:141:LEU:O	1:C:145:THR:HG23	1.84	0.77
1:A:90:LYS:HD3	1:A:122:PHE:CE1	2.19	0.77
1:C:281:TRP:CZ2	1:C:283:PRO:HG3	2.19	0.77
1:C:112:THR:HG22	1:C:124:GLY:HA3	1.65	0.76
1:B:93:ILE:HD11	1:B:95:TYR:HE1	1.50	0.76
1:C:178:TRP:O	1:C:182:THR:HG23	1.86	0.76
1:F:38:GLU:CG	1:F:39:GLU:N	2.46	0.76
1:F:497:GLY:O	1:F:498:VAL:HG13	1.86	0.76
1:C:219:VAL:HA	1:C:373:LEU:HD22	1.67	0.76
1:C:65:ILE:HG13	1:C:144:ILE:HG12	1.68	0.76
1:A:12:MET:HG3	1:A:354:PRO:HD3	1.68	0.76
1:F:201:LYS:NZ	1:F:388:ASN:HD21	1.83	0.76
1:B:112:THR:HG22	1:B:124:GLY:H	1.51	0.76
1:D:112:THR:HG22	1:D:124:GLY:HA3	1.68	0.75
1:A:219:VAL:HA	1:A:373:LEU:CD2	2.16	0.75
1:C:32:LEU:HD13	1:C:494:ASN:ND2	2.00	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:93:ILE:HD11	1:F:95:TYR:HE1	1.46	0.75
1:C:38:GLU:CG	1:C:39:GLU:H	1.85	0.75
1:B:336:ALA:N	1:B:337:PRO:HD2	2.02	0.75
1:E:38:GLU:CG	1:E:39:GLU:N	2.45	0.75
1:A:217:ARG:HB2	1:A:262:TYR:CE1	2.21	0.75
1:E:417:LEU:HD13	1:F:417:LEU:HD21	1.67	0.74
1:F:112:THR:HG22	1:F:124:GLY:CA	2.17	0.74
1:A:353:THR:HB	1:A:354:PRO:HD2	1.68	0.74
1:F:20:GLY:O	1:F:24:VAL:HG22	1.87	0.74
1:F:82:HIS:CD2	1:F:112:THR:CG2	2.69	0.74
1:A:201:LYS:NZ	1:A:388:ASN:HD21	1.84	0.74
1:A:25:GLU:O	1:A:29:VAL:HG23	1.88	0.74
1:A:91:GLY:HA3	1:A:125:ALA:O	1.87	0.74
1:B:346:GLU:OE1	1:B:352:THR:HG23	1.88	0.74
1:F:99:VAL:HA	1:F:103:GLU:OE2	1.88	0.74
1:E:281:TRP:CZ2	1:E:283:PRO:HG3	2.22	0.74
1:B:255:VAL:HG22	1:B:325:ALA:HB1	1.68	0.73
1:F:248:VAL:HG12	1:F:319:CYS:SG	2.28	0.73
1:F:196:ALA:HA	1:F:388:ASN:HD22	1.52	0.73
1:B:112:THR:HG22	1:B:124:GLY:N	2.04	0.73
1:F:346:GLU:HG2	1:F:351:PRO:HG2	1.69	0.73
1:C:32:LEU:HD13	1:C:494:ASN:HD22	1.51	0.73
1:C:48:ILE:O	1:C:52:ILE:HG13	1.89	0.73
1:D:201:LYS:NZ	1:D:388:ASN:HD21	1.87	0.73
1:A:19:ARG:HG2	1:A:479:THR:HG21	1.71	0.73
1:D:443:ALA:HB2	1:E:401:TYR:CD2	2.24	0.73
1:C:210:GLY:O	1:C:214:ALA:HB2	1.89	0.73
1:E:409:LEU:HD13	1:F:409:LEU:HD11	1.70	0.73
1:D:392:VAL:HG11	1:D:397:LEU:CD1	2.14	0.72
1:E:82:HIS:HD2	1:E:112:THR:HG21	1.52	0.72
1:E:246:THR:HG22	1:E:320:ASP:H	1.54	0.72
1:F:281:TRP:CZ2	1:F:283:PRO:HG3	2.24	0.72
1:E:19:ARG:HG2	1:E:479:THR:HG21	1.71	0.72
1:A:166:ALA:HB1	1:A:167:PRO:CD	2.18	0.72
1:A:255:VAL:HG22	1:A:325:ALA:HB1	1.70	0.72
1:F:372:TYR:OH	1:F:461:ALA:HB2	1.88	0.72
1:A:408:HIS:NE2	1:B:435:GLU:HG2	2.03	0.72
1:C:82:HIS:CD2	1:C:112:THR:CG2	2.73	0.72
1:A:107:LEU:CB	1:A:126:LYS:HG2	2.18	0.72
1:B:247:PHE:CZ	1:B:270:CYS:HB2	2.22	0.72
1:C:126:LYS:HZ3	2:C:502:GLU:N	1.87	0.72
1:A:258:HIS:HD2	1:A:261:ARG:HH11	1.35	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:329:LYS:HG2	1:A:353:THR:HG22	1.72	0.72
1:E:271:ILE:HD12	1:E:272:THR:CG2	2.20	0.72
1:F:392:VAL:HG11	1:F:397:LEU:HD11	1.71	0.72
1:C:146:ARG:HE	1:C:182:THR:HG22	1.54	0.72
1:D:96:SER:O	1:D:99:VAL:HG13	1.90	0.72
1:F:427:THR:O	1:F:429:PRO:HD3	1.90	0.72
1:C:326:ALA:HB1	3:C:552:NDP:C8A	2.20	0.72
1:C:281:TRP:O	1:C:307:ALA:HB1	1.90	0.71
1:C:247:PHE:CZ	1:C:270:CYS:HB2	2.25	0.71
1:E:91:GLY:HA3	1:E:125:ALA:O	1.90	0.71
1:C:35:ARG:CD	1:C:35:ARG:H	2.03	0.71
1:F:374:ASN:HB2	3:F:552:NDP:H5N	1.72	0.71
1:E:175:GLU:O	1:E:179:ILE:HG13	1.91	0.71
1:B:417:LEU:HD21	1:C:417:LEU:CD1	2.21	0.71
1:C:346:GLU:HG2	1:C:351:PRO:HG2	1.73	0.71
1:B:38:GLU:HG3	1:B:40:GLN:H	1.56	0.71
1:C:112:THR:CG2	1:C:124:GLY:H	2.03	0.71
1:C:337:PRO:HD3	1:C:359:ILE:CD1	2.20	0.71
1:A:178:TRP:O	1:A:182:THR:HG23	1.90	0.70
1:E:304:PHE:CD1	1:E:305:PRO:HD2	2.25	0.70
1:F:252:PHE:CE2	1:F:291:LEU:HD13	2.26	0.70
1:A:315:LEU:HD13	1:A:331:LEU:HD13	1.72	0.70
1:A:219:VAL:HA	1:A:373:LEU:HD22	1.72	0.70
1:C:214:ALA:HB1	1:C:380:VAL:HG21	1.72	0.70
1:C:146:ARG:NH2	1:C:181:ASP:OD2	2.24	0.70
1:F:65:ILE:HG13	1:F:144:ILE:CG1	2.21	0.70
1:D:457:MET:HA	1:D:457:MET:CE	2.21	0.70
1:B:344:ILE:HB	1:B:367:VAL:HG12	1.72	0.70
1:E:24:VAL:HG11	1:E:483:VAL:HG13	1.73	0.70
1:C:72:TRP:HB2	1:F:47:SER:HB3	1.73	0.70
1:B:219:VAL:HA	1:B:373:LEU:CD2	2.22	0.69
1:E:172:GLY:H	1:E:175:GLU:HG2	1.57	0.69
1:E:32:LEU:HD13	1:E:494:ASN:HD21	1.57	0.69
1:F:56:ASN:HD22	1:F:84:GLN:NE2	1.89	0.69
1:A:417:LEU:HD13	1:C:417:LEU:HD21	1.73	0.69
1:F:107:LEU:HG	1:F:126:LYS:HE3	1.73	0.69
1:C:258:HIS:HD2	1:C:261:ARG:HH11	1.36	0.69
1:D:38:GLU:CG	1:D:39:GLU:N	2.43	0.69
1:F:496:ALA:C	1:F:498:VAL:H	1.95	0.69
1:C:370:ASP:HB2	1:C:374:ASN:HD21	1.57	0.69
1:A:409:LEU:HD13	1:C:409:LEU:HD11	1.75	0.69
1:E:271:ILE:HD12	1:E:272:THR:HG23	1.74	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:303:GLY:H	1:D:309:ILE:HD11	1.58	0.69
1:B:213:SER:HB2	1:B:258:HIS:CD2	2.27	0.69
1:E:321:ILE:HG23	1:E:343:ILE:HB	1.73	0.69
1:D:141:LEU:O	1:D:145:THR:HG23	1.93	0.69
1:D:281:TRP:CZ2	1:D:283:PRO:HG3	2.27	0.69
1:B:271:ILE:HD11	1:B:319:CYS:HB3	1.73	0.69
1:C:346:GLU:OE1	1:C:352:THR:HG23	1.92	0.69
1:D:379:THR:O	1:D:382:TYR:HB3	1.92	0.69
1:D:248:VAL:HG23	1:D:272:THR:O	1.93	0.69
1:E:117:VAL:HG21	1:E:371:LEU:HD22	1.75	0.69
1:B:400:LYS:HB2	1:C:455:TYR:HB2	1.75	0.69
1:A:272:THR:HG21	1:A:317:VAL:HG11	1.75	0.68
1:A:344:ILE:HB	1:A:367:VAL:HG12	1.75	0.68
1:C:432:PRO:HB2	1:C:437:GLN:HG2	1.75	0.68
1:C:126:LYS:NZ	2:C:502:GLU:N	2.41	0.68
1:B:232:TYR:HE2	1:B:465:MET:HG2	1.58	0.68
1:C:231:SER:O	1:C:235:ILE:HD13	1.93	0.68
1:F:422:GLY:C	1:F:423:LYS:HD2	2.14	0.68
1:A:114:LYS:HA	1:A:371:LEU:HD23	1.73	0.68
1:C:107:LEU:HB3	1:C:126:LYS:HG2	1.74	0.68
1:A:257:LEU:O	1:A:257:LEU:HD12	1.92	0.68
1:B:147:ARG:O	1:B:151:GLU:HG2	1.94	0.68
1:E:495:GLU:OE1	1:F:204:SER:HB3	1.93	0.68
1:A:117:VAL:HG21	1:A:371:LEU:HD22	1.76	0.68
1:B:9:PHE:O	1:B:9:PHE:HD2	1.77	0.68
1:F:396:ARG:HD2	1:F:396:ARG:O	1.92	0.68
1:B:35:ARG:CD	1:B:35:ARG:H	2.01	0.68
1:C:336:ALA:N	1:C:337:PRO:HD2	2.09	0.68
1:C:246:THR:OG1	1:C:271:ILE:HG12	1.94	0.68
1:D:139:ASN:OD1	1:F:501:THR:HG21	1.92	0.68
1:C:322:LEU:HB3	1:C:344:ILE:CD1	2.23	0.68
1:A:133:PRO:HG2	1:A:170:SER:HB3	1.75	0.68
1:D:95:TYR:HB3	1:D:133:PRO:HG3	1.76	0.68
1:A:79:ARG:HD2	1:A:127:ALA:HB2	1.76	0.68
1:D:107:LEU:HB3	1:D:126:LYS:HE3	1.75	0.68
1:D:24:VAL:CG1	1:D:483:VAL:HG13	2.24	0.68
1:B:427:THR:O	1:B:429:PRO:HD3	1.94	0.68
1:C:366:MET:HG3	1:C:475:LEU:HD22	1.76	0.68
1:E:107:LEU:HG	1:E:126:LYS:HE3	1.76	0.67
1:A:112:THR:CG2	1:A:124:GLY:H	2.06	0.67
1:B:65:ILE:HG13	1:B:144:ILE:HG12	1.76	0.67
1:F:91:GLY:HA3	1:F:125:ALA:O	1.95	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:196:ALA:HA	1:B:388:ASN:HD22	1.60	0.67
1:A:6:ASP:OD1	1:A:329:LYS:HD2	1.95	0.67
1:A:271:ILE:HD12	1:A:272:THR:HG22	1.77	0.67
1:A:57:HIS:CE1	1:A:84:GLN:HE22	2.13	0.67
1:C:75:ILE:C	1:C:75:ILE:HD13	2.14	0.67
1:B:392:VAL:HG11	1:B:397:LEU:HD11	1.75	0.67
1:E:259:SER:O	1:E:263:LEU:HD12	1.94	0.67
1:C:232:TYR:HE2	1:C:465:MET:HG2	1.60	0.67
1:C:458:GLU:HG3	1:C:459:ARG:N	2.09	0.67
1:A:159:GLY:HA3	1:A:162:VAL:HG13	1.77	0.67
1:D:32:LEU:HD13	1:D:494:ASN:OD1	1.95	0.66
1:C:99:VAL:HA	1:C:103:GLU:OE2	1.95	0.66
1:C:158:ILE:HG12	1:C:159:GLY:N	2.10	0.66
1:C:462:ARG:HG3	1:C:466:ARG:HH22	1.60	0.66
1:F:338:ARG:HG3	1:F:338:ARG:O	1.95	0.66
1:B:303:GLY:N	1:B:309:ILE:HD11	2.10	0.66
1:A:392:VAL:HG11	1:A:397:LEU:HD11	1.77	0.66
1:A:82:HIS:CD2	1:A:112:THR:CG2	2.76	0.66
1:A:146:ARG:HE	1:A:182:THR:CG2	2.09	0.66
1:A:146:ARG:NE	1:A:182:THR:HG22	2.10	0.66
1:A:390:ASN:O	1:A:392:VAL:HG23	1.96	0.66
1:F:478:ARG:HH11	1:F:478:ARG:HG3	1.59	0.66
1:E:353:THR:HB	1:E:354:PRO:HD2	1.76	0.66
1:E:75:ILE:C	1:E:75:ILE:HD13	2.16	0.66
1:E:146:ARG:HA	1:E:182:THR:HG21	1.77	0.66
1:E:37:THR:HG22	1:E:41:LYS:HE3	1.76	0.66
1:E:53:LYS:O	1:E:82:HIS:HE1	1.79	0.66
1:D:116:ALA:O	1:D:488:LYS:HD2	1.95	0.65
1:F:141:LEU:O	1:F:145:THR:CG2	2.44	0.65
1:E:10:PHE:HA	1:E:106:ALA:HB2	1.77	0.65
1:A:90:LYS:HD3	1:A:122:PHE:CD1	2.32	0.65
1:E:427:THR:O	1:E:429:PRO:HD3	1.97	0.65
1:F:252:PHE:CZ	1:F:291:LEU:HD13	2.31	0.65
1:A:117:VAL:CG2	1:A:371:LEU:HD22	2.27	0.65
1:C:146:ARG:NE	1:C:182:THR:HG22	2.11	0.65
1:E:223:ILE:HD11	1:E:345:ALA:CB	2.26	0.65
1:B:260:MET:HG2	1:B:288:PRO:HG3	1.78	0.65
1:D:435:GLU:HG2	1:E:408:HIS:CE1	2.31	0.65
1:C:248:VAL:HB	1:C:272:THR:HG23	1.78	0.65
1:D:409:LEU:HD11	1:F:409:LEU:HD13	1.78	0.65
1:A:427:THR:O	1:A:429:PRO:HD3	1.96	0.65
1:E:52:ILE:HG12	1:E:493:TYR:CE1	2.32	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:133:PRO:HG2	1:B:170:SER:HB3	1.79	0.65
1:B:273:VAL:HG21	1:B:291:LEU:HD12	1.79	0.65
1:D:112:THR:HG22	1:D:124:GLY:CA	2.26	0.65
1:C:219:VAL:HA	1:C:373:LEU:CD2	2.27	0.65
1:D:219:VAL:HA	1:D:373:LEU:CD2	2.27	0.65
1:D:433:THR:HG23	1:E:412:SER:HA	1.78	0.65
1:A:19:ARG:CG	1:A:479:THR:HG21	2.27	0.64
1:D:255:VAL:HG22	1:D:325:ALA:HB1	1.79	0.64
1:B:271:ILE:CG2	1:B:283:PRO:HA	2.28	0.64
1:F:65:ILE:HG13	1:F:144:ILE:HG13	1.79	0.64
1:B:315:LEU:HD13	1:B:331:LEU:HD13	1.79	0.64
1:B:263:LEU:CD1	1:B:323:ILE:HD11	2.28	0.64
1:B:47:SER:O	1:B:51:ILE:HG13	1.96	0.64
1:E:413:VAL:HG12	1:E:430:ILE:HG13	1.78	0.64
1:C:55:CYS:O	1:F:62:SER:HB2	1.97	0.64
1:F:353:THR:HB	1:F:354:PRO:HD2	1.78	0.64
1:C:3:ARG:HD3	1:C:3:ARG:N	2.11	0.64
1:E:89:CYS:HB3	1:E:125:ALA:HB2	1.77	0.64
1:E:211:ARG:HD2	1:E:211:ARG:O	1.97	0.64
1:B:112:THR:CG2	1:B:124:GLY:H	2.11	0.64
1:B:114:LYS:HA	1:B:371:LEU:CD2	2.28	0.64
1:B:258:HIS:HD2	1:B:261:ARG:HH11	1.45	0.64
1:A:435:GLU:HG2	1:C:408:HIS:NE2	2.13	0.64
1:E:75:ILE:O	1:E:75:ILE:HD13	1.97	0.64
1:D:175:GLU:HA	1:D:178:TRP:CE3	2.33	0.64
1:C:322:LEU:HB3	1:C:344:ILE:HD13	1.80	0.64
1:B:37:THR:O	1:B:38:GLU:CG	2.41	0.64
1:D:53:LYS:O	1:D:82:HIS:HE1	1.80	0.64
1:B:32:LEU:HD13	1:B:494:ASN:HD21	1.62	0.64
1:C:332:THR:HG22	1:C:353:THR:CG2	2.28	0.64
1:F:95:TYR:OH	1:F:145:THR:HB	1.97	0.63
1:C:261:ARG:NH2	4:C:503:GTP:C8	2.66	0.63
1:E:196:ALA:HA	1:E:388:ASN:HD22	1.63	0.63
1:A:272:THR:CG2	1:A:317:VAL:HG11	2.29	0.63
1:C:277:ASP:O	1:C:302:LEU:HD11	1.99	0.63
1:E:346:GLU:HG2	1:E:351:PRO:HG2	1.79	0.63
1:E:32:LEU:CD1	1:E:494:ASN:HD21	2.10	0.63
1:E:435:GLU:HG2	1:F:408:HIS:NE2	2.13	0.63
1:B:210:GLY:O	1:B:214:ALA:HB2	1.98	0.63
1:E:258:HIS:HD2	1:E:261:ARG:NH1	1.95	0.63
1:A:232:TYR:HE2	1:A:465:MET:HG2	1.63	0.63
1:C:315:LEU:HD13	1:C:331:LEU:HD12	1.79	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:37:THR:HG22	1:D:41:LYS:HE3	1.80	0.63
1:E:248:VAL:HG12	1:E:319:CYS:SG	2.38	0.63
1:C:223:ILE:HD12	1:C:263:LEU:HD11	1.81	0.63
1:B:255:VAL:CG2	1:B:325:ALA:HB1	2.27	0.63
1:B:303:GLY:H	1:B:309:ILE:HD11	1.63	0.63
1:E:232:TYR:O	1:E:236:LEU:HB2	1.99	0.63
1:E:112:THR:HG22	1:E:124:GLY:CA	2.27	0.63
1:C:93:ILE:HG13	1:C:93:ILE:O	1.99	0.62
1:B:201:LYS:HZ1	1:B:388:ASN:HD21	1.46	0.62
1:E:272:THR:HG22	1:E:281:TRP:HD1	1.64	0.62
1:E:24:VAL:CG1	1:E:483:VAL:HG13	2.29	0.62
1:F:153:ALA:HB1	1:F:187:ILE:HG13	1.80	0.62
1:A:346:GLU:HG2	1:A:351:PRO:HG2	1.80	0.62
1:B:446:LYS:HZ3	1:B:446:LYS:HB2	1.63	0.62
1:A:417:LEU:CD1	1:C:417:LEU:HD21	2.29	0.62
1:B:271:ILE:HG22	1:B:283:PRO:HA	1.81	0.62
1:B:315:LEU:HD13	1:B:331:LEU:CD1	2.29	0.62
1:F:153:ALA:HA	1:F:158:ILE:HG22	1.81	0.62
1:C:9:PHE:CE1	1:C:107:LEU:HD13	2.34	0.62
1:E:368:ILE:HB	1:E:373:LEU:HD12	1.81	0.62
1:E:63:PHE:CD1	1:E:147:ARG:HG3	2.35	0.62
1:C:3:ARG:H	1:C:3:ARG:CD	2.10	0.62
1:C:271:ILE:HD12	1:C:272:THR:CG2	2.28	0.62
1:D:248:VAL:HB	1:D:272:THR:HG23	1.81	0.62
1:E:91:GLY:O	1:E:165:PRO:HA	2.00	0.62
1:B:271:ILE:HD12	1:B:272:THR:CG2	2.29	0.62
1:F:201:LYS:HZ1	1:F:388:ASN:HD21	1.48	0.62
1:F:271:ILE:HD12	1:F:272:THR:CG2	2.30	0.62
1:D:107:LEU:HG	1:D:126:LYS:HE3	1.81	0.62
1:A:24:VAL:CG1	1:A:483:VAL:HG13	2.29	0.62
1:A:202:PRO:HB2	1:A:205:GLN:HG3	1.81	0.62
1:F:247:PHE:CZ	1:F:270:CYS:HB2	2.35	0.62
1:A:95:TYR:HB3	1:A:133:PRO:HG3	1.81	0.61
1:D:458:GLU:HG3	1:D:459:ARG:N	2.16	0.61
1:D:219:VAL:HA	1:D:373:LEU:HD22	1.83	0.61
1:F:146:ARG:HA	1:F:182:THR:HG21	1.82	0.61
1:D:172:GLY:H	1:D:175:GLU:HG2	1.64	0.61
1:B:214:ALA:HB1	1:B:380:VAL:HG21	1.83	0.61
1:D:336:ALA:N	1:D:337:PRO:HD2	2.15	0.61
1:E:217:ARG:HB2	1:E:262:TYR:CE1	2.35	0.61
1:D:35:ARG:H	1:D:35:ARG:CD	2.02	0.61
1:F:255:VAL:HG22	1:F:325:ALA:HB1	1.81	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:47:SER:O	1:D:51:ILE:HG13	2.01	0.61
1:D:485:ALA:O	1:D:489:VAL:HG23	2.01	0.61
1:C:92:GLY:O	1:C:126:LYS:HD3	2.00	0.61
1:F:24:VAL:CG1	1:F:483:VAL:HG13	2.31	0.61
1:C:117:VAL:HG21	1:C:371:LEU:HD22	1.83	0.61
1:F:457:MET:HA	1:F:457:MET:HE2	1.83	0.61
1:A:336:ALA:N	1:A:337:PRO:HD2	2.15	0.61
1:C:201:LYS:HZ1	1:C:388:ASN:HD21	1.49	0.61
1:F:148:PHE:CE2	1:F:152:LEU:HD11	2.35	0.61
1:F:315:LEU:HD13	1:F:331:LEU:CD1	2.30	0.61
1:B:57:HIS:HD2	1:E:61:LEU:HD12	1.66	0.61
1:B:24:VAL:CG1	1:B:483:VAL:HG13	2.30	0.61
1:E:201:LYS:NZ	1:E:388:ASN:ND2	2.48	0.60
1:A:153:ALA:HB1	1:A:187:ILE:HG13	1.81	0.60
1:B:126:LYS:HG3	1:B:127:ALA:N	2.16	0.60
1:A:91:GLY:O	1:A:165:PRO:HA	2.01	0.60
1:E:117:VAL:CG2	1:E:371:LEU:HD22	2.30	0.60
1:A:392:VAL:HG22	1:B:386:LEU:HD11	1.83	0.60
1:D:167:PRO:HD3	1:D:200:GLY:HA3	1.83	0.60
1:C:217:ARG:CZ	1:C:450:HIS:CD2	2.85	0.60
1:B:164:VAL:HG13	1:B:198:VAL:HA	1.83	0.60
1:D:92:GLY:O	1:D:126:LYS:HD3	2.02	0.60
1:D:395:GLY:HA3	1:D:399:PHE:CZ	2.37	0.60
1:C:20:GLY:O	1:C:24:VAL:HG22	2.01	0.60
1:A:313:SER:HB3	1:A:316:GLU:HG3	1.81	0.60
1:A:52:ILE:HD13	1:A:489:VAL:HG12	1.84	0.60
1:F:325:ALA:HA	1:F:348:ALA:HB2	1.83	0.60
1:F:37:THR:O	1:F:38:GLU:HB3	2.01	0.60
1:A:446:LYS:HG3	1:A:447:ASP:H	1.67	0.60
1:C:47:SER:HB3	1:F:72:TRP:HB2	1.82	0.60
1:D:231:SER:O	1:D:235:ILE:HD13	2.01	0.60
1:B:408:HIS:HB3	1:C:436:PHE:HB2	1.83	0.60
1:D:417:LEU:HD21	1:F:417:LEU:HD13	1.83	0.60
1:C:211:ARG:HD2	1:C:211:ARG:O	2.00	0.60
1:B:153:ALA:HB1	1:B:187:ILE:HG13	1.83	0.60
1:B:150:MET:O	1:B:154:LYS:HG3	2.01	0.60
1:B:457:MET:HA	1:B:457:MET:CE	2.31	0.60
1:D:263:LEU:CD1	1:D:323:ILE:HD11	2.32	0.60
1:A:166:ALA:HB1	1:A:167:PRO:HD3	1.81	0.60
1:C:57:HIS:HD2	1:F:61:LEU:HD12	1.67	0.60
1:F:82:HIS:CG	1:F:109:SER:HA	2.37	0.60
1:F:219:VAL:HA	1:F:373:LEU:HD22	1.82	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:8:ASN:OD1	1:F:11:LYS:HG3	2.02	0.60
1:C:427:THR:O	1:C:429:PRO:HD3	2.02	0.60
1:C:315:LEU:HD13	1:C:331:LEU:HD13	1.83	0.59
1:E:336:ALA:N	1:E:337:PRO:HD2	2.15	0.59
1:B:64:PRO:O	1:B:65:ILE:HD13	2.02	0.59
1:F:369:PRO:HG3	1:F:478:ARG:HA	1.82	0.59
1:C:24:VAL:HG13	1:C:483:VAL:HG22	1.83	0.59
1:E:203:ILE:HD11	1:E:209:HIS:HA	1.83	0.59
1:F:199:THR:HG22	1:F:384:GLU:HG2	1.82	0.59
1:B:146:ARG:HG2	1:B:182:THR:HG21	1.82	0.59
1:B:95:TYR:OH	1:B:145:THR:HG22	2.02	0.59
1:D:369:PRO:HG3	1:D:478:ARG:HA	1.84	0.59
1:D:114:LYS:HZ2	2:D:502:GLU:N	2.00	0.59
1:B:390:ASN:O	1:B:392:VAL:HG23	2.01	0.59
1:E:219:VAL:HA	1:E:373:LEU:HD22	1.84	0.59
1:A:24:VAL:HG11	1:A:483:VAL:HG13	1.82	0.59
1:E:229:GLU:HG3	1:E:231:SER:HB3	1.84	0.59
1:B:89:CYS:HB3	1:B:125:ALA:HB2	1.84	0.59
1:C:245:LYS:HD2	1:C:245:LYS:N	2.17	0.59
1:C:271:ILE:CG2	1:C:283:PRO:HA	2.31	0.59
1:B:96:SER:O	1:B:99:VAL:CG1	2.50	0.59
1:A:247:PHE:CZ	1:A:270:CYS:HB2	2.38	0.59
1:D:457:MET:HE2	1:D:457:MET:HA	1.83	0.59
1:B:24:VAL:HG11	1:B:483:VAL:HG13	1.84	0.59
1:A:63:PHE:CZ	1:A:75:ILE:CD1	2.85	0.59
1:C:281:TRP:O	1:C:282:ASN:HB2	2.03	0.59
1:C:271:ILE:HG22	1:C:283:PRO:HA	1.85	0.59
1:A:446:LYS:HG3	1:A:447:ASP:N	2.17	0.59
1:F:112:THR:HG22	1:F:124:GLY:N	2.18	0.59
1:F:9:PHE:CE1	1:F:107:LEU:HD13	2.38	0.59
1:E:227:ILE:HD11	1:E:245:LYS:HG2	1.85	0.59
1:A:271:ILE:HD11	1:A:319:CYS:HB3	1.83	0.59
1:D:223:ILE:HD11	1:D:345:ALA:CB	2.32	0.59
1:A:8:ASN:OD1	1:A:11:LYS:HG3	2.02	0.59
1:E:422:GLY:C	1:E:423:LYS:HD2	2.23	0.59
1:C:298:HIS:O	1:C:300:THR:N	2.36	0.59
1:D:397:LEU:O	1:F:448:ILE:HD12	2.02	0.59
1:B:408:HIS:ND1	1:C:439:ARG:HD2	2.18	0.59
1:E:315:LEU:HD13	1:E:331:LEU:HD13	1.84	0.59
1:A:417:LEU:HD21	1:B:417:LEU:CD1	2.33	0.58
1:B:107:LEU:HB3	1:B:126:LYS:HE3	1.85	0.58
1:C:246:THR:O	1:C:320:ASP:HB2	2.03	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:63:PHE:CZ	1:C:75:ILE:CD1	2.86	0.58
1:A:433:THR:HG23	1:C:412:SER:OG	2.03	0.58
1:C:18:ASP:O	1:C:21:ALA:HB3	2.03	0.58
1:D:414:GLN:HG3	1:D:428:ILE:O	2.03	0.58
1:D:96:SER:O	1:D:99:VAL:CG1	2.51	0.58
1:B:271:ILE:HD12	1:B:272:THR:HG23	1.86	0.58
1:A:490:PHE:O	1:A:491:ARG:CB	2.51	0.58
1:C:321:ILE:HG23	1:C:343:ILE:HB	1.84	0.58
1:F:322:LEU:HB3	1:F:344:ILE:HD12	1.86	0.58
1:D:422:GLY:C	1:D:423:LYS:HD2	2.23	0.58
1:D:95:TYR:OH	1:D:145:THR:HB	2.03	0.58
1:F:32:LEU:HD13	1:F:494:ASN:ND2	2.15	0.58
1:C:258:HIS:HD2	1:C:261:ARG:NH1	2.01	0.58
1:A:422:GLY:C	1:A:423:LYS:HD2	2.24	0.58
1:E:118:VAL:HG23	1:E:120:VAL:HG23	1.84	0.58
1:A:257:LEU:C	1:A:257:LEU:HD12	2.24	0.58
1:C:68:ASP:OD1	1:C:137:THR:HG21	2.03	0.58
1:F:172:GLY:H	1:F:175:GLU:HG2	1.69	0.58
1:C:421:PHE:N	1:C:421:PHE:CD2	2.69	0.58
1:F:108:ALA:O	1:F:111:MET:HB2	2.03	0.58
1:E:95:TYR:OH	1:E:145:THR:HG22	2.04	0.58
1:F:107:LEU:CB	1:F:126:LYS:HG2	2.32	0.58
1:F:65:ILE:HG13	1:F:144:ILE:HG12	1.86	0.58
1:D:152:LEU:HD22	1:D:157:PHE:HB3	1.85	0.58
1:E:150:MET:O	1:E:154:LYS:HG3	2.04	0.58
1:E:246:THR:CG2	1:E:320:ASP:H	2.15	0.58
1:A:85:HIS:CD2	1:A:86:ARG:HG2	2.38	0.58
1:A:271:ILE:HD12	1:A:272:THR:CG2	2.34	0.58
1:D:271:ILE:HD12	1:D:272:THR:CG2	2.33	0.58
1:E:432:PRO:HB3	1:E:436:PHE:CD2	2.36	0.58
1:D:342:LYS:N	1:D:342:LYS:HD3	2.19	0.58
1:A:131:ILE:O	1:A:133:PRO:HD3	2.04	0.57
1:E:95:TYR:HB3	1:E:133:PRO:HG3	1.85	0.57
1:A:154:LYS:HD3	1:E:185:SER:O	2.04	0.57
1:C:332:THR:HG22	1:C:353:THR:HG21	1.86	0.57
1:E:291:LEU:HD21	1:E:301:ILE:HG22	1.84	0.57
1:C:215:THR:O	1:C:219:VAL:HG23	2.04	0.57
1:A:232:TYR:CE2	1:A:465:MET:HG2	2.38	0.57
1:D:412:SER:OG	1:F:433:THR:HG23	2.04	0.57
1:F:35:ARG:H	1:F:35:ARG:CD	2.10	0.57
1:C:339:VAL:O	1:C:340:LYS:HB2	2.05	0.57
1:F:90:LYS:HE3	1:F:381:SER:HB3	1.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:17:PHE:CE1	1:B:486:ILE:HG12	2.40	0.57
1:B:111:MET:HE1	2:B:502:GLU:HG3	1.87	0.57
1:D:336:ALA:HB2	1:D:356:ALA:HB1	1.86	0.57
1:E:463:GLN:OE1	1:E:488:LYS:NZ	2.35	0.57
1:E:23:ILE:HG22	1:E:471:TYR:CD1	2.40	0.57
1:A:17:PHE:CE1	1:A:486:ILE:HG12	2.40	0.57
1:D:248:VAL:HG12	1:D:319:CYS:SG	2.45	0.57
1:C:63:PHE:CZ	1:C:75:ILE:HD12	2.40	0.57
1:B:250:GLN:NE2	1:B:315:LEU:HD21	2.20	0.57
1:F:368:ILE:HB	1:F:373:LEU:HD12	1.85	0.57
1:E:308:LYS:HG3	1:E:309:ILE:O	2.05	0.57
1:E:427:THR:HG23	1:E:427:THR:O	2.04	0.57
1:C:196:ALA:HA	1:C:388:ASN:HD22	1.70	0.57
1:D:89:CYS:HA	1:D:123:GLY:O	2.05	0.57
1:B:146:ARG:HE	1:B:182:THR:HG22	1.69	0.57
1:B:326:ALA:O	3:B:552:NDP:H4D	2.05	0.57
1:E:196:ALA:HB2	1:E:388:ASN:HB2	1.87	0.57
1:D:370:ASP:OD1	1:D:371:LEU:N	2.34	0.57
1:C:37:THR:HG22	1:C:41:LYS:HE3	1.85	0.56
1:B:38:GLU:CG	1:B:39:GLU:N	2.61	0.56
1:D:63:PHE:CZ	1:D:75:ILE:CD1	2.87	0.56
1:C:310:TYR:CZ	1:C:317:VAL:HG22	2.40	0.56
1:E:96:SER:O	1:E:99:VAL:CG1	2.53	0.56
1:F:93:ILE:CD1	1:F:95:TYR:HE1	2.11	0.56
1:E:29:VAL:HG13	1:E:41:LYS:HB3	1.87	0.56
1:A:114:LYS:HA	1:A:371:LEU:CD2	2.35	0.56
1:F:346:GLU:HG2	1:F:351:PRO:CG	2.35	0.56
1:F:258:HIS:HD2	1:F:261:ARG:NH1	1.97	0.56
1:D:107:LEU:HB3	1:D:126:LYS:HG2	1.86	0.56
1:D:64:PRO:O	1:D:65:ILE:HD13	2.05	0.56
1:F:59:LEU:O	1:F:78:TYR:HA	2.05	0.56
1:B:233:MET:HA	1:B:233:MET:HE2	1.86	0.56
1:D:12:MET:HG3	1:D:354:PRO:HD3	1.87	0.56
1:F:24:VAL:HG13	1:F:483:VAL:HG13	1.88	0.56
1:C:370:ASP:HB2	1:C:374:ASN:ND2	2.20	0.56
1:E:89:CYS:HA	1:E:123:GLY:O	2.05	0.56
1:B:260:MET:HE1	1:B:288:PRO:HA	1.86	0.56
1:F:382:TYR:O	1:F:386:LEU:HD22	2.05	0.56
1:F:227:ILE:HD11	1:F:245:LYS:HG2	1.86	0.56
1:C:146:ARG:HE	1:C:182:THR:CG2	2.18	0.56
1:B:337:PRO:HD3	1:B:359:ILE:HD13	1.87	0.56
1:E:20:GLY:O	1:E:24:VAL:HG22	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:482:TYR:O	1:B:486:ILE:HD12	2.05	0.56
1:E:274:GLY:O	1:E:275:GLU:HG2	2.05	0.56
1:C:133:PRO:HG2	1:C:170:SER:HB3	1.88	0.56
1:E:75:ILE:HD11	1:E:129:VAL:HG13	1.87	0.56
1:C:466:ARG:HB2	1:C:466:ARG:NH1	2.20	0.56
1:A:107:LEU:CG	1:A:126:LYS:HE3	2.30	0.56
1:E:272:THR:OG1	1:E:314:ILE:HD11	2.04	0.56
1:C:371:LEU:HD12	1:C:482:TYR:CE1	2.41	0.56
1:A:432:PRO:HB2	1:A:437:GLN:HG2	1.87	0.56
1:A:37:THR:HG22	1:A:41:LYS:HE3	1.87	0.56
1:D:205:GLN:NE2	1:F:496:ALA:HB2	2.20	0.56
1:F:271:ILE:C	1:F:272:THR:HG22	2.26	0.56
1:F:63:PHE:CZ	1:F:75:ILE:CD1	2.89	0.56
1:B:38:GLU:H	1:B:41:LYS:HD2	1.71	0.56
1:A:370:ASP:OD1	1:A:371:LEU:N	2.29	0.56
1:E:23:ILE:CG2	1:E:471:TYR:CD1	2.89	0.56
1:D:3:ARG:HD2	1:D:4:GLU:N	2.20	0.56
1:A:458:GLU:HG3	1:A:459:ARG:N	2.21	0.55
1:B:222:GLY:HA2	1:B:372:TYR:OH	2.06	0.55
1:B:42:ARG:O	1:B:46:ARG:HG3	2.06	0.55
1:B:381:SER:O	1:B:384:GLU:HB3	2.06	0.55
1:E:99:VAL:HG13	1:E:130:LYS:HA	1.88	0.55
1:A:211:ARG:HH22	3:A:552:NDP:H72N	1.53	0.55
1:F:374:ASN:HB2	3:F:552:NDP:C5N	2.36	0.55
1:A:196:ALA:HB2	1:A:388:ASN:HB2	1.88	0.55
1:E:90:LYS:HD3	1:E:122:PHE:CD1	2.41	0.55
1:F:201:LYS:HZ2	1:F:388:ASN:HD21	1.52	0.55
1:E:175:GLU:H	1:E:175:GLU:CD	2.10	0.55
1:F:84:GLN:C	1:F:86:ARG:H	2.08	0.55
1:D:24:VAL:HG13	1:D:483:VAL:HG13	1.88	0.55
1:F:457:MET:HA	1:F:457:MET:CE	2.37	0.55
1:F:150:MET:HA	1:F:150:MET:HE3	1.88	0.55
1:D:17:PHE:CE1	1:D:486:ILE:HG12	2.42	0.55
1:F:211:ARG:HH22	3:F:552:NDP:H72N	1.55	0.55
1:A:345:ALA:HB1	1:A:373:LEU:CD1	2.33	0.55
1:B:201:LYS:HZ2	1:B:388:ASN:HD21	1.53	0.55
1:D:459:ARG:O	1:D:463:GLN:HG2	2.06	0.55
1:A:23:ILE:HD12	1:A:473:LEU:HD21	1.88	0.55
1:A:113:TYR:C	1:A:371:LEU:HD21	2.27	0.55
1:F:496:ALA:HB3	1:F:498:VAL:O	2.05	0.55
1:B:409:LEU:HD11	1:C:409:LEU:HD13	1.87	0.55
1:F:75:ILE:HG12	1:F:76:GLU:N	2.20	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:39:GLU:C	1:C:41:LYS:H	2.09	0.55
1:F:495:GLU:O	1:F:497:GLY:N	2.37	0.55
1:C:368:ILE:HB	1:C:373:LEU:HD12	1.88	0.55
1:F:201:LYS:HZ2	1:F:388:ASN:ND2	2.04	0.55
1:D:167:PRO:CD	1:D:200:GLY:HA3	2.37	0.55
1:D:315:LEU:HD13	1:D:331:LEU:HD13	1.88	0.55
1:A:281:TRP:CZ2	1:A:283:PRO:CG	2.90	0.55
1:D:443:ALA:HB2	1:E:401:TYR:CE2	2.42	0.55
1:E:495:GLU:OE1	1:F:204:SER:CB	2.55	0.55
1:A:427:THR:O	1:A:427:THR:HG23	2.06	0.55
1:C:203:ILE:HD11	1:C:209:HIS:HA	1.89	0.55
1:E:489:VAL:O	1:E:492:VAL:HG13	2.07	0.55
1:E:79:ARG:NH2	1:E:163:ASP:OD2	2.39	0.55
1:D:186:THR:O	1:D:189:HIS:ND1	2.30	0.55
1:D:346:GLU:HG2	1:D:351:PRO:CG	2.34	0.55
1:D:248:VAL:CG2	1:D:272:THR:HG23	2.37	0.55
1:E:246:THR:CG2	1:E:319:CYS:HA	2.37	0.55
1:F:142:GLU:O	1:F:146:ARG:HG3	2.07	0.55
1:B:96:SER:O	1:B:99:VAL:HG13	2.06	0.55
1:F:95:TYR:HB3	1:F:133:PRO:HG3	1.88	0.55
1:C:24:VAL:CG1	1:C:483:VAL:HG13	2.37	0.55
1:C:47:SER:O	1:C:51:ILE:HG13	2.07	0.55
1:E:94:ARG:HB2	1:E:168:ASP:OD1	2.07	0.55
1:B:177:SER:HB2	1:B:202:PRO:HG2	1.89	0.55
1:E:63:PHE:CZ	1:E:75:ILE:HD12	2.42	0.54
1:B:141:LEU:O	1:B:145:THR:HG23	2.07	0.54
1:D:314:ILE:HG23	1:D:315:LEU:N	2.20	0.54
1:F:478:ARG:NH1	1:F:478:ARG:HG3	2.22	0.54
1:A:232:TYR:O	1:A:236:LEU:HB2	2.07	0.54
1:F:131:ILE:O	1:F:133:PRO:HD3	2.07	0.54
1:B:90:LYS:HD2	1:B:164:VAL:O	2.06	0.54
1:B:273:VAL:HG21	1:B:291:LEU:CD1	2.35	0.54
1:A:154:LYS:HD2	1:E:189:HIS:HB3	1.88	0.54
1:B:444:SER:O	1:B:447:ASP:HB2	2.07	0.54
1:D:146:ARG:NH2	1:D:181:ASP:OD2	2.40	0.54
1:F:271:ILE:HD12	1:F:272:THR:HG22	1.90	0.54
1:F:146:ARG:NH2	1:F:181:ASP:OD2	2.40	0.54
1:C:24:VAL:HB	1:C:28:LEU:HD22	1.90	0.54
1:F:174:ARG:O	1:F:177:SER:HB3	2.08	0.54
1:F:294:PHE:CE2	1:F:298:HIS:ND1	2.75	0.54
1:E:166:ALA:HB1	1:E:167:PRO:HD2	1.88	0.54
1:B:248:VAL:HG23	1:B:272:THR:OG1	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:84:GLN:C	1:F:86:ARG:N	2.61	0.54
1:B:408:HIS:CE1	1:C:435:GLU:HG2	2.43	0.54
1:C:37:THR:O	1:C:38:GLU:HB3	2.08	0.54
1:B:378:VAL:HA	1:B:381:SER:HB2	1.87	0.54
1:F:178:TRP:O	1:F:182:THR:HG22	2.07	0.54
1:A:112:THR:CG2	1:A:124:GLY:HA3	2.30	0.54
1:A:172:GLY:H	1:A:175:GLU:HG2	1.72	0.54
1:F:32:LEU:CD1	1:F:494:ASN:HD21	2.19	0.54
1:D:201:LYS:HZ1	1:D:388:ASN:HD21	1.55	0.54
1:A:19:ARG:HG2	1:A:479:THR:CG2	2.37	0.54
1:C:344:ILE:HB	1:C:367:VAL:CG1	2.38	0.54
1:F:219:VAL:HA	1:F:373:LEU:CD2	2.38	0.54
1:B:95:TYR:HB3	1:B:133:PRO:HG3	1.89	0.54
1:E:90:LYS:HD2	1:E:164:VAL:HB	1.90	0.54
1:A:490:PHE:O	1:A:491:ARG:HB3	2.07	0.54
1:C:90:LYS:HD2	1:C:164:VAL:HB	1.89	0.54
1:F:210:GLY:O	1:F:214:ALA:HB2	2.08	0.54
1:A:344:ILE:HB	1:A:367:VAL:CG1	2.38	0.54
1:B:89:CYS:HA	1:B:123:GLY:O	2.08	0.54
1:C:63:PHE:CE1	1:C:75:ILE:HD12	2.42	0.54
1:D:108:ALA:O	1:D:111:MET:HB2	2.08	0.54
1:F:427:THR:HG23	1:F:427:THR:O	2.08	0.54
1:E:114:LYS:HA	1:E:371:LEU:HD23	1.89	0.54
1:C:158:ILE:HG12	1:C:159:GLY:H	1.72	0.54
1:E:346:GLU:OE1	1:E:352:THR:HG23	2.08	0.54
1:C:108:ALA:O	1:C:111:MET:HB2	2.08	0.54
1:C:308:LYS:HG3	1:C:309:ILE:O	2.07	0.54
1:B:19:ARG:HG2	1:B:479:THR:HG21	1.90	0.54
1:F:112:THR:HG22	1:F:124:GLY:H	1.71	0.53
1:C:114:LYS:HA	1:C:371:LEU:HD23	1.89	0.53
1:F:2:ASP:O	1:F:3:ARG:HB2	2.07	0.53
1:A:400:LYS:HB2	1:B:455:TYR:HB2	1.89	0.53
1:B:272:THR:HG21	1:B:317:VAL:HG21	1.90	0.53
1:D:201:LYS:HZ2	1:D:388:ASN:HD21	1.56	0.53
1:D:303:GLY:N	1:D:309:ILE:HD11	2.22	0.53
1:D:326:ALA:O	3:D:552:NDP:H4D	2.08	0.53
1:C:21:ALA:HA	1:C:486:ILE:HD13	1.90	0.53
1:C:186:THR:OG1	1:C:187:ILE:N	2.36	0.53
1:F:68:ASP:OD1	1:F:137:THR:HG21	2.09	0.53
1:B:368:ILE:HB	1:B:373:LEU:HD12	1.90	0.53
1:E:32:LEU:HD13	1:E:494:ASN:ND2	2.22	0.53
1:B:146:ARG:NE	1:B:182:THR:HG22	2.24	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:39:GLU:C	1:E:41:LYS:H	2.10	0.53
1:A:107:LEU:HB3	1:A:126:LYS:CG	2.28	0.53
1:C:117:VAL:CG2	1:C:371:LEU:HD22	2.38	0.53
1:F:47:SER:O	1:F:51:ILE:HG13	2.09	0.53
1:D:2:ASP:CG	1:D:3:ARG:N	2.61	0.53
1:F:232:TYR:CE2	1:F:465:MET:HG2	2.43	0.53
1:C:44:ARG:HH22	1:C:494:ASN:HB2	1.73	0.53
1:D:26:ASP:HA	1:D:42:ARG:NH2	2.24	0.53
1:B:172:GLY:H	1:B:175:GLU:HG2	1.73	0.53
1:D:53:LYS:O	1:D:82:HIS:CE1	2.62	0.53
1:D:314:ILE:HA	1:D:317:VAL:HG23	1.90	0.53
1:D:19:ARG:HG2	1:D:479:THR:CG2	2.37	0.53
1:D:432:PRO:HB2	1:D:437:GLN:HG2	1.89	0.53
1:B:446:LYS:NZ	1:B:446:LYS:HB2	2.24	0.53
1:B:82:HIS:HD2	1:B:112:THR:CG2	2.03	0.53
1:D:346:GLU:CG	1:D:351:PRO:HG2	2.37	0.53
1:A:248:VAL:CB	1:A:272:THR:HG23	2.37	0.53
1:C:114:LYS:NZ	2:C:502:GLU:O	2.42	0.53
1:C:374:ASN:HB2	3:C:552:NDP:C5N	2.39	0.53
1:E:255:VAL:HG22	1:E:325:ALA:HB1	1.90	0.53
1:D:222:GLY:HA2	1:D:372:TYR:OH	2.08	0.53
1:D:24:VAL:HG11	1:D:483:VAL:HG13	1.90	0.53
1:B:166:ALA:HA	1:B:199:THR:O	2.08	0.53
1:B:12:MET:HG3	1:B:354:PRO:HD3	1.91	0.53
1:F:114:LYS:HA	1:F:371:LEU:HD23	1.91	0.53
1:E:201:LYS:HZ2	1:E:388:ASN:ND2	2.07	0.53
1:D:271:ILE:C	1:D:272:THR:HG22	2.28	0.53
1:D:314:ILE:CG2	1:D:315:LEU:N	2.71	0.53
1:D:19:ARG:CG	1:D:479:THR:HG21	2.38	0.53
1:E:246:THR:O	1:E:320:ASP:HB2	2.09	0.52
1:A:489:VAL:HG12	1:A:490:PHE:N	2.24	0.52
1:A:57:HIS:HE1	1:A:84:GLN:HE22	1.54	0.52
1:A:328:GLU:HB2	1:A:350:GLY:O	2.09	0.52
1:C:255:VAL:HG22	1:C:325:ALA:HB1	1.91	0.52
1:E:432:PRO:HA	1:F:412:SER:HB3	1.91	0.52
1:D:417:LEU:HD21	1:F:417:LEU:CD1	2.39	0.52
1:A:17:PHE:CE2	1:A:53:LYS:HG3	2.44	0.52
1:E:378:VAL:HA	1:E:381:SER:HB2	1.91	0.52
1:B:422:GLY:C	1:B:423:LYS:HD2	2.30	0.52
1:B:85:HIS:HD2	1:B:492:VAL:HG21	1.73	0.52
1:B:171:THR:HB	1:B:175:GLU:HG3	1.91	0.52
2:E:502:GLU:HA	3:E:552:NDP:H41N	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:ARG:HD2	1:A:140:GLU:OE1	2.10	0.52
1:E:199:THR:HA	1:E:384:GLU:OE1	2.09	0.52
1:B:346:GLU:HG2	1:B:351:PRO:HG2	1.90	0.52
1:E:346:GLU:HG2	1:E:351:PRO:CG	2.40	0.52
1:D:75:ILE:HG12	1:D:76:GLU:N	2.24	0.52
1:B:38:GLU:HG2	1:B:40:GLN:HG2	1.91	0.52
1:A:55:CYS:HA	1:A:82:HIS:HA	1.91	0.52
1:E:291:LEU:CD2	1:E:301:ILE:HG22	2.40	0.52
1:B:227:ILE:HD11	1:B:245:LYS:HG2	1.92	0.52
1:E:252:PHE:CZ	1:E:257:LEU:HD13	2.44	0.52
1:A:371:LEU:HD12	1:A:482:TYR:CD1	2.44	0.52
1:D:89:CYS:HB3	1:D:125:ALA:HB2	1.91	0.52
1:E:59:LEU:O	1:E:78:TYR:HA	2.09	0.52
1:B:478:ARG:HG3	1:B:478:ARG:HH11	1.75	0.52
1:E:112:THR:CG2	1:E:124:GLY:H	2.12	0.52
1:E:417:LEU:CD1	1:F:417:LEU:HD21	2.40	0.52
1:C:462:ARG:NH1	1:C:465:MET:HE1	2.25	0.52
1:C:217:ARG:NH2	1:C:450:HIS:CD2	2.78	0.52
1:C:220:PHE:CD2	1:C:221:HIS:N	2.78	0.52
1:C:10:PHE:HA	1:C:106:ALA:HB2	1.90	0.52
1:B:346:GLU:HG2	1:B:351:PRO:CG	2.40	0.52
1:B:457:MET:HA	1:B:457:MET:HE1	1.92	0.52
1:B:107:LEU:HB3	1:B:126:LYS:HG2	1.93	0.51
1:B:213:SER:CB	1:B:258:HIS:CD2	2.92	0.51
1:A:277:ASP:O	1:A:302:LEU:HD11	2.09	0.51
1:C:163:ASP:O	1:C:165:PRO:HD3	2.10	0.51
1:F:339:VAL:HG12	1:F:341:ALA:H	1.75	0.51
1:E:103:GLU:O	1:E:107:LEU:HB2	2.10	0.51
1:E:53:LYS:O	1:E:82:HIS:CE1	2.62	0.51
1:B:248:VAL:O	1:B:248:VAL:HG13	2.10	0.51
1:A:90:LYS:HE3	1:A:381:SER:HB3	1.92	0.51
1:E:245:LYS:HA	1:E:320:ASP:OD1	2.10	0.51
1:F:272:THR:OG1	1:F:273:VAL:N	2.42	0.51
1:F:372:TYR:CZ	1:F:461:ALA:HB2	2.46	0.51
1:C:236:LEU:HD21	1:C:343:ILE:HG12	1.92	0.51
1:B:446:LYS:HZ3	1:B:446:LYS:CB	2.24	0.51
1:F:321:ILE:HG23	1:F:343:ILE:HB	1.92	0.51
1:D:248:VAL:HG21	1:D:314:ILE:HG12	1.91	0.51
1:B:84:GLN:O	1:B:86:ARG:N	2.44	0.51
1:C:214:ALA:CB	1:C:380:VAL:HG21	2.39	0.51
1:B:414:GLN:HG3	1:B:428:ILE:O	2.10	0.51
1:C:39:GLU:C	1:C:41:LYS:N	2.62	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:37:THR:O	1:F:38:GLU:CB	2.58	0.51
1:B:107:LEU:CG	1:B:126:LYS:HE3	2.39	0.51
1:C:96:SER:O	1:C:99:VAL:CG1	2.59	0.51
1:C:252:PHE:CZ	1:C:291:LEU:HD13	2.46	0.51
1:C:396:ARG:HD2	1:C:396:ARG:O	2.10	0.51
1:E:345:ALA:HB1	1:E:373:LEU:CD1	2.41	0.51
1:D:133:PRO:HG2	1:D:170:SER:HB3	1.93	0.51
1:C:374:ASN:HB2	3:C:552:NDP:H5N	1.91	0.51
1:F:353:THR:HB	1:F:354:PRO:CD	2.39	0.51
1:E:435:GLU:HB3	1:F:408:HIS:CD2	2.45	0.51
1:B:146:ARG:CG	1:B:182:THR:HG21	2.40	0.51
1:C:94:ARG:O	1:C:128:GLY:HA2	2.11	0.51
1:C:359:ILE:O	1:C:363:ARG:HB2	2.11	0.51
1:F:211:ARG:NH2	2:F:502:GLU:HG3	2.26	0.51
1:A:142:GLU:OE2	1:A:146:ARG:NH1	2.44	0.51
1:C:248:VAL:HG22	1:C:249:VAL:N	2.25	0.51
1:F:232:TYR:HE2	1:F:465:MET:HG2	1.74	0.51
1:A:252:PHE:CZ	1:A:291:LEU:HD13	2.46	0.51
1:E:392:VAL:HG11	1:E:397:LEU:HD11	1.92	0.51
1:C:245:LYS:HA	1:C:320:ASP:OD1	2.11	0.51
1:B:323:ILE:HG12	1:B:345:ALA:HB3	1.93	0.51
1:B:407:TYR:CZ	1:B:440:ILE:HD13	2.45	0.51
1:E:473:LEU:HB3	1:E:476:ASP:HB3	1.92	0.51
1:D:258:HIS:HD2	1:D:261:ARG:HH11	1.58	0.51
1:F:133:PRO:HG2	1:F:170:SER:HB3	1.93	0.51
1:A:196:ALA:HB2	1:A:388:ASN:CB	2.40	0.51
1:D:417:LEU:HD13	1:E:417:LEU:HD21	1.93	0.51
1:E:19:ARG:HG2	1:E:479:THR:CG2	2.41	0.51
1:F:214:ALA:HB1	1:F:380:VAL:HG21	1.92	0.51
1:C:95:TYR:OH	1:C:145:THR:HB	2.11	0.50
1:B:337:PRO:HD3	1:B:359:ILE:CD1	2.41	0.50
1:F:118:VAL:HG11	1:F:375:ALA:HB3	1.91	0.50
1:E:421:PHE:CD2	1:E:421:PHE:N	2.77	0.50
1:B:211:ARG:HD2	1:B:211:ARG:O	2.11	0.50
1:E:370:ASP:CG	1:E:371:LEU:H	2.13	0.50
1:B:32:LEU:HD11	1:B:44:ARG:HH12	1.75	0.50
1:F:214:ALA:CB	1:F:380:VAL:HG21	2.40	0.50
1:A:291:LEU:O	1:A:291:LEU:HD22	2.11	0.50
1:D:58:VAL:HG11	1:D:101:VAL:HG23	1.94	0.50
1:E:249:VAL:HG22	1:E:251:GLY:O	2.12	0.50
1:B:75:ILE:O	1:B:75:ILE:HD13	2.11	0.50
1:A:478:ARG:HH11	1:A:478:ARG:CG	2.03	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:349:ASN:ND2	2:C:502:GLU:OXT	2.37	0.50
1:E:219:VAL:HA	1:E:373:LEU:CD2	2.41	0.50
1:F:416:SER:HA	1:F:419:ARG:NH1	2.26	0.50
1:E:166:ALA:HB1	1:E:167:PRO:CD	2.41	0.50
1:E:111:MET:SD	2:E:502:GLU:OXT	2.69	0.50
1:A:69:ASP:C	1:A:69:ASP:OD2	2.50	0.50
1:C:2:ASP:O	1:C:6:ASP:HB2	2.12	0.50
1:C:232:TYR:CE2	1:C:465:MET:HG2	2.42	0.50
1:E:217:ARG:HA	1:E:262:TYR:CD1	2.46	0.50
1:B:483:VAL:O	1:B:487:GLU:HB2	2.10	0.50
1:A:185:SER:O	1:E:154:LYS:HD3	2.11	0.50
1:C:165:PRO:O	1:C:166:ALA:HB2	2.10	0.50
1:A:274:GLY:HA3	1:A:314:ILE:HD12	1.94	0.50
1:B:126:LYS:NZ	1:B:168:ASP:OD2	2.45	0.50
1:E:303:GLY:H	1:E:309:ILE:HD11	1.76	0.50
1:E:492:VAL:O	1:F:205:GLN:NE2	2.44	0.50
1:F:114:LYS:HA	1:F:371:LEU:CD2	2.41	0.50
1:B:336:ALA:N	1:B:337:PRO:CD	2.73	0.50
1:C:110:LEU:O	1:C:114:LYS:HB2	2.11	0.50
1:A:483:VAL:O	1:A:487:GLU:HB2	2.12	0.50
1:A:248:VAL:HG13	1:A:322:LEU:HD12	1.92	0.50
1:B:336:ALA:HB3	1:B:359:ILE:HD12	1.94	0.50
1:D:460:SER:HA	1:D:463:GLN:CG	2.42	0.50
1:C:421:PHE:O	1:C:422:GLY:C	2.50	0.50
1:B:245:LYS:HD2	1:B:245:LYS:N	2.26	0.50
1:B:75:ILE:HD11	1:B:129:VAL:HG13	1.93	0.50
1:A:172:GLY:O	1:A:176:MET:HG2	2.10	0.50
1:E:10:PHE:CA	1:E:106:ALA:HB2	2.42	0.50
1:F:118:VAL:HG11	1:F:375:ALA:CB	2.42	0.50
1:D:409:LEU:HD13	1:E:409:LEU:HD11	1.93	0.50
1:F:163:ASP:O	1:F:165:PRO:HD3	2.12	0.50
1:A:339:VAL:O	1:A:340:LYS:HB2	2.12	0.50
1:A:189:HIS:HE1	1:E:187:ILE:HD12	1.77	0.49
1:A:111:MET:HE1	1:A:378:VAL:HG11	1.94	0.49
1:D:3:ARG:C	1:D:5:ASP:H	2.14	0.49
1:E:56:ASN:HD22	1:E:84:GLN:NE2	2.10	0.49
1:B:113:TYR:C	1:B:371:LEU:HD21	2.33	0.49
1:F:271:ILE:HD11	1:F:319:CYS:HB3	1.94	0.49
1:E:423:LYS:N	1:E:423:LYS:HD2	2.26	0.49
1:C:372:TYR:OH	1:C:461:ALA:HB2	2.12	0.49
1:F:366:MET:HG3	1:F:475:LEU:HD22	1.94	0.49
1:F:264:HIS:CD2	1:F:288:PRO:HD3	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:88:PRO:HG3	1:B:160:PRO:O	2.12	0.49
1:B:91:GLY:O	1:B:165:PRO:HA	2.13	0.49
1:B:246:THR:CG2	1:B:319:CYS:HA	2.42	0.49
1:C:65:ILE:HG13	1:C:144:ILE:CG1	2.40	0.49
1:F:84:GLN:O	1:F:86:ARG:N	2.45	0.49
1:D:107:LEU:CB	1:D:126:LYS:HE3	2.43	0.49
1:A:446:LYS:O	1:A:447:ASP:C	2.50	0.49
1:C:44:ARG:NH2	1:C:494:ASN:HB2	2.26	0.49
1:A:412:SER:HA	1:B:433:THR:HG23	1.93	0.49
1:F:199:THR:HA	1:F:384:GLU:OE1	2.13	0.49
1:D:252:PHE:CZ	1:D:291:LEU:HD13	2.47	0.49
1:A:321:ILE:HG23	1:A:343:ILE:CG2	2.42	0.49
1:F:495:GLU:C	1:F:497:GLY:H	2.16	0.49
1:E:272:THR:HB	1:E:280:ILE:O	2.13	0.49
1:F:271:ILE:O	1:F:272:THR:HG22	2.13	0.49
1:B:199:THR:HA	1:B:384:GLU:OE1	2.11	0.49
1:E:433:THR:HG23	1:F:412:SER:OG	2.13	0.49
1:D:427:THR:O	1:D:427:THR:HG23	2.12	0.49
1:E:112:THR:HG22	1:E:124:GLY:HA3	1.94	0.49
1:D:272:THR:HG21	1:D:317:VAL:HG21	1.94	0.49
1:D:276:SER:HB2	3:D:552:NDP:O2X	2.13	0.49
1:C:316:GLU:CD	1:C:338:ARG:HD2	2.32	0.49
1:F:19:ARG:HG2	1:F:479:THR:HG21	1.95	0.49
1:B:163:ASP:OD2	1:B:163:ASP:C	2.51	0.49
1:A:95:TYR:OH	1:A:145:THR:HG22	2.13	0.49
1:B:258:HIS:HD2	1:B:261:ARG:NH1	2.11	0.49
1:B:263:LEU:HD11	1:B:323:ILE:HD11	1.94	0.49
1:B:112:THR:CB	1:B:124:GLY:H	2.26	0.49
1:C:214:ALA:HB1	1:C:380:VAL:CG2	2.42	0.49
1:D:423:LYS:HD2	1:D:423:LYS:N	2.27	0.49
1:F:202:PRO:HD2	1:F:205:GLN:HB2	1.94	0.49
1:F:17:PHE:CE1	1:F:486:ILE:HG12	2.48	0.49
1:F:92:GLY:O	1:F:126:LYS:HD3	2.12	0.49
1:D:142:GLU:OE1	1:F:498:VAL:HG21	2.12	0.49
1:E:427:THR:O	1:E:429:PRO:CD	2.60	0.49
1:D:215:THR:O	1:D:219:VAL:HG23	2.13	0.49
1:C:223:ILE:CD1	1:C:263:LEU:HD11	2.43	0.49
1:A:337:PRO:HD3	1:A:359:ILE:HD13	1.95	0.49
1:E:67:ARG:NE	1:E:73:GLU:OE1	2.46	0.49
1:B:399:PHE:HA	1:B:441:SER:O	2.13	0.49
1:A:211:ARG:HD3	1:A:380:VAL:HG12	1.94	0.48
1:D:95:TYR:HB3	1:D:133:PRO:CG	2.41	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:55:CYS:HA	1:E:82:HIS:HA	1.95	0.48
1:E:35:ARG:CD	1:E:35:ARG:H	2.08	0.48
1:F:374:ASN:CB	3:F:552:NDP:H5N	2.43	0.48
1:E:258:HIS:CD2	1:E:261:ARG:NH1	2.73	0.48
1:D:178:TRP:HE1	1:F:498:VAL:HG21	1.78	0.48
1:D:5:ASP:OD2	1:D:332:THR:HB	2.13	0.48
1:E:271:ILE:HD12	1:E:272:THR:HG22	1.92	0.48
1:A:408:HIS:CD2	1:B:435:GLU:HB3	2.48	0.48
1:F:75:ILE:HD11	1:F:129:VAL:HG13	1.95	0.48
1:A:456:THR:OG1	1:C:396:ARG:NH2	2.45	0.48
1:B:363:ARG:NH1	1:B:365:ILE:HD11	2.29	0.48
1:D:468:ALA:HA	1:D:473:LEU:HD12	1.94	0.48
1:F:35:ARG:O	1:F:37:THR:HG23	2.14	0.48
1:A:353:THR:HB	1:A:354:PRO:CD	2.42	0.48
1:C:494:ASN:OD1	1:C:495:GLU:N	2.46	0.48
1:B:324:PRO:HD2	1:B:345:ALA:O	2.13	0.48
1:F:186:THR:OG1	1:F:187:ILE:N	2.44	0.48
1:F:12:MET:CE	1:F:16:PHE:HE1	2.25	0.48
1:D:232:TYR:CE2	1:D:465:MET:HG2	2.48	0.48
1:C:341:ALA:O	1:C:365:ILE:HG23	2.14	0.48
1:B:198:VAL:HG22	1:B:199:THR:N	2.28	0.48
1:B:219:VAL:HA	1:B:373:LEU:HD23	1.95	0.48
1:D:178:TRP:HE1	1:F:498:VAL:HG22	1.78	0.48
1:A:9:PHE:HD2	1:A:9:PHE:O	1.96	0.48
1:B:278:GLY:HA3	1:B:302:LEU:HD21	1.96	0.48
1:A:493:TYR:O	1:A:494:ASN:ND2	2.47	0.48
1:E:93:ILE:HD11	1:E:95:TYR:HE1	1.70	0.48
1:B:317:VAL:CG1	1:B:318:ASP:N	2.77	0.48
1:C:248:VAL:CG2	1:C:249:VAL:N	2.76	0.48
1:A:186:THR:O	1:A:189:HIS:ND1	2.46	0.48
1:B:414:GLN:OE1	1:B:429:PRO:HA	2.14	0.48
1:E:315:LEU:HD13	1:E:331:LEU:CD1	2.44	0.48
1:E:325:ALA:O	3:E:552:NDP:H51N	2.14	0.48
1:B:97:THR:HG23	1:B:132:ASN:HB2	1.95	0.48
1:C:41:LYS:O	1:C:45:VAL:HG23	2.13	0.48
1:E:37:THR:O	1:E:38:GLU:HB3	2.14	0.48
1:C:131:ILE:O	1:C:133:PRO:HD3	2.14	0.48
1:A:371:LEU:HD12	1:A:482:TYR:CE1	2.49	0.48
1:E:82:HIS:CD2	1:E:112:THR:CG2	2.92	0.48
1:E:186:THR:OG1	1:E:187:ILE:N	2.47	0.48
1:D:174:ARG:HD2	1:D:178:TRP:CH2	2.49	0.48
1:A:75:ILE:HD11	1:A:129:VAL:HG13	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:339:VAL:HG11	1:E:344:ILE:HD11	1.95	0.48
1:E:275:GLU:HG3	1:E:301:ILE:CD1	2.44	0.48
1:B:84:GLN:C	1:B:86:ARG:N	2.67	0.48
1:B:167:PRO:HD3	1:B:200:GLY:HA3	1.96	0.48
1:E:93:ILE:HB	1:E:127:ALA:HB3	1.95	0.48
1:D:408:HIS:CE1	1:F:435:GLU:HG2	2.49	0.48
1:A:186:THR:OG1	1:A:187:ILE:N	2.47	0.48
1:D:248:VAL:HG21	1:D:314:ILE:CG1	2.44	0.48
1:F:272:THR:HG21	1:F:317:VAL:HG21	1.96	0.48
1:E:382:TYR:OH	1:F:392:VAL:HG13	2.14	0.48
1:C:278:GLY:HA3	1:C:302:LEU:HD21	1.96	0.48
1:E:291:LEU:O	1:E:291:LEU:HD22	2.14	0.48
1:B:342:LYS:HD3	1:B:342:LYS:N	2.29	0.48
1:D:160:PRO:O	1:E:192:ILE:HD12	2.14	0.48
1:F:186:THR:O	1:F:189:HIS:ND1	2.47	0.48
1:A:468:ALA:HA	1:A:473:LEU:HD12	1.96	0.48
1:A:9:PHE:CE1	1:A:328:GLU:HG3	2.49	0.48
1:B:75:ILE:C	1:B:75:ILE:HD13	2.33	0.48
1:F:165:PRO:HD2	1:F:197:CYS:O	2.14	0.48
1:E:247:PHE:CZ	1:E:270:CYS:HB2	2.48	0.48
1:E:398:THR:O	1:E:399:PHE:C	2.53	0.48
1:B:35:ARG:O	1:B:37:THR:N	2.46	0.47
1:E:282:ASN:C	1:E:282:ASN:OD1	2.52	0.47
1:D:88:PRO:HD2	1:D:122:PHE:CE2	2.49	0.47
1:D:396:ARG:O	1:D:396:ARG:HD2	2.13	0.47
1:D:236:LEU:HA	1:D:236:LEU:HD12	1.67	0.47
1:A:47:SER:CB	1:D:72:TRP:HB2	2.36	0.47
1:D:99:VAL:HG21	1:D:128:GLY:C	2.34	0.47
1:A:61:LEU:HD12	1:D:57:HIS:HD2	1.79	0.47
1:C:339:VAL:HG21	1:C:360:PHE:CZ	2.49	0.47
1:C:339:VAL:HG12	1:C:341:ALA:H	1.79	0.47
1:F:126:LYS:NZ	2:F:502:GLU:N	2.62	0.47
1:B:232:TYR:CE2	1:B:465:MET:HG2	2.43	0.47
1:C:147:ARG:O	1:C:151:GLU:HG2	2.14	0.47
1:A:99:VAL:O	1:A:99:VAL:HG22	2.13	0.47
1:C:462:ARG:NH1	1:C:465:MET:CE	2.77	0.47
1:F:345:ALA:HB1	1:F:373:LEU:CD1	2.45	0.47
1:C:61:LEU:HD12	1:F:57:HIS:HD2	1.78	0.47
1:B:294:PHE:CE2	1:B:298:HIS:ND1	2.76	0.47
1:B:82:HIS:N	1:B:124:GLY:O	2.47	0.47
1:F:336:ALA:N	1:F:337:PRO:CD	2.75	0.47
1:E:175:GLU:HA	1:E:178:TRP:CE3	2.49	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:56:ASN:HD22	1:F:84:GLN:HE21	1.60	0.47
1:A:173:GLU:OE2	1:A:202:PRO:HA	2.14	0.47
1:D:263:LEU:HD11	1:D:323:ILE:HD11	1.97	0.47
1:F:378:VAL:HA	1:F:381:SER:HB2	1.96	0.47
1:B:458:GLU:HG3	1:B:459:ARG:N	2.29	0.47
1:C:174:ARG:O	1:C:177:SER:HB3	2.14	0.47
1:B:2:ASP:HB3	1:B:3:ARG:H	1.51	0.47
1:D:53:LYS:N	1:D:54:PRO:HD2	2.30	0.47
1:E:63:PHE:CZ	1:E:75:ILE:CD1	2.98	0.47
1:C:363:ARG:NH1	1:C:365:ILE:HD11	2.30	0.47
1:D:107:LEU:CG	1:D:126:LYS:HE3	2.45	0.47
1:C:153:ALA:HB1	1:C:187:ILE:HG13	1.96	0.47
1:A:96:SER:O	1:A:130:LYS:HA	2.15	0.47
1:B:141:LEU:HA	1:B:141:LEU:HD23	1.70	0.47
1:C:271:ILE:H	1:C:271:ILE:HG13	1.51	0.47
1:E:152:LEU:O	1:E:153:ALA:C	2.53	0.47
1:E:271:ILE:O	1:E:272:THR:HG22	2.15	0.47
1:A:409:LEU:C	1:A:409:LEU:HD23	2.35	0.47
1:A:79:ARG:CD	1:A:127:ALA:HB2	2.43	0.47
1:F:49:LEU:HA	1:F:49:LEU:HD12	1.64	0.47
1:E:158:ILE:HG12	1:E:159:GLY:N	2.30	0.47
1:F:448:ILE:HD13	1:F:448:ILE:HA	1.72	0.47
1:C:211:ARG:HA	1:C:380:VAL:HG11	1.96	0.47
1:B:291:LEU:HD21	1:B:301:ILE:HG22	1.97	0.47
1:C:414:GLN:OE1	1:C:429:PRO:HA	2.15	0.47
1:F:171:THR:HB	1:F:175:GLU:HG3	1.96	0.47
1:B:421:PHE:N	1:B:421:PHE:CD2	2.81	0.47
1:A:118:VAL:HG23	1:A:120:VAL:CG2	2.41	0.47
1:B:248:VAL:HG13	1:B:322:LEU:HD12	1.96	0.47
1:A:89:CYS:HB3	1:A:125:ALA:HB2	1.97	0.47
1:F:272:THR:OG1	1:F:314:ILE:HD11	2.15	0.47
1:E:19:ARG:CG	1:E:479:THR:HG21	2.44	0.47
1:C:344:ILE:HB	1:C:367:VAL:HG12	1.97	0.47
1:E:339:VAL:HG21	1:E:360:PHE:CE1	2.50	0.47
1:C:246:THR:CG2	1:C:319:CYS:HA	2.45	0.47
1:A:163:ASP:C	1:A:163:ASP:OD2	2.53	0.47
1:D:248:VAL:CG2	1:D:314:ILE:HD11	2.45	0.47
1:D:314:ILE:HG23	1:D:315:LEU:HD23	1.97	0.47
1:F:271:ILE:HD12	1:F:272:THR:HG23	1.97	0.47
1:B:9:PHE:O	1:B:9:PHE:CD2	2.63	0.47
1:B:99:VAL:HG22	1:B:99:VAL:O	2.13	0.47
1:A:433:THR:HG23	1:C:412:SER:HA	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:313:SER:HB3	1:C:316:GLU:HG3	1.96	0.47
1:A:304:PHE:CD1	1:A:305:PRO:HD2	2.50	0.47
1:B:371:LEU:HD12	1:B:482:TYR:CE1	2.49	0.46
1:A:37:THR:HG22	1:A:41:LYS:CE	2.46	0.46
1:D:112:THR:HG22	1:D:124:GLY:N	2.30	0.46
1:D:82:HIS:CG	1:D:109:SER:HA	2.50	0.46
1:C:478:ARG:HG2	1:C:482:TYR:CE1	2.50	0.46
1:F:153:ALA:HA	1:F:158:ILE:CG2	2.45	0.46
1:A:72:TRP:HB2	1:D:47:SER:HB3	1.97	0.46
1:C:196:ALA:HA	1:C:388:ASN:ND2	2.28	0.46
1:F:322:LEU:HB3	1:F:344:ILE:CD1	2.45	0.46
1:A:114:LYS:NZ	2:A:502:GLU:OXT	2.42	0.46
1:E:103:GLU:OE1	1:E:328:GLU:OE1	2.33	0.46
1:E:242:PHE:CE1	1:E:263:LEU:HD23	2.51	0.46
1:D:196:ALA:HA	1:D:388:ASN:HD22	1.81	0.46
1:A:408:HIS:CE1	1:B:435:GLU:HG2	2.49	0.46
1:C:96:SER:O	1:C:99:VAL:HG13	2.15	0.46
1:C:5:ASP:HB3	1:C:332:THR:HB	1.97	0.46
1:C:332:THR:HG22	1:C:353:THR:HG23	1.95	0.46
1:F:341:ALA:O	1:F:365:ILE:HG23	2.14	0.46
1:D:313:SER:HB3	1:D:316:GLU:HG3	1.98	0.46
1:A:51:ILE:O	1:A:51:ILE:HG22	2.14	0.46
1:A:201:LYS:NZ	1:A:388:ASN:ND2	2.59	0.46
1:E:142:GLU:O	1:E:146:ARG:HG3	2.14	0.46
1:A:236:LEU:HA	1:A:236:LEU:HD12	1.62	0.46
1:E:232:TYR:HE2	1:E:465:MET:HG2	1.81	0.46
1:E:287:ASP:HA	1:E:288:PRO:HD3	1.77	0.46
1:C:172:GLY:H	1:C:175:GLU:HG2	1.80	0.46
1:C:33:LYS:HB2	1:C:33:LYS:HE3	1.82	0.46
1:A:371:LEU:HD13	1:A:481:ALA:HB1	1.97	0.46
1:B:211:ARG:HH12	3:B:552:NDP:H72N	1.63	0.46
1:C:314:ILE:HG12	1:C:314:ILE:O	2.14	0.46
1:E:172:GLY:H	1:E:175:GLU:CG	2.27	0.46
1:D:436:PHE:HB2	1:E:408:HIS:HB3	1.98	0.46
1:C:84:GLN:C	1:C:86:ARG:H	2.18	0.46
1:C:84:GLN:C	1:C:86:ARG:N	2.68	0.46
1:D:400:LYS:HB2	1:F:455:TYR:HB2	1.97	0.46
1:F:89:CYS:HA	1:F:123:GLY:O	2.15	0.46
1:C:141:LEU:O	1:C:145:THR:CG2	2.61	0.46
1:F:28:LEU:O	1:F:31:ASP:HB2	2.15	0.46
1:B:328:GLU:HA	1:B:351:PRO:HA	1.96	0.46
1:D:114:LYS:HA	1:D:371:LEU:CD2	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:161:GLY:HA3	1:C:192:ILE:HA	1.97	0.46
1:B:118:VAL:HG23	1:B:120:VAL:HG23	1.96	0.46
1:C:315:LEU:HB3	1:C:331:LEU:HD11	1.96	0.46
1:D:246:THR:CG2	1:D:319:CYS:HA	2.46	0.46
1:F:248:VAL:HB	1:F:272:THR:HG23	1.97	0.46
1:A:79:ARG:CG	1:A:127:ALA:HB2	2.45	0.46
1:C:332:THR:HA	1:C:356:ALA:HB2	1.96	0.46
1:B:33:LYS:O	1:B:34:THR:C	2.54	0.46
1:F:94:ARG:O	1:F:128:GLY:HA2	2.16	0.46
1:E:39:GLU:C	1:E:41:LYS:N	2.68	0.46
1:B:36:GLU:O	1:B:37:THR:O	2.34	0.46
1:F:281:TRP:O	1:F:282:ASN:HB2	2.16	0.46
1:C:409:LEU:C	1:C:409:LEU:HD23	2.35	0.46
1:B:213:SER:HA	1:B:258:HIS:CG	2.51	0.46
1:A:85:HIS:CE1	1:A:489:VAL:HG22	2.51	0.46
1:B:233:MET:CE	1:B:233:MET:HA	2.45	0.46
1:B:403:ARG:O	1:B:407:TYR:CD1	2.69	0.46
1:B:459:ARG:O	1:B:463:GLN:HG2	2.16	0.46
1:A:271:ILE:C	1:A:272:THR:HG22	2.36	0.46
1:F:245:LYS:HD2	1:F:245:LYS:N	2.31	0.46
1:C:275:GLU:HG3	1:C:301:ILE:HD13	1.98	0.46
1:C:15:GLY:O	1:C:16:PHE:C	2.53	0.46
1:B:114:LYS:HA	1:B:371:LEU:HD23	1.96	0.46
1:C:281:TRP:CG	1:C:282:ASN:N	2.84	0.46
1:C:211:ARG:HD3	1:C:380:VAL:HG12	1.97	0.46
1:E:232:TYR:CE2	1:E:465:MET:HG2	2.50	0.46
1:B:53:LYS:O	1:B:82:HIS:HE1	1.99	0.46
1:E:94:ARG:O	1:E:128:GLY:HA2	2.16	0.46
1:B:342:LYS:O	1:B:365:ILE:HG22	2.15	0.46
1:F:112:THR:CG2	1:F:124:GLY:H	2.29	0.45
1:D:141:LEU:O	1:D:145:THR:CG2	2.63	0.45
1:F:150:MET:HA	1:F:150:MET:CE	2.43	0.45
1:C:187:ILE:HD13	1:C:187:ILE:N	2.31	0.45
1:D:217:ARG:HA	1:D:262:TYR:CD1	2.51	0.45
1:B:477:LEU:O	1:B:480:ALA:HB3	2.16	0.45
1:E:40:GLN:HE21	1:E:40:GLN:HB3	1.60	0.45
1:E:131:ILE:HG13	1:E:131:ILE:O	2.16	0.45
1:E:133:PRO:HG2	1:E:170:SER:HB3	1.98	0.45
1:A:57:HIS:HE1	1:A:84:GLN:NE2	2.14	0.45
1:E:332:THR:HG22	1:E:353:THR:CG2	2.46	0.45
1:E:96:SER:O	1:E:99:VAL:HG12	2.16	0.45
1:A:321:ILE:HG23	1:A:343:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:131:ILE:HB	1:C:136:TYR:CE2	2.51	0.45
1:D:186:THR:OG1	1:D:187:ILE:N	2.47	0.45
1:C:201:LYS:NZ	1:C:388:ASN:HD21	2.15	0.45
1:B:202:PRO:O	1:B:203:ILE:C	2.55	0.45
1:D:248:VAL:CB	1:D:272:THR:HG23	2.45	0.45
1:E:165:PRO:HD2	1:E:197:CYS:O	2.16	0.45
1:A:52:ILE:HD13	1:A:489:VAL:CG1	2.45	0.45
1:A:459:ARG:O	1:A:463:GLN:HG2	2.17	0.45
1:F:178:TRP:O	1:F:182:THR:CG2	2.65	0.45
1:D:336:ALA:N	1:D:337:PRO:CD	2.78	0.45
1:E:65:ILE:HG13	1:E:144:ILE:HG12	1.98	0.45
1:B:381:SER:O	1:B:384:GLU:N	2.49	0.45
1:F:347:GLY:O	1:F:374:ASN:HB3	2.16	0.45
1:A:373:LEU:O	1:A:373:LEU:HD22	2.17	0.45
1:A:248:VAL:HG21	1:A:314:ILE:HG12	1.99	0.45
1:D:314:ILE:O	1:D:317:VAL:HG23	2.16	0.45
1:C:216:GLY:O	1:C:219:VAL:HB	2.17	0.45
1:D:434:ALA:O	1:D:437:GLN:HB2	2.16	0.45
1:F:247:PHE:HB2	1:F:321:ILE:O	2.16	0.45
1:D:220:PHE:CE1	1:D:242:PHE:CE2	3.05	0.45
1:E:451:SER:HB2	1:F:400:LYS:HB3	1.97	0.45
1:B:416:SER:HA	1:B:419:ARG:NH1	2.31	0.45
2:A:502:GLU:HA	3:A:552:NDP:H41N	1.98	0.45
1:C:336:ALA:H	1:C:337:PRO:HD2	1.81	0.45
1:B:80:ALA:O	1:B:125:ALA:HA	2.17	0.45
1:A:258:HIS:HD2	1:A:261:ARG:NH1	2.11	0.45
1:B:409:LEU:O	1:B:412:SER:HB2	2.16	0.45
1:F:402:GLU:O	1:F:403:ARG:C	2.53	0.45
1:B:271:ILE:C	1:B:272:THR:HG22	2.36	0.45
1:B:409:LEU:C	1:B:409:LEU:HD23	2.37	0.45
1:D:371:LEU:HD23	1:D:371:LEU:HA	1.75	0.45
1:B:16:PHE:O	1:B:19:ARG:HB3	2.17	0.45
1:B:19:ARG:HG2	1:B:479:THR:CG2	2.46	0.45
1:B:158:ILE:HG12	1:B:159:GLY:N	2.32	0.45
1:C:185:SER:O	1:D:154:LYS:HD3	2.16	0.45
1:D:455:TYR:HB2	1:E:400:LYS:HB2	1.98	0.45
1:D:79:ARG:CG	1:D:127:ALA:HB2	2.47	0.45
1:A:417:LEU:HD21	1:B:417:LEU:HD11	1.98	0.45
1:A:219:VAL:HA	1:A:373:LEU:HD21	1.94	0.45
1:A:189:HIS:CE1	1:E:187:ILE:HD12	2.51	0.45
1:D:255:VAL:HG13	3:D:552:NDP:O2N	2.16	0.45
1:A:204:SER:OG	1:A:205:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:58:VAL:HG11	1:F:101:VAL:HG23	1.99	0.45
1:A:424:HIS:ND1	1:A:424:HIS:N	2.65	0.45
1:E:319:CYS:O	1:E:341:ALA:HA	2.17	0.45
1:A:65:ILE:HG13	1:A:144:ILE:HG12	1.97	0.45
1:A:126:LYS:NZ	2:A:502:GLU:N	2.65	0.45
1:F:82:HIS:CE1	1:F:109:SER:HB3	2.52	0.45
1:A:409:LEU:CD1	1:C:409:LEU:HD11	2.46	0.45
1:E:117:VAL:HG11	1:E:372:TYR:HB2	1.99	0.45
1:A:282:ASN:OD1	1:A:284:ASP:HB2	2.17	0.45
1:C:110:LEU:HD12	1:C:110:LEU:HA	1.63	0.44
1:C:462:ARG:HG3	1:C:466:ARG:NH2	2.29	0.44
1:D:75:ILE:C	1:D:75:ILE:HD13	2.37	0.44
1:D:249:VAL:HG22	1:D:251:GLY:O	2.16	0.44
1:D:296:LEU:HD22	1:D:296:LEU:HA	1.76	0.44
1:D:273:VAL:HG12	1:D:274:GLY:N	2.32	0.44
1:B:317:VAL:HG12	1:B:318:ASP:N	2.32	0.44
1:B:196:ALA:HB2	1:B:388:ASN:HB3	1.98	0.44
1:A:316:GLU:OE2	1:A:338:ARG:HD2	2.17	0.44
1:F:421:PHE:O	1:F:422:GLY:C	2.55	0.44
1:C:91:GLY:O	1:C:165:PRO:HA	2.17	0.44
1:C:12:MET:HE2	1:C:16:PHE:HE1	1.83	0.44
1:F:446:LYS:CB	1:F:446:LYS:NZ	2.80	0.44
1:C:342:LYS:N	1:C:342:LYS:HD3	2.33	0.44
1:B:296:LEU:HD22	1:B:296:LEU:HA	1.79	0.44
1:D:272:THR:CG2	1:D:317:VAL:HG11	2.47	0.44
1:A:39:GLU:C	1:A:41:LYS:H	2.18	0.44
1:B:169:MET:CG	3:B:552:NDP:H3D	2.48	0.44
1:D:408:HIS:ND1	1:F:439:ARG:HD2	2.33	0.44
1:C:72:TRP:HB3	1:F:51:ILE:HD11	2.00	0.44
1:C:367:VAL:O	1:C:369:PRO:HD3	2.16	0.44
1:F:353:THR:O	1:F:357:ASP:HB2	2.17	0.44
1:F:214:ALA:HB1	1:F:380:VAL:CG2	2.48	0.44
1:E:59:LEU:HB2	1:E:157:PHE:CZ	2.52	0.44
1:F:167:PRO:HD3	1:F:200:GLY:HA3	2.00	0.44
1:B:234:SER:O	1:B:237:GLY:N	2.50	0.44
1:D:444:SER:OG	1:D:446:LYS:HG3	2.17	0.44
1:A:309:ILE:HD12	1:A:309:ILE:N	2.33	0.44
1:C:446:LYS:CB	1:C:446:LYS:NZ	2.80	0.44
1:F:246:THR:O	1:F:320:ASP:HB2	2.16	0.44
1:B:9:PHE:C	1:B:9:PHE:CD2	2.90	0.44
1:D:337:PRO:HD3	1:D:359:ILE:HD13	1.99	0.44
1:B:99:VAL:HG13	1:B:130:LYS:HA	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:152:LEU:HD22	1:D:157:PHE:CB	2.46	0.44
1:B:202:PRO:HB2	1:B:205:GLN:HG3	1.99	0.44
1:B:63:PHE:CZ	1:B:75:ILE:CD1	3.00	0.44
1:F:93:ILE:O	1:F:93:ILE:HG13	2.15	0.44
1:E:95:TYR:HB3	1:E:133:PRO:CG	2.47	0.44
1:E:90:LYS:HB2	1:E:122:PHE:CG	2.53	0.44
1:C:242:PHE:CE1	1:C:263:LEU:CD2	3.00	0.44
1:C:480:ALA:O	1:C:483:VAL:HB	2.17	0.44
1:D:316:GLU:OE2	1:D:338:ARG:HD2	2.16	0.44
1:A:161:GLY:CA	1:C:192:ILE:HG13	2.48	0.44
1:C:463:GLN:HB3	1:C:463:GLN:HE21	1.60	0.44
1:C:424:HIS:N	1:C:424:HIS:ND1	2.66	0.44
1:B:217:ARG:HA	1:B:262:TYR:CD1	2.53	0.44
1:B:25:GLU:O	1:B:29:VAL:HG23	2.18	0.44
1:F:82:HIS:ND1	1:F:109:SER:HB3	2.33	0.44
1:E:282:ASN:OD1	1:E:284:ASP:N	2.51	0.44
1:F:272:THR:HB	1:F:280:ILE:O	2.17	0.44
1:A:313:SER:HB3	1:A:316:GLU:CG	2.47	0.44
1:F:340:LYS:HE2	1:F:340:LYS:HB2	1.73	0.44
1:D:456:THR:HG22	1:D:457:MET:HE3	2.00	0.44
1:F:457:MET:CA	1:F:457:MET:HE2	2.46	0.44
1:F:12:MET:HE2	1:F:16:PHE:HE1	1.82	0.44
1:C:46:ARG:O	1:C:50:ARG:HB2	2.17	0.44
1:D:432:PRO:HB3	1:D:436:PHE:HD2	1.83	0.44
1:C:298:HIS:C	1:C:300:THR:H	2.21	0.44
1:F:26:ASP:HA	1:F:42:ARG:NH2	2.33	0.44
1:D:37:THR:HG22	1:D:41:LYS:CE	2.47	0.43
1:A:95:TYR:OH	1:A:145:THR:HB	2.18	0.43
1:D:93:ILE:HA	1:D:127:ALA:O	2.18	0.43
1:A:188:GLY:O	1:A:189:HIS:C	2.54	0.43
1:B:344:ILE:HB	1:B:367:VAL:CG1	2.45	0.43
1:D:242:PHE:O	1:D:245:LYS:HB2	2.18	0.43
1:C:10:PHE:CA	1:C:106:ALA:HB2	2.48	0.43
1:B:231:SER:O	1:B:235:ILE:HD13	2.18	0.43
1:D:68:ASP:OD1	1:D:137:THR:HG21	2.18	0.43
1:F:236:LEU:HD12	1:F:236:LEU:HA	1.84	0.43
1:D:33:LYS:HB2	1:D:33:LYS:HE3	1.81	0.43
1:D:37:THR:O	1:D:40:GLN:HG2	2.17	0.43
1:A:178:TRP:O	1:A:182:THR:CG2	2.64	0.43
1:A:274:GLY:HA2	1:A:279:SER:HA	2.00	0.43
1:E:148:PHE:CE2	1:E:152:LEU:HD11	2.52	0.43
1:C:326:ALA:O	3:C:552:NDP:H4D	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:31:ASP:O	1:B:32:LEU:C	2.56	0.43
1:F:142:GLU:O	1:F:143:LYS:C	2.55	0.43
1:E:99:VAL:HG21	1:E:128:GLY:C	2.38	0.43
1:E:108:ALA:O	1:E:111:MET:HB2	2.19	0.43
1:C:37:THR:O	1:C:38:GLU:CB	2.66	0.43
1:B:348:ALA:HB3	1:B:351:PRO:HB3	2.01	0.43
1:D:272:THR:HG21	1:D:317:VAL:HG11	2.00	0.43
1:B:107:LEU:HD12	1:B:107:LEU:HA	1.81	0.43
1:F:395:GLY:O	1:F:397:LEU:N	2.51	0.43
1:A:159:GLY:CA	1:A:162:VAL:HG13	2.44	0.43
1:D:17:PHE:HZ	1:D:49:LEU:HD12	1.83	0.43
1:C:95:TYR:HB3	1:C:133:PRO:HG3	1.99	0.43
1:B:248:VAL:HG13	1:B:322:LEU:CD1	2.48	0.43
1:B:79:ARG:HG3	1:B:127:ALA:HB2	2.01	0.43
1:F:423:LYS:N	1:F:423:LYS:HD2	2.33	0.43
1:B:331:LEU:HA	1:B:331:LEU:HD12	1.77	0.43
1:D:448:ILE:HA	1:D:448:ILE:HD13	1.81	0.43
1:B:371:LEU:HD23	1:B:371:LEU:HA	1.66	0.43
1:B:165:PRO:C	1:B:198:VAL:HG23	2.39	0.43
1:C:245:LYS:CD	1:C:245:LYS:N	2.81	0.43
1:B:373:LEU:O	1:B:373:LEU:HD23	2.18	0.43
1:C:169:MET:CG	3:C:552:NDP:H3D	2.49	0.43
1:C:75:ILE:HD13	1:C:75:ILE:O	2.18	0.43
1:A:462:ARG:NH1	1:A:465:MET:HE1	2.34	0.43
1:B:187:ILE:HD12	1:F:189:HIS:HE1	1.83	0.43
1:F:146:ARG:CB	1:F:182:THR:HG21	2.48	0.43
1:F:230:ALA:O	1:F:231:SER:C	2.55	0.43
1:C:264:HIS:HA	1:C:268:ALA:O	2.19	0.43
1:E:11:LYS:HA	1:E:14:GLU:HB2	2.01	0.43
1:F:424:HIS:N	1:F:424:HIS:ND1	2.65	0.43
1:B:29:VAL:HG13	1:B:41:LYS:HB3	2.00	0.43
1:A:255:VAL:HG13	3:A:552:NDP:O2N	2.19	0.43
1:A:84:GLN:C	1:A:86:ARG:N	2.72	0.43
1:E:188:GLY:O	1:E:189:HIS:C	2.57	0.43
1:A:99:VAL:HG21	1:A:128:GLY:C	2.39	0.43
1:E:299:GLY:O	1:E:300:THR:HB	2.18	0.43
1:A:180:ALA:HB2	1:A:198:VAL:CG1	2.49	0.43
1:A:450:HIS:CE1	4:A:503:GTP:O1B	2.72	0.43
1:D:36:GLU:HB3	1:D:40:GLN:OE1	2.18	0.43
1:D:37:THR:O	1:D:38:GLU:CB	2.67	0.43
2:B:502:GLU:CA	3:B:552:NDP:H41N	2.38	0.43
1:E:248:VAL:HG23	1:E:272:THR:OG1	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:172:GLY:O	1:E:176:MET:HG2	2.19	0.43
1:F:49:LEU:HD12	1:F:52:ILE:HD12	2.00	0.43
1:C:118:VAL:HG11	1:C:375:ALA:HB3	2.00	0.43
1:C:410:LEU:HD12	1:C:410:LEU:HA	1.75	0.43
1:B:107:LEU:CB	1:B:126:LYS:HE3	2.48	0.43
1:C:126:LYS:HB2	1:C:126:LYS:HE2	1.85	0.43
1:A:85:HIS:HB2	1:A:492:VAL:HG11	2.00	0.43
1:B:291:LEU:HD23	1:B:291:LEU:HA	1.76	0.43
1:D:114:LYS:HA	1:D:371:LEU:HD23	2.00	0.43
1:A:9:PHE:CD1	1:A:328:GLU:HG3	2.54	0.43
1:C:56:ASN:HD22	1:C:84:GLN:NE2	2.16	0.43
1:E:450:HIS:CE1	4:E:503:GTP:O1B	2.72	0.43
1:D:11:LYS:HA	1:D:14:GLU:HB2	2.01	0.43
1:C:29:VAL:HG22	1:C:45:VAL:HG21	2.00	0.43
1:B:371:LEU:HD12	1:B:482:TYR:CD1	2.54	0.43
1:B:282:ASN:C	1:B:282:ASN:OD1	2.57	0.43
1:B:78:TYR:O	1:B:127:ALA:HA	2.18	0.43
1:E:248:VAL:CG1	1:E:319:CYS:SG	3.06	0.43
1:A:459:ARG:O	1:A:462:ARG:HB3	2.19	0.43
1:D:242:PHE:CE1	1:D:263:LEU:CD2	3.02	0.43
1:C:446:LYS:HB2	1:C:446:LYS:HZ2	1.84	0.43
1:E:477:LEU:HA	1:E:477:LEU:HD23	1.75	0.43
1:F:496:ALA:C	1:F:498:VAL:N	2.66	0.43
1:E:246:THR:HG23	1:E:319:CYS:HA	2.01	0.43
1:F:65:ILE:CG1	1:F:144:ILE:HG12	2.48	0.43
1:E:44:ARG:HH12	1:E:494:ASN:ND2	2.17	0.43
1:A:257:LEU:O	1:A:260:MET:HB3	2.18	0.43
1:E:273:VAL:HG12	1:E:274:GLY:N	2.34	0.43
1:F:462:ARG:NH1	1:F:465:MET:CE	2.82	0.43
1:B:391:HIS:O	1:C:382:TYR:OH	2.28	0.43
1:E:215:THR:HG23	1:E:216:GLY:N	2.34	0.43
1:D:410:LEU:HA	1:D:410:LEU:HD12	1.64	0.43
1:A:37:THR:O	1:A:38:GLU:HB3	2.18	0.42
1:A:126:LYS:NZ	1:A:168:ASP:OD2	2.48	0.42
1:A:347:GLY:O	1:A:374:ASN:HB3	2.19	0.42
1:F:55:CYS:HA	1:F:82:HIS:HA	2.00	0.42
1:D:95:TYR:OH	1:D:145:THR:CB	2.67	0.42
1:F:337:PRO:O	1:F:363:ARG:NE	2.52	0.42
1:A:177:SER:HB2	1:A:202:PRO:HG2	2.01	0.42
1:B:146:ARG:CB	1:B:182:THR:HG21	2.48	0.42
1:B:146:ARG:NH2	1:B:181:ASP:OD2	2.52	0.42
1:C:191:ASP:HB3	1:C:194:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:150:MET:O	1:C:154:LYS:HG3	2.19	0.42
1:F:361:LEU:HA	1:F:361:LEU:HD22	1.77	0.42
1:C:390:ASN:O	1:C:392:VAL:HG23	2.19	0.42
1:C:82:HIS:CG	1:C:109:SER:HA	2.55	0.42
1:D:79:ARG:HA	1:D:127:ALA:HA	2.01	0.42
1:F:31:ASP:O	1:F:32:LEU:C	2.57	0.42
1:A:196:ALA:HA	1:A:388:ASN:HD22	1.85	0.42
1:E:224:GLU:HB2	1:E:242:PHE:HE2	1.84	0.42
1:D:443:ALA:N	1:E:401:TYR:CE2	2.87	0.42
1:E:171:THR:HB	1:E:175:GLU:HG3	2.01	0.42
1:D:335:ASN:C	1:D:337:PRO:HD2	2.40	0.42
1:B:476:ASP:OD2	1:B:479:THR:HG23	2.18	0.42
1:B:175:GLU:HA	1:B:178:TRP:CE3	2.53	0.42
1:A:273:VAL:HG21	1:A:291:LEU:HD12	2.01	0.42
1:A:249:VAL:HG22	1:A:251:GLY:O	2.19	0.42
1:A:401:TYR:CD2	1:B:443:ALA:HB2	2.53	0.42
1:A:37:THR:O	1:A:38:GLU:CB	2.68	0.42
1:A:95:TYR:OH	1:A:145:THR:CG2	2.68	0.42
1:A:215:THR:HG23	1:A:216:GLY:H	1.85	0.42
1:A:118:VAL:HG11	1:A:375:ALA:HB3	2.00	0.42
1:B:271:ILE:HD12	1:B:272:THR:HG22	2.00	0.42
1:B:252:PHE:CZ	1:B:291:LEU:HD13	2.55	0.42
1:A:336:ALA:N	1:A:337:PRO:CD	2.82	0.42
1:E:331:LEU:HA	1:E:331:LEU:HD12	1.76	0.42
1:B:160:PRO:HD3	1:B:197:CYS:HB3	2.01	0.42
1:B:395:GLY:HA3	1:B:399:PHE:CZ	2.54	0.42
1:A:234:SER:O	1:A:235:ILE:C	2.57	0.42
1:A:389:LEU:O	1:A:391:HIS:ND1	2.52	0.42
1:F:39:GLU:C	1:F:41:LYS:H	2.23	0.42
1:E:196:ALA:HB1	1:E:385:TRP:CD1	2.54	0.42
1:D:417:LEU:HD23	1:D:417:LEU:HA	1.78	0.42
1:A:313:SER:C	1:A:315:LEU:N	2.73	0.42
1:F:421:PHE:N	1:F:421:PHE:CD2	2.87	0.42
1:E:233:MET:HA	1:E:233:MET:HE2	2.02	0.42
1:F:242:PHE:CE1	1:F:263:LEU:CD2	3.03	0.42
1:A:215:THR:HG23	1:A:216:GLY:N	2.35	0.42
1:E:272:THR:HG21	1:E:317:VAL:HG21	2.01	0.42
1:A:489:VAL:C	1:A:490:PHE:O	2.57	0.42
1:B:142:GLU:OE2	1:B:146:ARG:NH1	2.53	0.42
1:E:303:GLY:N	1:E:309:ILE:HD11	2.33	0.42
1:D:291:LEU:O	1:D:294:PHE:N	2.52	0.42
1:A:96:SER:O	1:A:99:VAL:CG1	2.67	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:328:GLU:HB2	1:F:350:GLY:O	2.19	0.42
1:D:131:ILE:O	1:D:131:ILE:HG13	2.17	0.42
1:E:38:GLU:HG3	1:E:39:GLU:HG2	2.00	0.42
1:D:29:VAL:HG13	1:D:41:LYS:HB3	2.02	0.42
1:C:141:LEU:HA	1:C:141:LEU:HD23	1.73	0.42
1:E:196:ALA:HB2	1:E:388:ASN:CB	2.48	0.42
1:F:498:VAL:HB	1:F:499:THR:H	1.69	0.42
1:E:272:THR:CG2	1:E:281:TRP:HD1	2.29	0.42
1:A:409:LEU:O	1:A:409:LEU:HD23	2.19	0.42
1:D:91:GLY:HA3	1:D:125:ALA:O	2.19	0.42
1:B:118:VAL:HB	1:B:456:THR:CG2	2.50	0.42
1:B:477:LEU:HA	1:B:477:LEU:HD23	1.86	0.42
1:F:234:SER:O	1:F:235:ILE:C	2.56	0.42
1:F:40:GLN:HB3	1:F:40:GLN:HE21	1.59	0.42
1:E:37:THR:O	1:E:38:GLU:CB	2.67	0.42
1:A:93:ILE:HG13	1:A:94:ARG:N	2.27	0.42
1:F:215:THR:HB	3:F:552:NDP:H42N	2.01	0.42
1:C:248:VAL:CG2	1:C:314:ILE:HD11	2.49	0.42
1:A:378:VAL:HA	1:A:381:SER:HB2	2.02	0.42
1:E:370:ASP:OD1	1:E:371:LEU:N	2.47	0.42
1:F:117:VAL:HG21	1:F:371:LEU:HD22	2.02	0.42
1:A:107:LEU:HD12	1:A:107:LEU:HA	1.73	0.42
1:C:51:ILE:HG23	1:F:64:PRO:HB3	2.02	0.42
1:A:75:ILE:HD11	1:A:129:VAL:CG1	2.49	0.42
1:E:344:ILE:HB	1:E:367:VAL:HG12	2.02	0.42
1:E:275:GLU:HG3	1:E:301:ILE:HD11	2.02	0.42
1:D:221:HIS:O	1:D:224:GLU:HB3	2.20	0.42
1:A:370:ASP:HB2	1:A:374:ASN:HD21	1.84	0.42
1:C:305:PRO:O	1:C:307:ALA:N	2.51	0.42
1:D:476:ASP:OD2	1:D:479:THR:HG23	2.20	0.42
1:F:337:PRO:HD3	1:F:359:ILE:HD13	2.01	0.42
1:D:142:GLU:OE2	1:D:146:ARG:NH1	2.53	0.42
1:C:208:ILE:HG22	1:C:211:ARG:HB2	2.02	0.42
1:C:446:LYS:HB2	1:C:446:LYS:NZ	2.35	0.42
1:F:33:LYS:O	1:F:34:THR:C	2.58	0.42
1:E:100:SER:O	1:E:101:VAL:C	2.59	0.42
1:C:53:LYS:N	1:C:54:PRO:CD	2.83	0.42
1:D:271:ILE:HD11	1:D:319:CYS:HB3	2.01	0.42
1:E:281:TRP:O	1:E:282:ASN:HB2	2.19	0.42
1:D:409:LEU:HD23	1:D:409:LEU:O	2.20	0.42
1:E:410:LEU:HG	1:E:430:ILE:HG22	2.01	0.42
1:A:462:ARG:NH1	1:A:465:MET:CE	2.83	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:227:ILE:HG23	1:B:227:ILE:O	2.20	0.42
1:B:229:GLU:HG3	1:B:231:SER:HB3	2.01	0.42
1:D:84:GLN:C	1:D:86:ARG:N	2.73	0.42
1:F:313:SER:HB3	1:F:316:GLU:CD	2.40	0.42
1:A:211:ARG:HA	1:A:380:VAL:HG11	2.01	0.41
1:E:213:SER:CB	1:E:258:HIS:CD2	3.03	0.41
1:C:31:ASP:O	1:C:32:LEU:C	2.58	0.41
1:F:281:TRP:CZ2	1:F:283:PRO:CG	3.00	0.41
1:E:12:MET:HG3	1:E:354:PRO:HD3	2.02	0.41
1:C:90:LYS:HD2	1:C:164:VAL:O	2.20	0.41
1:E:253:GLY:HA3	3:E:552:NDP:O5B	2.20	0.41
1:C:25:GLU:OE2	1:C:42:ARG:NH1	2.53	0.41
1:B:82:HIS:CG	1:B:109:SER:HA	2.55	0.41
1:E:169:MET:O	1:E:170:SER:HB2	2.20	0.41
1:D:79:ARG:HB2	1:D:127:ALA:HB2	2.03	0.41
1:D:248:VAL:CG2	1:D:314:ILE:HG12	2.50	0.41
1:A:201:LYS:HZ1	1:A:388:ASN:ND2	2.09	0.41
1:B:382:TYR:CE1	1:B:386:LEU:HD22	2.55	0.41
1:B:252:PHE:CE2	1:B:291:LEU:HD13	2.54	0.41
1:C:353:THR:HB	1:C:354:PRO:HD2	2.01	0.41
1:D:65:ILE:HG13	1:D:144:ILE:HG13	2.02	0.41
1:C:274:GLY:HA2	1:C:279:SER:HA	2.01	0.41
1:C:142:GLU:OE2	1:C:146:ARG:NH1	2.53	0.41
1:E:224:GLU:HB2	1:E:242:PHE:CE2	2.54	0.41
1:C:63:PHE:CD1	1:C:147:ARG:HG3	2.55	0.41
1:A:435:GLU:HG2	1:C:408:HIS:CE1	2.55	0.41
1:C:224:GLU:HB2	1:C:242:PHE:CE2	2.54	0.41
1:C:436:PHE:CG	1:C:436:PHE:O	2.74	0.41
1:F:368:ILE:HB	1:F:373:LEU:CD1	2.50	0.41
1:B:416:SER:O	1:B:419:ARG:HB3	2.20	0.41
1:C:227:ILE:HA	1:C:233:MET:SD	2.60	0.41
1:A:379:THR:O	1:A:382:TYR:HB3	2.20	0.41
1:F:79:ARG:HG3	1:F:127:ALA:HB2	2.01	0.41
1:B:38:GLU:CG	1:B:39:GLU:H	1.92	0.41
1:A:272:THR:HG21	1:A:317:VAL:HG21	2.02	0.41
1:C:65:ILE:HA	1:C:65:ILE:HD13	1.68	0.41
1:A:57:HIS:HD2	1:D:61:LEU:HD12	1.85	0.41
1:C:75:ILE:HD11	1:C:129:VAL:HG13	2.02	0.41
1:A:63:PHE:CZ	1:A:75:ILE:HD12	2.56	0.41
1:C:309:ILE:N	1:C:309:ILE:HD12	2.35	0.41
1:D:100:SER:O	1:D:101:VAL:C	2.59	0.41
1:F:487:GLU:OE2	1:F:491:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:9:PHE:HD2	1:E:9:PHE:O	2.04	0.41
1:F:35:ARG:O	1:F:37:THR:N	2.54	0.41
1:B:349:ASN:ND2	3:B:552:NDP:O2D	2.46	0.41
1:A:189:HIS:CE1	1:E:187:ILE:CD1	3.03	0.41
1:E:10:PHE:HD2	1:E:106:ALA:HA	1.86	0.41
1:B:453:LEU:O	1:B:453:LEU:HD12	2.20	0.41
1:F:28:LEU:HA	1:F:28:LEU:HD12	1.77	0.41
1:B:281:TRP:O	1:B:282:ASN:HB2	2.20	0.41
1:F:337:PRO:O	1:F:363:ARG:CZ	2.68	0.41
1:F:201:LYS:NZ	1:F:388:ASN:ND2	2.57	0.41
1:B:303:GLY:H	1:B:309:ILE:CD1	2.31	0.41
1:C:316:GLU:OE1	1:C:338:ARG:HD2	2.20	0.41
1:C:338:ARG:O	1:C:338:ARG:HG3	2.20	0.41
1:D:87:THR:HB	1:D:88:PRO:HA	2.02	0.41
1:D:78:TYR:CD1	1:D:78:TYR:N	2.88	0.41
1:A:246:THR:HG22	1:A:320:ASP:H	1.86	0.41
1:C:29:VAL:CG2	1:C:45:VAL:HG21	2.50	0.41
1:A:276:SER:OG	3:A:552:NDP:P2B	2.79	0.41
1:A:175:GLU:HA	1:A:178:TRP:CE3	2.55	0.41
1:E:386:LEU:HD21	1:F:392:VAL:HG13	2.01	0.41
1:C:344:ILE:HB	1:C:367:VAL:HG13	2.01	0.41
1:F:146:ARG:CA	1:F:182:THR:HG21	2.49	0.41
1:B:84:GLN:HE21	1:B:84:GLN:HB2	1.69	0.41
1:C:291:LEU:HD23	1:C:291:LEU:HA	1.89	0.41
1:E:65:ILE:HD13	1:E:65:ILE:HA	1.63	0.41
1:A:333:LYS:HD2	1:A:355:GLU:HG2	2.03	0.41
1:B:236:LEU:HD12	1:B:236:LEU:HA	1.85	0.41
1:F:39:GLU:C	1:F:41:LYS:N	2.72	0.41
1:B:35:ARG:HD3	1:B:35:ARG:N	2.14	0.41
1:F:374:ASN:OD1	1:F:374:ASN:C	2.59	0.41
1:B:346:GLU:HB2	1:B:368:ILE:O	2.19	0.41
1:B:281:TRP:CZ2	1:B:283:PRO:HG3	2.55	0.41
1:A:63:PHE:CE1	1:A:75:ILE:HD12	2.56	0.41
1:E:162:VAL:O	1:E:163:ASP:HB2	2.21	0.41
1:B:17:PHE:CE2	1:B:53:LYS:CG	3.03	0.41
1:A:37:THR:HG22	1:A:41:LYS:NZ	2.35	0.41
1:E:107:LEU:HD12	1:E:107:LEU:HA	1.88	0.41
1:E:95:TYR:CD1	1:E:129:VAL:HB	2.56	0.41
1:C:339:VAL:HG21	1:C:360:PHE:CE1	2.55	0.41
1:C:281:TRP:O	1:C:282:ASN:CB	2.67	0.41
1:A:158:ILE:HA	1:A:163:ASP:O	2.20	0.41
1:B:314:ILE:HA	1:B:317:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:346:GLU:HG2	1:A:351:PRO:CG	2.50	0.41
1:E:90:LYS:HB2	1:E:122:PHE:CD1	2.56	0.41
1:A:111:MET:CA	1:A:111:MET:HE3	2.50	0.41
1:E:224:GLU:HA	1:E:227:ILE:HG22	2.03	0.41
1:C:107:LEU:HD12	1:C:107:LEU:HA	1.89	0.41
1:D:460:SER:HA	1:D:463:GLN:HG2	2.03	0.41
1:C:196:ALA:HB2	1:C:388:ASN:CB	2.51	0.41
1:D:167:PRO:HG3	1:D:176:MET:CG	2.50	0.41
1:D:486:ILE:O	1:D:487:GLU:C	2.58	0.41
1:F:371:LEU:HA	1:F:371:LEU:HD23	1.81	0.41
1:B:398:THR:O	1:B:399:PHE:C	2.59	0.41
1:A:65:ILE:HA	1:A:65:ILE:HD13	1.62	0.41
1:D:90:LYS:HD2	1:D:164:VAL:HB	2.03	0.41
1:D:191:ASP:C	1:D:193:ASN:H	2.23	0.41
1:F:159:GLY:HA3	1:F:162:VAL:HG13	2.03	0.41
1:D:119:ASP:O	1:E:396:ARG:NH1	2.53	0.41
1:F:257:LEU:HD12	1:F:257:LEU:O	2.21	0.41
1:D:79:ARG:CB	1:D:127:ALA:HB2	2.51	0.41
1:B:90:LYS:HE2	1:B:164:VAL:HG12	2.03	0.41
1:A:153:ALA:HA	1:A:158:ILE:HG22	2.03	0.41
1:D:175:GLU:HA	1:D:178:TRP:HE3	1.82	0.41
1:E:430:ILE:HA	1:F:416:SER:HB3	2.03	0.41
1:F:462:ARG:HG3	1:F:466:ARG:HH22	1.86	0.41
2:E:502:GLU:HA	3:E:552:NDP:C4N	2.51	0.41
1:F:96:SER:OG	1:F:98:ASP:HB2	2.21	0.41
1:A:32:LEU:HD11	1:A:44:ARG:NH1	2.36	0.41
1:E:289:LYS:HD2	1:E:289:LYS:HA	1.83	0.41
1:D:416:SER:CB	1:F:430:ILE:HA	2.50	0.41
1:C:45:VAL:HG12	1:C:49:LEU:HD23	2.01	0.40
1:C:82:HIS:HD2	1:C:112:THR:CG2	2.04	0.40
1:A:53:LYS:O	1:A:82:HIS:HE1	2.03	0.40
1:B:276:SER:HB2	3:B:552:NDP:O2X	2.21	0.40
1:F:201:LYS:HB2	1:F:201:LYS:HE2	1.85	0.40
1:F:65:ILE:HA	1:F:65:ILE:HD13	1.64	0.40
1:E:31:ASP:O	1:E:32:LEU:C	2.59	0.40
1:C:232:TYR:O	1:C:236:LEU:HB2	2.21	0.40
1:E:229:GLU:O	1:E:230:ALA:C	2.60	0.40
1:E:213:SER:HB2	1:E:258:HIS:CD2	2.56	0.40
1:A:196:ALA:HB1	1:A:385:TRP:CD1	2.56	0.40
1:C:8:ASN:O	1:C:9:PHE:C	2.60	0.40
1:E:176:MET:O	1:E:177:SER:C	2.58	0.40
1:A:409:LEU:O	1:A:412:SER:HB2	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:234:SER:O	1:C:235:ILE:C	2.60	0.40
1:C:5:ASP:OD2	1:C:332:THR:HB	2.20	0.40
1:F:113:TYR:C	1:F:371:LEU:HD21	2.42	0.40
1:F:42:ARG:O	1:F:45:VAL:HB	2.21	0.40
1:F:286:ILE:HG23	1:F:304:PHE:HE2	1.87	0.40
1:A:421:PHE:CD2	1:A:421:PHE:N	2.86	0.40
1:A:457:MET:CE	1:A:457:MET:HA	2.38	0.40
1:F:370:ASP:HB2	1:F:374:ASN:ND2	2.36	0.40
1:B:32:LEU:HD11	1:B:44:ARG:NH1	2.37	0.40
1:C:427:THR:HG23	1:C:427:THR:O	2.21	0.40
1:C:294:PHE:CE1	1:C:300:THR:O	2.74	0.40
1:F:371:LEU:HD13	1:F:481:ALA:HB1	2.03	0.40
1:A:96:SER:OG	1:A:97:THR:N	2.54	0.40
1:D:66:ARG:CZ	1:D:70:GLY:O	2.69	0.40
1:B:424:HIS:ND1	1:B:424:HIS:N	2.69	0.40
1:D:417:LEU:HB3	1:D:428:ILE:HD13	2.03	0.40
1:F:271:ILE:C	1:F:272:THR:CG2	2.90	0.40
1:E:175:GLU:N	1:E:175:GLU:CD	2.74	0.40
1:B:291:LEU:CD2	1:B:301:ILE:HG22	2.51	0.40
1:D:167:PRO:HG3	1:D:176:MET:HG2	2.03	0.40
1:E:331:LEU:HG	1:E:360:PHE:HZ	1.86	0.40
1:D:2:ASP:OD1	1:D:5:ASP:O	2.39	0.40
1:E:255:VAL:HG11	3:E:552:NDP:O4D	2.21	0.40
1:A:466:ARG:NH1	1:A:466:ARG:HB2	2.37	0.40
1:F:107:LEU:HA	1:F:107:LEU:HD12	1.72	0.40
1:A:216:GLY:HA2	1:A:219:VAL:HB	2.03	0.40
1:A:118:VAL:HG11	1:A:375:ALA:CB	2.52	0.40
1:C:211:ARG:NH2	2:C:502:GLU:HG2	2.36	0.40
1:E:24:VAL:HG13	1:E:483:VAL:HG22	2.03	0.40
1:D:436:PHE:O	1:D:440:ILE:HB	2.22	0.40
1:B:186:THR:OG1	1:B:187:ILE:N	2.53	0.40
1:A:423:LYS:HD2	1:A:423:LYS:N	2.36	0.40
1:F:172:GLY:H	1:F:175:GLU:CG	2.34	0.40
1:E:273:VAL:HG21	1:E:291:LEU:HD12	2.02	0.40
1:E:301:ILE:HG13	1:E:302:LEU:N	2.37	0.40
1:C:80:ALA:O	1:C:125:ALA:HA	2.22	0.40
1:D:304:PHE:HA	1:D:305:PRO:HD2	1.94	0.40
1:E:296:LEU:HA	1:E:296:LEU:HD22	1.70	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	493/501 (98%)	428 (87%)	52 (10%)	13 (3%)	8	31
1	B	493/501 (98%)	429 (87%)	49 (10%)	15 (3%)	7	26
1	C	493/501 (98%)	424 (86%)	55 (11%)	14 (3%)	8	29
1	D	493/501 (98%)	427 (87%)	57 (12%)	9 (2%)	13	43
1	E	493/501 (98%)	427 (87%)	56 (11%)	10 (2%)	11	40
1	F	499/501 (100%)	424 (85%)	62 (12%)	13 (3%)	8	31
All	All	2964/3006 (99%)	2559 (86%)	331 (11%)	74 (2%)	9	32

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	371	LEU
1	B	34	THR
1	B	37	THR
1	B	38	GLU
1	C	38	GLU
1	C	282	ASN
1	D	4	GLU
1	D	38	GLU
1	D	404	ASP
1	E	38	GLU
1	E	371	LEU
1	F	38	GLU
1	F	496	ALA
1	F	498	VAL
1	A	234	SER
1	A	422	GLY
1	B	85	HIS
1	B	306	LYS
1	B	422	GLY
1	C	36	GLU

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Mol	Chain	Res	Type
1	C	299	GLY
1	C	306	LYS
1	C	422	GLY
1	D	405	SER
1	D	422	GLY
1	E	370	ASP
1	E	422	GLY
1	F	3	ARG
1	F	36	GLU
1	F	396	ARG
1	F	422	GLY
1	A	235	ILE
1	A	396	ARG
1	A	491	ARG
1	B	348	ALA
1	D	204	SER
1	E	31	ASP
1	E	36	GLU
1	A	31	ASP
1	A	32	LEU
1	B	31	ASP
1	B	474	GLY
1	C	2	ASP
1	C	31	ASP
1	E	32	LEU
1	E	209	HIS
1	F	34	THR
1	F	231	SER
1	F	371	LEU
1	A	493	TYR
1	B	396	ARG
1	B	494	ASN
1	C	126	LYS
1	C	166	ALA
1	C	340	LYS
1	D	36	GLU
1	E	187	ILE
1	E	210	GLY
1	F	31	ASP
1	F	500	PHE
1	A	168	ASP
1	B	32	LEU

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Mol	Chain	Res	Type
1	B	36	GLU
1	B	305	PRO
1	B	371	LEU
1	C	305	PRO
1	D	487	GLU
1	A	99	VAL
1	A	166	ALA
1	C	165	PRO
1	F	165	PRO
1	C	240	PRO
1	D	203	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	416/420 (99%)	356 (86%)	60 (14%)	5	13
1	B	416/420 (99%)	353 (85%)	63 (15%)	4	11
1	C	416/420 (99%)	358 (86%)	58 (14%)	5	14
1	D	416/420 (99%)	352 (85%)	64 (15%)	4	11
1	E	416/420 (99%)	355 (85%)	61 (15%)	4	12
1	F	420/420 (100%)	356 (85%)	64 (15%)	4	11
All	All	2500/2520 (99%)	2130 (85%)	370 (15%)	4	12

All (370) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	GLU
1	A	9	PHE
1	A	28	LEU
1	A	33	LYS
1	A	35	ARG
1	A	38	GLU
1	A	44	ARG

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Mol	Chain	Res	Type
1	A	49	LEU
1	A	61	LEU
1	A	65	ILE
1	A	75	ILE
1	A	84	GLN
1	A	93	ILE
1	A	99	VAL
1	A	101	VAL
1	A	107	LEU
1	A	110	LEU
1	A	112	THR
1	A	145	THR
1	A	158	ILE
1	A	162	VAL
1	A	182	THR
1	A	203	ILE
1	A	212	ILE
1	A	227	ILE
1	A	238	MET
1	A	239	THR
1	A	249	VAL
1	A	255	VAL
1	A	272	THR
1	A	291	LEU
1	A	296	LEU
1	A	297	GLN
1	A	306	LYS
1	A	311	GLU
1	A	321	ILE
1	A	331	LEU
1	A	340	LYS
1	A	352	THR
1	A	361	LEU
1	A	364	ASN
1	A	365	ILE
1	A	367	VAL
1	A	371	LEU
1	A	373	LEU
1	A	378	VAL
1	A	386	LEU
1	A	392	VAL
1	A	393	SER

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Mol	Chain	Res	Type
1	A	397	LEU
1	A	405	SER
1	A	410	LEU
1	A	424	HIS
1	A	446	LYS
1	A	458	GLU
1	A	463	GLN
1	A	478	ARG
1	A	487	GLU
1	A	495	GLU
1	B	2	ASP
1	B	9	PHE
1	B	28	LEU
1	B	33	LYS
1	B	35	ARG
1	B	40	GLN
1	B	44	ARG
1	B	49	LEU
1	B	66	ARG
1	B	75	ILE
1	B	78	TYR
1	B	84	GLN
1	B	93	ILE
1	B	96	SER
1	B	99	VAL
1	B	101	VAL
1	B	104	VAL
1	B	107	LEU
1	B	112	THR
1	B	137	THR
1	B	145	THR
1	B	150	MET
1	B	162	VAL
1	B	176	MET
1	B	182	THR
1	B	212	ILE
1	B	238	MET
1	B	239	THR
1	B	245	LYS
1	B	246	THR
1	B	249	VAL
1	B	272	THR

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Mol	Chain	Res	Type
1	B	291	LEU
1	B	296	LEU
1	B	297	GLN
1	B	306	LYS
1	B	311	GLU
1	B	321	ILE
1	B	331	LEU
1	B	340	LYS
1	B	352	THR
1	B	357	ASP
1	B	361	LEU
1	B	364	ASN
1	B	365	ILE
1	B	367	VAL
1	B	371	LEU
1	B	373	LEU
1	B	378	VAL
1	B	386	LEU
1	B	392	VAL
1	B	393	SER
1	B	397	LEU
1	B	405	SER
1	B	423	LYS
1	B	424	HIS
1	B	437	GLN
1	B	446	LYS
1	B	458	GLU
1	B	487	GLU
1	B	492	VAL
1	B	494	ASN
1	B	495	GLU
1	C	3	ARG
1	C	9	PHE
1	C	24	VAL
1	C	28	LEU
1	C	33	LYS
1	C	35	ARG
1	C	38	GLU
1	C	40	GLN
1	C	44	ARG
1	C	49	LEU
1	C	61	LEU

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Mol	Chain	Res	Type
1	C	66	ARG
1	C	75	ILE
1	C	78	TYR
1	C	84	GLN
1	C	93	ILE
1	C	96	SER
1	C	99	VAL
1	C	107	LEU
1	C	110	LEU
1	C	112	THR
1	C	145	THR
1	C	162	VAL
1	C	175	GLU
1	C	182	THR
1	C	203	ILE
1	C	212	ILE
1	C	238	MET
1	C	239	THR
1	C	245	LYS
1	C	255	VAL
1	C	272	THR
1	C	291	LEU
1	C	296	LEU
1	C	297	GLN
1	C	306	LYS
1	C	311	GLU
1	C	321	ILE
1	C	331	LEU
1	C	340	LYS
1	C	352	THR
1	C	361	LEU
1	C	364	ASN
1	C	365	ILE
1	C	367	VAL
1	C	368	ILE
1	C	371	LEU
1	C	373	LEU
1	C	378	VAL
1	C	386	LEU
1	C	392	VAL
1	C	393	SER
1	C	410	LEU

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Mol	Chain	Res	Type
1	C	423	LYS
1	C	424	HIS
1	C	446	LYS
1	C	458	GLU
1	C	487	GLU
1	D	3	ARG
1	D	9	PHE
1	D	28	LEU
1	D	31	ASP
1	D	33	LYS
1	D	35	ARG
1	D	38	GLU
1	D	43	ASN
1	D	44	ARG
1	D	49	LEU
1	D	61	LEU
1	D	65	ILE
1	D	66	ARG
1	D	75	ILE
1	D	78	TYR
1	D	84	GLN
1	D	93	ILE
1	D	96	SER
1	D	99	VAL
1	D	104	VAL
1	D	107	LEU
1	D	112	THR
1	D	145	THR
1	D	162	VAL
1	D	175	GLU
1	D	182	THR
1	D	212	ILE
1	D	236	LEU
1	D	238	MET
1	D	239	THR
1	D	246	THR
1	D	255	VAL
1	D	272	THR
1	D	291	LEU
1	D	296	LEU
1	D	297	GLN
1	D	306	LYS

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Mol	Chain	Res	Type
1	D	311	GLU
1	D	313	SER
1	D	321	ILE
1	D	331	LEU
1	D	340	LYS
1	D	342	LYS
1	D	352	THR
1	D	357	ASP
1	D	361	LEU
1	D	364	ASN
1	D	365	ILE
1	D	367	VAL
1	D	371	LEU
1	D	373	LEU
1	D	378	VAL
1	D	386	LEU
1	D	393	SER
1	D	397	LEU
1	D	405	SER
1	D	410	LEU
1	D	423	LYS
1	D	424	HIS
1	D	446	LYS
1	D	458	GLU
1	D	463	GLN
1	D	487	GLU
1	D	494	ASN
1	E	3	ARG
1	E	4	GLU
1	E	9	PHE
1	E	28	LEU
1	E	33	LYS
1	E	35	ARG
1	E	38	GLU
1	E	44	ARG
1	E	49	LEU
1	E	61	LEU
1	E	65	ILE
1	E	66	ARG
1	E	75	ILE
1	E	78	TYR
1	E	84	GLN

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Mol	Chain	Res	Type
1	E	93	ILE
1	E	96	SER
1	E	99	VAL
1	E	107	LEU
1	E	112	THR
1	E	145	THR
1	E	182	THR
1	E	203	ILE
1	E	212	ILE
1	E	239	THR
1	E	246	THR
1	E	249	VAL
1	E	255	VAL
1	E	272	THR
1	E	291	LEU
1	E	296	LEU
1	E	297	GLN
1	E	300	THR
1	E	306	LYS
1	E	311	GLU
1	E	313	SER
1	E	321	ILE
1	E	331	LEU
1	E	340	LYS
1	E	352	THR
1	E	361	LEU
1	E	364	ASN
1	E	365	ILE
1	E	367	VAL
1	E	371	LEU
1	E	373	LEU
1	E	378	VAL
1	E	386	LEU
1	E	392	VAL
1	E	393	SER
1	E	397	LEU
1	E	405	SER
1	E	410	LEU
1	E	423	LYS
1	E	424	HIS
1	E	446	LYS
1	E	458	GLU

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Mol	Chain	Res	Type
1	E	463	GLN
1	E	487	GLU
1	E	492	VAL
1	E	495	GLU
1	F	9	PHE
1	F	24	VAL
1	F	28	LEU
1	F	33	LYS
1	F	35	ARG
1	F	38	GLU
1	F	43	ASN
1	F	44	ARG
1	F	49	LEU
1	F	60	SER
1	F	65	ILE
1	F	66	ARG
1	F	75	ILE
1	F	78	TYR
1	F	84	GLN
1	F	93	ILE
1	F	96	SER
1	F	101	VAL
1	F	107	LEU
1	F	112	THR
1	F	145	THR
1	F	162	VAL
1	F	182	THR
1	F	203	ILE
1	F	212	ILE
1	F	217	ARG
1	F	239	THR
1	F	244	ASP
1	F	245	LYS
1	F	249	VAL
1	F	255	VAL
1	F	272	THR
1	F	291	LEU
1	F	296	LEU
1	F	297	GLN
1	F	306	LYS
1	F	311	GLU
1	F	321	ILE

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Mol	Chain	Res	Type
1	F	331	LEU
1	F	340	LYS
1	F	342	LYS
1	F	352	THR
1	F	361	LEU
1	F	364	ASN
1	F	365	ILE
1	F	367	VAL
1	F	368	ILE
1	F	371	LEU
1	F	373	LEU
1	F	378	VAL
1	F	386	LEU
1	F	392	VAL
1	F	393	SER
1	F	397	LEU
1	F	398	THR
1	F	400	LYS
1	F	410	LEU
1	F	424	HIS
1	F	446	LYS
1	F	458	GLU
1	F	487	GLU
1	F	495	GLU
1	F	498	VAL
1	F	500	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	82	HIS
1	A	84	GLN
1	A	139	ASN
1	A	258	HIS
1	A	388	ASN
1	A	406	ASN
1	A	494	ASN
1	B	82	HIS
1	B	84	GLN
1	B	258	HIS
1	B	388	ASN

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Mol	Chain	Res	Type
1	B	406	ASN
1	B	494	ASN
1	C	82	HIS
1	C	84	GLN
1	C	139	ASN
1	C	258	HIS
1	C	388	ASN
1	D	82	HIS
1	D	84	GLN
1	D	388	ASN
1	E	40	GLN
1	E	82	HIS
1	E	84	GLN
1	E	258	HIS
1	E	297	GLN
1	E	388	ASN
1	E	406	ASN
1	E	494	ASN
1	F	40	GLN
1	F	82	HIS
1	F	84	GLN
1	F	139	ASN
1	F	258	HIS
1	F	264	HIS
1	F	388	ASN
1	F	406	ASN
1	F	494	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 30 ligands modelled in this entry, 12 are monoatomic - leaving 18 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	502	-	9,9,9	0.94	0	11,11,11	1.34	1 (9%)
4	GTP	A	503	5	34,34,34	1.28	4 (11%)	51,54,54	2.04	10 (19%)
3	NDP	A	552	-	52,52,52	1.36	5 (9%)	80,80,80	1.67	12 (15%)
2	GLU	B	502	-	9,9,9	0.93	0	11,11,11	1.05	1 (9%)
4	GTP	B	503	5	34,34,34	1.11	1 (2%)	51,54,54	1.80	13 (25%)
3	NDP	B	552	-	52,52,52	1.38	5 (9%)	80,80,80	1.69	9 (11%)
2	GLU	C	502	-	9,9,9	0.97	1 (11%)	11,11,11	1.22	1 (9%)
4	GTP	C	503	5	34,34,34	0.98	1 (2%)	51,54,54	1.86	7 (13%)
3	NDP	C	552	-	52,52,52	1.41	5 (9%)	80,80,80	1.56	7 (8%)
2	GLU	D	502	-	9,9,9	0.89	0	11,11,11	0.94	0
4	GTP	D	503	5	34,34,34	0.98	1 (2%)	51,54,54	1.53	8 (15%)
3	NDP	D	552	-	52,52,52	1.36	5 (9%)	80,80,80	1.80	12 (15%)
2	GLU	E	502	-	9,9,9	0.92	0	11,11,11	1.09	1 (9%)
4	GTP	E	503	5	34,34,34	0.99	1 (2%)	51,54,54	1.53	9 (17%)
3	NDP	E	552	-	52,52,52	1.44	5 (9%)	80,80,80	1.73	10 (12%)
2	GLU	F	502	-	9,9,9	0.91	0	11,11,11	1.31	1 (9%)
4	GTP	F	503	5	34,34,34	0.98	1 (2%)	51,54,54	1.72	11 (21%)
3	NDP	F	552	-	52,52,52	1.39	4 (7%)	80,80,80	1.61	9 (11%)

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	502	-	-	0/9/9/9	0/0/0/0
4	GTP	A	503	5	-	0/22/38/38	0/1/3/3
3	NDP	A	552	-	-	0/35/77/77	0/3/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	B	502	-	-	0/9/9/9	0/0/0/0
4	GTP	B	503	5	-	0/22/38/38	0/1/3/3
3	NDP	B	552	-	-	0/35/77/77	0/3/5/5
2	GLU	C	502	-	-	0/9/9/9	0/0/0/0
4	GTP	C	503	5	-	0/22/38/38	0/1/3/3
3	NDP	C	552	-	-	0/35/77/77	0/3/5/5
2	GLU	D	502	-	-	0/9/9/9	0/0/0/0
4	GTP	D	503	5	-	0/22/38/38	0/1/3/3
3	NDP	D	552	-	-	0/35/77/77	0/3/5/5
2	GLU	E	502	-	-	0/9/9/9	0/0/0/0
4	GTP	E	503	5	-	0/22/38/38	0/1/3/3
3	NDP	E	552	-	-	0/35/77/77	0/3/5/5
2	GLU	F	502	-	-	0/9/9/9	0/0/0/0
4	GTP	F	503	5	-	0/22/38/38	0/1/3/3
3	NDP	F	552	-	-	0/35/77/77	0/3/5/5

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	552	NDP	O7N-C7N	6.77	1.42	1.24
3	E	552	NDP	O7N-C7N	6.67	1.41	1.24
3	C	552	NDP	O7N-C7N	6.55	1.41	1.24
3	D	552	NDP	O7N-C7N	6.32	1.41	1.24
3	A	552	NDP	O7N-C7N	6.22	1.40	1.24
3	F	552	NDP	O7N-C7N	6.09	1.40	1.24
4	C	503	GTP	C2-N3	3.61	1.38	1.33
3	F	552	NDP	C2A-N3A	3.33	1.38	1.32
3	C	552	NDP	C2A-N3A	3.30	1.38	1.32
3	C	552	NDP	C6N-C5N	3.28	1.40	1.33
4	B	503	GTP	C2-N3	3.23	1.37	1.33
4	A	503	GTP	C2-N3	3.22	1.37	1.33
3	E	552	NDP	C2N-C3N	3.20	1.41	1.34
3	D	552	NDP	C2A-N3A	3.13	1.38	1.32
3	E	552	NDP	C2A-N3A	3.08	1.38	1.32
3	A	552	NDP	C2N-C3N	3.07	1.40	1.34
4	D	503	GTP	C2-N3	3.01	1.37	1.33
4	F	503	GTP	C2-N3	2.96	1.37	1.33
3	A	552	NDP	C6N-C5N	2.96	1.39	1.33
3	F	552	NDP	C2N-C3N	2.93	1.40	1.34
3	A	552	NDP	C2A-N3A	2.90	1.37	1.32
3	F	552	NDP	C6N-C5N	2.83	1.39	1.33
3	B	552	NDP	C2A-N3A	2.81	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	552	NDP	C2N-C3N	2.78	1.40	1.34
4	E	503	GTP	C2-N3	2.75	1.37	1.33
3	D	552	NDP	C6N-C5N	2.61	1.38	1.33
3	C	552	NDP	C2N-C3N	2.59	1.39	1.34
3	D	552	NDP	C2N-C3N	2.58	1.39	1.34
3	E	552	NDP	C2A-N1A	2.54	1.38	1.33
3	E	552	NDP	C6N-C5N	2.52	1.38	1.33
3	B	552	NDP	C6N-C5N	2.52	1.38	1.33
4	A	503	GTP	O4'-C4'	-2.24	1.39	1.45
3	D	552	NDP	C2A-N1A	2.23	1.38	1.33
3	A	552	NDP	C2A-N1A	2.16	1.38	1.33
4	A	503	GTP	C6-C5	-2.13	1.37	1.41
4	A	503	GTP	C2-N1	2.14	1.40	1.36
3	C	552	NDP	C2A-N1A	2.13	1.38	1.33
2	C	502	GLU	OXT-C	-2.10	1.22	1.30
3	B	552	NDP	C2A-N1A	2.08	1.38	1.33

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	552	NDP	N3A-C2A-N1A	-10.89	119.61	128.71
3	E	552	NDP	N3A-C2A-N1A	-10.51	119.92	128.71
3	D	552	NDP	N3A-C2A-N1A	-10.18	120.20	128.71
3	F	552	NDP	N3A-C2A-N1A	-9.96	120.39	128.71
3	C	552	NDP	N3A-C2A-N1A	-9.85	120.47	128.71
4	A	503	GTP	C6-C5-N7	-9.71	132.83	134.14
3	A	552	NDP	N3A-C2A-N1A	-9.51	120.76	128.71
4	C	503	GTP	C6-C5-N7	-8.87	132.94	134.14
4	F	503	GTP	O4'-C1'-N9	5.52	113.58	108.44
4	A	503	GTP	N2-C2-N1	5.34	123.74	117.86
4	D	503	GTP	PB-O3B-PG	-4.62	118.12	131.68
4	B	503	GTP	C6-C5-N7	-4.62	133.52	134.14
3	A	552	NDP	PN-O3-PA	-4.52	118.44	131.68
3	D	552	NDP	O4B-C1B-N9A	4.49	112.62	108.44
3	D	552	NDP	PN-O3-PA	-4.23	119.27	131.68
4	C	503	GTP	PB-O3B-PG	-4.23	119.29	131.68
4	E	503	GTP	N2-C2-N1	4.16	122.43	117.86
4	F	503	GTP	C6-C5-N7	-4.15	133.58	134.14
3	A	552	NDP	N3A-C4A-N9A	3.99	132.63	125.43
4	B	503	GTP	N2-C2-N1	3.94	122.19	117.86
4	B	503	GTP	PB-O3B-PG	-3.90	120.23	131.68
3	B	552	NDP	N3A-C4A-N9A	3.87	132.42	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	GTP	O3A-PB-O3B	3.87	109.53	101.66
3	D	552	NDP	N3A-C4A-N9A	3.86	132.40	125.43
3	E	552	NDP	N3A-C4A-N9A	3.84	132.36	125.43
3	C	552	NDP	N3A-C4A-N9A	3.81	132.32	125.43
3	F	552	NDP	N3A-C4A-N9A	3.65	132.02	125.43
4	E	503	GTP	PB-O3B-PG	-3.64	121.01	131.68
3	E	552	NDP	O4B-C1B-C2B	-3.55	103.63	106.95
4	B	503	GTP	C2-N3-C4	3.54	120.06	115.09
3	E	552	NDP	PN-O3-PA	-3.51	121.39	131.68
4	D	503	GTP	C2-N3-C4	3.42	119.89	115.09
4	A	503	GTP	C1'-N9-C4	-3.34	120.87	126.64
4	D	503	GTP	C5-C4-N3	-3.27	121.20	125.94
3	B	552	NDP	PN-O3-PA	-3.26	122.13	131.68
4	C	503	GTP	C2-N3-C4	3.23	119.62	115.09
4	E	503	GTP	C1'-N9-C4	-3.20	121.10	126.64
4	D	503	GTP	C4-C5-N7	-3.18	106.80	109.52
3	F	552	NDP	O4B-C1B-N9A	3.18	111.39	108.44
4	C	503	GTP	C5-C4-N3	-3.18	121.34	125.94
3	F	552	NDP	O4B-C1B-C2B	-3.15	104.00	106.95
4	A	503	GTP	PB-O3B-PG	-3.15	122.45	131.68
2	A	502	GLU	OXT-C-O	-3.14	116.96	124.07
4	F	503	GTP	PB-O3B-PG	-3.09	122.61	131.68
4	F	503	GTP	C2-N3-C4	3.04	119.36	115.09
4	D	503	GTP	N2-C2-N1	3.01	121.17	117.86
4	C	503	GTP	N3-C4-N9	3.00	131.32	126.91
2	F	502	GLU	OXT-C-O	-2.98	117.33	124.07
4	A	503	GTP	C2-N3-C4	2.97	119.27	115.09
4	E	503	GTP	O4'-C1'-N9	2.97	111.20	108.44
4	E	503	GTP	C2-N3-C4	2.97	119.26	115.09
4	F	503	GTP	PA-O3A-PB	-2.95	123.03	131.68
4	F	503	GTP	O3'-C3'-C2'	-2.88	102.47	111.83
4	F	503	GTP	C5-C4-N3	-2.83	121.84	125.94
3	B	552	NDP	O4B-C1B-C2B	-2.83	104.30	106.95
4	E	503	GTP	C4-C5-N7	-2.81	107.11	109.52
3	A	552	NDP	C4A-C5A-N7A	-2.79	107.13	109.52
3	C	552	NDP	C5A-C4A-N3A	-2.76	119.69	125.70
4	D	503	GTP	O3A-PB-O3B	2.75	107.26	101.66
4	B	503	GTP	C5-C4-N3	-2.74	121.97	125.94
3	E	552	NDP	P2B-O2B-C2B	-2.74	116.19	121.96
4	F	503	GTP	C2'-C1'-N9	-2.71	106.32	113.27
3	D	552	NDP	C5A-C4A-N3A	-2.70	119.83	125.70
3	F	552	NDP	C5A-C4A-N3A	-2.67	119.88	125.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	552	NDP	C1D-N1N-C6N	-2.67	114.88	120.79
3	A	552	NDP	C5A-C4A-N3A	-2.64	119.94	125.70
3	D	552	NDP	C4A-C5A-N7A	-2.64	107.26	109.52
3	E	552	NDP	C1D-N1N-C6N	-2.63	114.97	120.79
3	E	552	NDP	C4A-C5A-N7A	-2.61	107.28	109.52
4	B	503	GTP	C1'-N9-C4	-2.60	122.15	126.64
4	F	503	GTP	N3-C4-N9	2.59	130.71	126.91
3	F	552	NDP	C4A-C5A-N7A	-2.57	107.32	109.52
3	E	552	NDP	C5A-C4A-N3A	-2.57	120.11	125.70
4	B	503	GTP	N7-C8-N9	-2.56	107.12	114.36
2	C	502	GLU	OXT-C-O	-2.55	118.30	124.07
3	B	552	NDP	O4B-C1B-N9A	2.55	110.81	108.44
4	B	503	GTP	C4-C5-N7	-2.52	107.36	109.52
3	D	552	NDP	C3N-C7N-N7N	-2.51	112.66	117.48
3	D	552	NDP	C3N-C2N-N1N	-2.50	119.50	123.05
2	B	502	GLU	OXT-C-O	-2.47	118.48	124.07
3	C	552	NDP	PN-O3-PA	-2.46	124.48	131.68
3	B	552	NDP	C1D-N1N-C6N	-2.41	115.45	120.79
4	D	503	GTP	N3-C4-N9	2.39	130.42	126.91
2	E	502	GLU	OXT-C-O	-2.38	118.69	124.07
3	A	552	NDP	O4B-C1B-N9A	2.37	110.64	108.44
3	E	552	NDP	C2A-N3A-C4A	2.36	120.74	114.01
4	C	503	GTP	N7-C8-N9	-2.36	107.68	114.36
3	F	552	NDP	C2A-N3A-C4A	2.35	120.70	114.01
4	B	503	GTP	N3-C4-N9	2.34	130.34	126.91
3	D	552	NDP	C4N-C3N-C7N	-2.33	112.03	118.38
4	F	503	GTP	N2-C2-N1	2.33	120.42	117.86
3	F	552	NDP	PN-O3-PA	-2.33	124.86	131.68
3	D	552	NDP	C2A-N3A-C4A	2.32	120.61	114.01
3	A	552	NDP	C2A-N3A-C4A	2.30	120.56	114.01
3	B	552	NDP	C5A-C4A-N3A	-2.30	120.69	125.70
4	E	503	GTP	N7-C8-N9	-2.29	107.88	114.36
3	D	552	NDP	C4N-C3N-C2N	2.28	124.47	121.68
3	C	552	NDP	C2B-C3B-C4B	2.28	107.36	101.94
3	C	552	NDP	C2A-N3A-C4A	2.25	120.42	114.01
4	A	503	GTP	N7-C8-N9	-2.25	108.00	114.36
3	B	552	NDP	N7A-C8A-N9A	-2.25	108.00	114.36
4	A	503	GTP	O3A-PB-O3B	2.24	106.21	101.66
4	B	503	GTP	O5'-PA-O1A	-2.23	100.62	109.37
4	A	503	GTP	N2-C2-N3	-2.23	117.28	120.30
3	B	552	NDP	C2A-N3A-C4A	2.23	120.35	114.01
4	E	503	GTP	C8-N9-C1'	2.23	130.77	126.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	GTP	C4-C5-N7	-2.22	107.62	109.52
4	D	503	GTP	N7-C8-N9	-2.20	108.13	114.36
4	A	503	GTP	C8-N9-C4	2.20	108.58	106.90
4	B	503	GTP	C8-N9-C4	2.19	108.57	106.90
3	A	552	NDP	O4B-C1B-C2B	-2.16	104.92	106.95
3	E	552	NDP	N7A-C8A-N9A	-2.16	108.24	114.36
4	E	503	GTP	C5-C4-N3	-2.16	122.82	125.94
4	F	503	GTP	N7-C8-N9	-2.16	108.26	114.36
3	D	552	NDP	N7A-C8A-N9A	-2.12	108.36	114.36
4	A	503	GTP	C8-N9-C1'	2.11	130.54	126.38
3	A	552	NDP	O4D-C1D-N1N	2.11	112.52	108.05
3	A	552	NDP	P2B-O2B-C2B	-2.10	117.54	121.96
3	C	552	NDP	C4A-C5A-N7A	-2.10	107.73	109.52
4	B	503	GTP	O3'-C3'-C4'	-2.05	105.05	111.08
3	F	552	NDP	N7A-C8A-N9A	-2.02	108.65	114.36
3	A	552	NDP	C3N-C2N-N1N	-2.01	120.19	123.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	495/501 (98%)	0.06	20 (4%)	36	45	15, 32, 68, 127	0
1	B	495/501 (98%)	0.17	22 (4%)	33	41	17, 34, 71, 128	0
1	C	495/501 (98%)	0.32	40 (8%)	12	15	18, 38, 71, 129	0
1	D	495/501 (98%)	0.20	32 (6%)	18	24	15, 32, 71, 131	0
1	E	495/501 (98%)	0.09	25 (5%)	27	34	16, 32, 71, 126	0
1	F	501/501 (100%)	-0.02	22 (4%)	33	41	14, 29, 73, 130	0
All	All	2976/3006 (99%)	0.14	161 (5%)	25	32	14, 32, 72, 131	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	424	HIS	9.5
1	B	2	ASP	8.0
1	F	498	VAL	7.4
1	A	1	ALA	7.3
1	C	3	ARG	6.8
1	E	424	HIS	6.7
1	F	424	HIS	6.4
1	C	424	HIS	6.0
1	C	230	ALA	5.8
1	B	425	GLY	5.7
1	E	425	GLY	5.5
1	A	3	ARG	5.5
1	B	1	ALA	5.2
1	C	33	LYS	5.2
1	C	4	GLU	5.1
1	F	425	GLY	5.1
1	A	424	HIS	5.0
1	D	1	ALA	4.9
1	E	1	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	32	LEU	4.8
1	E	72	TRP	4.8
1	B	39	GLU	4.7
1	F	429	PRO	4.5
1	D	235	ILE	4.4
1	A	2	ASP	4.4
1	D	248	VAL	4.4
1	F	496	ALA	4.4
1	F	497	GLY	4.4
1	C	35	ARG	4.4
1	F	500	PHE	4.3
1	A	35	ARG	4.2
1	C	428	ILE	4.2
1	D	309	ILE	4.2
1	F	499	THR	4.1
1	B	3	ARG	4.1
1	E	3	ARG	4.1
1	D	424	HIS	4.1
1	C	34	THR	3.9
1	C	44	ARG	3.8
1	C	36	GLU	3.8
1	B	33	LYS	3.7
1	D	281	TRP	3.7
1	D	36	GLU	3.7
1	C	1	ALA	3.6
1	D	236	LEU	3.6
1	D	266	PHE	3.6
1	A	21	ALA	3.5
1	F	430	ILE	3.5
1	C	426	GLY	3.5
1	E	36	GLU	3.5
1	C	311	GLU	3.5
1	F	1	ALA	3.4
1	C	334	SER	3.4
1	C	302	LEU	3.4
1	F	36	GLU	3.4
1	A	33	LYS	3.4
1	D	317	VAL	3.3
1	C	40	GLN	3.3
1	B	312	GLY	3.3
1	D	2	ASP	3.3
1	B	35	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	36	GLU	3.2
1	B	44	ARG	3.2
1	D	270	CYS	3.2
1	E	428	ILE	3.2
1	B	298	HIS	3.1
1	C	339	VAL	3.1
1	B	297	GLN	3.1
1	E	71	SER	3.0
1	B	36	GLU	3.0
1	E	426	GLY	3.0
1	D	416	SER	2.9
1	F	29	VAL	2.9
1	C	232	TYR	2.9
1	C	72	TRP	2.9
1	B	417	LEU	2.9
1	D	246	THR	2.9
1	E	272	THR	2.9
1	A	417	LEU	2.8
1	F	501	THR	2.8
1	A	44	ARG	2.7
1	F	428	ILE	2.7
1	D	35	ARG	2.7
1	C	25	GLU	2.7
1	C	364	ASN	2.7
1	A	47	SER	2.7
1	D	339	VAL	2.7
1	E	2	ASP	2.6
1	B	43	ASN	2.6
1	B	296	LEU	2.6
1	F	32	LEU	2.6
1	C	365	ILE	2.6
1	E	407	TYR	2.6
1	C	31	ASP	2.5
1	D	426	GLY	2.5
1	E	427	THR	2.5
1	C	329	LYS	2.5
1	D	72	TRP	2.5
1	C	272	THR	2.5
1	E	37	THR	2.5
1	F	31	ASP	2.5
1	D	39	GLU	2.5
1	B	421	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	431	VAL	2.4
1	D	31	ASP	2.4
1	F	421	PHE	2.4
1	A	19	ARG	2.4
1	E	47	SER	2.4
1	C	66	ARG	2.4
1	F	417	LEU	2.4
1	D	272	THR	2.4
1	C	303	GLY	2.4
1	A	415	GLU	2.4
1	E	412	SER	2.3
1	C	2	ASP	2.3
1	E	35	ARG	2.3
1	F	44	ARG	2.3
1	A	34	THR	2.3
1	C	5	ASP	2.3
1	C	304	PHE	2.3
1	A	28	LEU	2.3
1	A	30	GLU	2.3
1	D	310	TYR	2.3
1	C	430	ILE	2.3
1	D	341	ALA	2.3
1	E	242	PHE	2.3
1	D	40	GLN	2.2
1	B	45	VAL	2.2
1	F	34	THR	2.2
1	E	66	ARG	2.2
1	C	285	GLY	2.2
1	D	247	PHE	2.2
1	C	494	ASN	2.2
1	F	47	SER	2.2
1	A	41	LYS	2.2
1	B	41	LYS	2.2
1	E	4	GLU	2.1
1	C	296	LEU	2.1
1	E	141	LEU	2.1
1	C	367	VAL	2.1
1	E	409	LEU	2.1
1	D	279	SER	2.1
1	D	3	ARG	2.1
1	B	431	VAL	2.1
1	E	32	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	19	ARG	2.1
1	C	243	GLY	2.1
1	C	465	MET	2.0
1	C	268	ALA	2.0
1	E	271	ILE	2.0
1	B	308	LYS	2.0
1	D	308	LYS	2.0
1	F	248	VAL	2.0
1	D	285	GLY	2.0
1	D	321	ILE	2.0
1	A	4	GLU	2.0
1	B	426	GLY	2.0
1	C	425	GLY	2.0
1	A	411	MET	2.0
1	A	294	PHE	2.0
1	D	342	LYS	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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GLU	F	502	10/10	0.18	1.06	19,20,26,26	0
5	ZN	C	506	1/1	0.20	0.70	46,46,46,46	0
2	GLU	A	502	10/10	0.18	0.63	19,26,31,31	0
2	GLU	D	502	10/10	0.19	0.48	20,24,26,33	0
5	ZN	F	504	1/1	0.18	0.37	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLU	B	502	10/10	0.17	0.32	22,26,31,31	0
5	ZN	B	505	1/1	0.18	0.09	43,43,43,43	0
2	GLU	E	502	10/10	0.15	-0.05	20,29,33,35	0
5	ZN	D	505	1/1	0.16	-0.11	42,42,42,42	0
3	NDP	A	552	48/48	0.15	-0.24	18,27,36,44	0
2	GLU	C	502	10/10	0.14	-0.39	25,31,33,34	0
3	NDP	D	552	48/48	0.15	-0.43	17,27,38,46	0
3	NDP	F	552	48/48	0.14	-0.62	14,21,32,35	0
4	GTP	D	503	32/32	0.15	-0.63	19,33,40,42	0
3	NDP	C	552	48/48	0.15	-0.75	23,39,55,60	0
3	NDP	B	552	48/48	0.13	-0.87	24,32,39,42	0
4	GTP	E	503	32/32	0.14	-0.92	16,27,33,38	0
3	NDP	E	552	48/48	0.14	-0.93	22,30,44,54	0
4	GTP	A	503	32/32	0.14	-1.11	24,34,37,44	0
4	GTP	C	503	32/32	0.14	-1.37	27,41,51,62	0
4	GTP	B	503	32/32	0.12	-1.48	24,36,43,48	0
4	GTP	F	503	32/32	0.11	-1.85	18,23,35,45	0
5	ZN	A	504	1/1	0.08	-2.50	58,58,58,58	0
5	ZN	E	505	1/1	0.12	-2.82	37,37,37,37	0
5	ZN	D	504	1/1	0.07	-3.16	65,65,65,65	0
5	ZN	C	504	1/1	0.05	-3.45	63,63,63,63	0
5	ZN	B	504	1/1	0.05	-3.83	64,64,64,64	0
5	ZN	A	505	1/1	0.09	-4.25	31,31,31,31	0
5	ZN	E	504	1/1	0.05	-4.61	50,50,50,50	0
5	ZN	C	505	1/1	0.04	-4.69	55,55,55,55	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.