



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 21, 2016 – 10:22 PM EDT

PDB ID : 5E9T  
Title : Crystal structure of GtfA/B complex  
Authors : Chen, Y.; Rapoport, T.A.  
Deposited on : 2015-10-15  
Resolution : 2.92 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

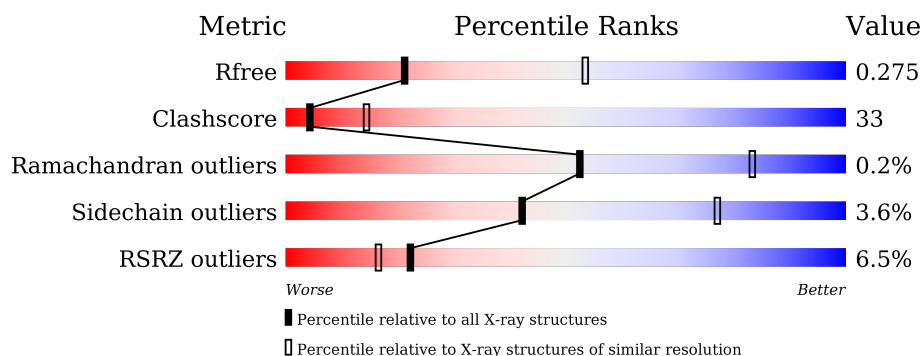
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.92 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	503	<div> <div>5%</div> <div> <div></div> <div>60%</div> <div>36%</div> <div>..</div> </div> </div>
1	C	503	<div> <div>7%</div> <div> <div></div> <div>55%</div> <div>40%</div> <div>5%</div> </div> </div>
2	B	447	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>44%</div> <div>.</div> </div> </div>
2	D	447	<div> <div>9%</div> <div> <div></div> <div>50%</div> <div>45%</div> <div>5%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15474 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Glycosyltransferase Gtf1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	Se	0	0	0
			4108	2624	687	789	2	6			
1	C	503	Total	C	N	O	S	Se	0	0	0
			4108	2624	687	789	2	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q9AET5
A	124	PHE	SER	engineered mutation	UNP Q9AET5
C	1	SER	-	expression tag	UNP Q9AET5
C	124	PHE	SER	engineered mutation	UNP Q9AET5

- Molecule 2 is a protein called Glycosyltransferase-stabilizing protein Gtf2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	447	Total	C	N	O	S	Se	0	0	0
			3615	2302	615	687	3	8			
2	D	445	Total	C	N	O	S	Se	0	0	0
			3607	2298	613	685	3	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MSE	-	initiating methionine	UNP Q79T00
D	1	MSE	-	initiating methionine	UNP Q79T00

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

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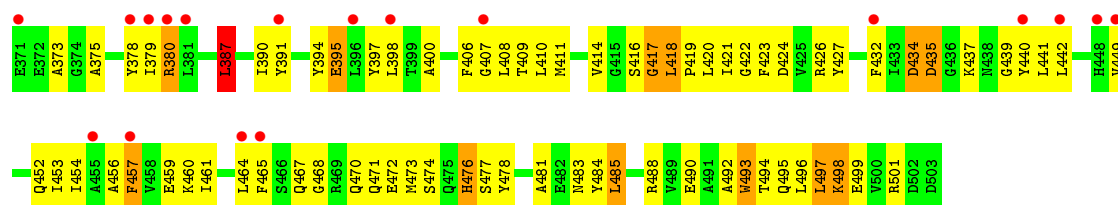
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

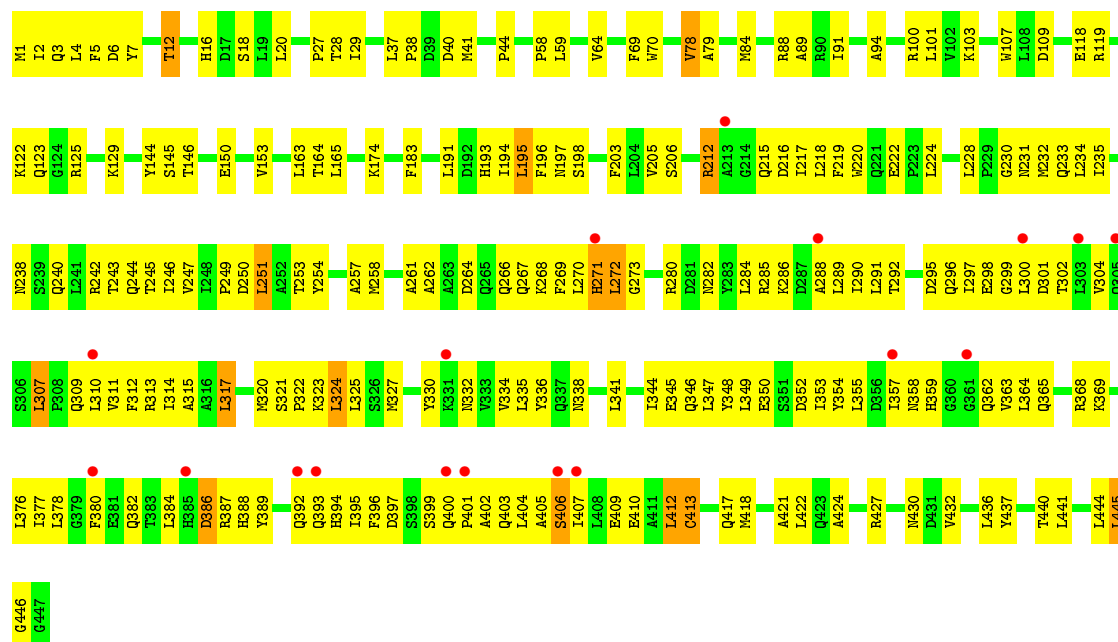
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	9	Total	O	0	0
			9	9		
4	C	8	Total	O	0	0
			8	8		
4	D	7	Total	O	0	0
			7	7		

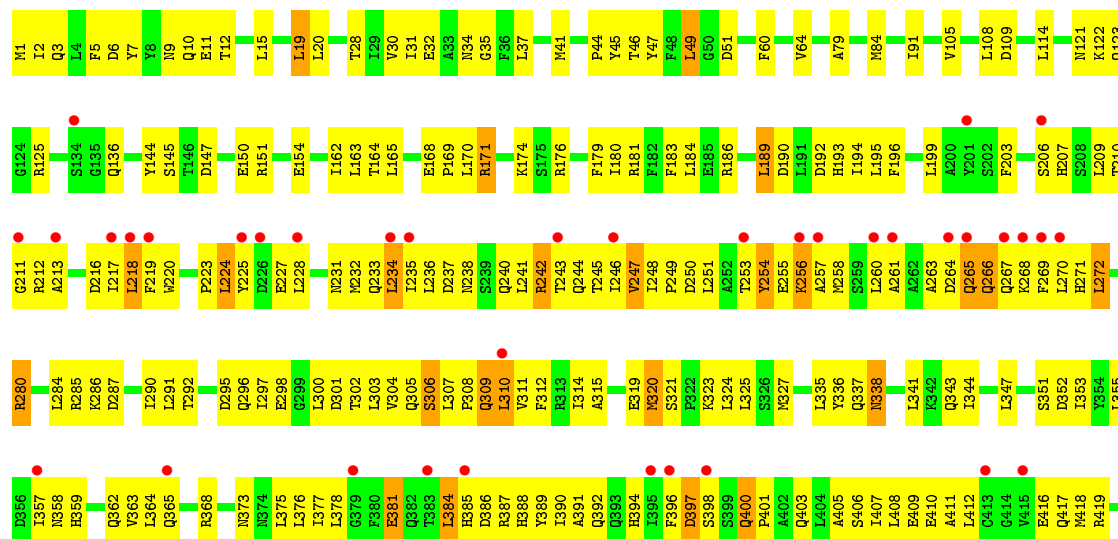


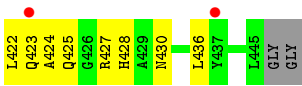


• Molecule 2: Glycosyltransferase-stabilizing protein Gtf2



• Molecule 2: Glycosyltransferase-stabilizing protein Gtf2





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.93Å 196.41Å 220.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.12 – 2.92 122.12 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.9 (122.12-2.92) 94.8 (122.12-2.62)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.95 (at 2.62Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.217 , 0.275 0.214 , 0.275	Depositor DCC
$R_{free}$ test set	3569 reflections (4.85%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 33.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 95954 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	15474	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.64	14/4196 (0.3%)	0.81	11/5678 (0.2%)
1	C	0.49	2/4196 (0.0%)	0.78	12/5678 (0.2%)
2	B	0.39	0/3686	0.67	8/4986 (0.2%)
2	D	0.54	5/3678 (0.1%)	0.87	19/4976 (0.4%)
All	All	0.53	21/15756 (0.1%)	0.79	50/21318 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	5
2	D	0	3
All	All	0	10

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	472	GLU	CD-OE1	-10.31	1.14	1.25
1	A	316	GLU	CD-OE2	-9.69	1.15	1.25
1	A	469	ARG	NE-CZ	-9.68	1.20	1.33
1	A	316	GLU	CD-OE1	-9.50	1.15	1.25
2	D	247	VAL	CB-CG1	-7.63	1.36	1.52
1	A	472	GLU	CD-OE2	-7.50	1.17	1.25
2	D	254	TYR	CE1-CZ	-7.27	1.29	1.38
1	A	469	ARG	CZ-NH1	-7.19	1.23	1.33
2	D	254	TYR	CD1-CE1	-7.08	1.28	1.39
1	A	363	GLU	CG-CD	-6.76	1.41	1.51
1	C	395	GLU	CG-CD	-6.53	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	ARG	CZ-NH2	-6.41	1.24	1.33
2	D	254	TYR	CB-CG	-6.23	1.42	1.51
1	A	484	TYR	CD2-CE2	6.18	1.48	1.39
2	D	256	LYS	CD-CE	-6.08	1.36	1.51
1	A	484	TYR	CZ-OH	6.05	1.48	1.37
1	C	418	LEU	N-CA	5.88	1.58	1.46
1	A	363	GLU	CD-OE2	-5.43	1.19	1.25
1	A	469	ARG	CD-NE	-5.42	1.37	1.46
1	A	472	GLU	CG-CD	-5.23	1.44	1.51
1	A	489	VAL	CB-CG2	-5.18	1.42	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	488	ARG	NE-CZ-NH2	25.97	133.29	120.30
1	C	329	LEU	CA-CB-CG	16.30	152.78	115.30
1	A	488	ARG	NE-CZ-NH1	-14.02	113.29	120.30
2	D	256	LYS	CD-CE-NZ	-12.70	82.49	111.70
1	C	364	ASP	CB-CG-OD2	-12.15	107.37	118.30
1	A	484	TYR	CD1-CE1-CZ	11.05	129.74	119.80
1	C	367	ARG	NE-CZ-NH1	-10.68	114.96	120.30
1	C	364	ASP	CB-CG-OD1	10.67	127.90	118.30
2	D	224	LEU	CB-CG-CD2	-8.29	96.90	111.00
2	D	254	TYR	CE1-CZ-OH	-8.13	98.14	120.10
2	D	254	TYR	OH-CZ-CE2	7.96	141.59	120.10
1	A	406	PHE	C-N-CA	-7.92	105.67	122.30
1	C	367	ARG	CD-NE-CZ	7.73	134.42	123.60
1	A	469	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	C	498	LYS	CD-CE-NZ	-7.48	94.49	111.70
2	B	195	LEU	CB-CG-CD1	-7.17	98.81	111.00
2	B	412	LEU	CA-CB-CG	7.09	131.61	115.30
1	A	484	TYR	CG-CD1-CE1	-6.88	115.79	121.30
2	D	218	LEU	CA-CB-CG	6.75	130.82	115.30
1	A	484	TYR	CB-CG-CD1	-6.75	116.95	121.00
2	B	445	LEU	CB-CG-CD1	-6.68	99.64	111.00
2	B	324	LEU	CB-CG-CD2	-6.49	99.98	111.00
2	D	320	MSE	CA-CB-CG	6.43	124.24	113.30
2	D	384	LEU	CB-CG-CD2	-6.42	100.09	111.00
2	D	218	LEU	CB-CG-CD2	6.38	121.84	111.00
1	C	366	LEU	CB-CG-CD2	-6.26	100.36	111.00
1	C	387	LEU	CA-CB-CG	6.21	129.59	115.30
1	A	382	LYS	CD-CE-NZ	-6.21	97.42	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	413	CYS	CA-CB-SG	6.21	125.17	114.00
2	B	251	LEU	CB-CG-CD2	-6.12	100.59	111.00
2	D	397	ASP	CB-CG-OD1	-6.05	112.85	118.30
1	C	497	LEU	CA-CB-CG	-6.00	101.51	115.30
2	D	224	LEU	CA-CB-CG	5.94	128.96	115.30
1	C	367	ARG	NH1-CZ-NH2	5.94	125.93	119.40
2	D	270	LEU	CA-CB-CG	5.87	128.79	115.30
1	A	398	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	488	ARG	NH1-CZ-NH2	-5.72	113.10	119.40
2	D	284	LEU	CB-CG-CD2	5.58	120.49	111.00
2	D	254	TYR	CA-CB-CG	-5.51	102.92	113.40
2	D	254	TYR	CD1-CE1-CZ	5.50	124.75	119.80
1	C	335	ILE	CG1-CB-CG2	-5.35	99.63	111.40
2	D	234	LEU	CB-CG-CD2	-5.30	101.98	111.00
1	A	315	LYS	C-N-CA	5.25	134.83	121.70
2	B	307	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	C	417	GLY	N-CA-C	5.19	126.07	113.10
2	B	272	LEU	CA-CB-CG	5.15	127.14	115.30
2	D	254	TYR	CZ-CE2-CD2	-5.12	115.19	119.80
2	D	19	LEU	CB-CG-CD2	-5.09	102.35	111.00
2	D	266	GLN	CA-CB-CG	-5.07	102.25	113.40
2	D	310	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	363	GLU	Peptide
1	A	466	SER	Peptide
1	C	108	GLN	Peptide
1	C	322	SER	Peptide
1	C	328	ARG	Peptide
1	C	380	ARG	Peptide
1	C	435	ASP	Peptide
2	D	265	GLN	Peptide
2	D	381	GLU	Peptide
2	D	400	GLN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4108	0	3965	240	0
1	C	4108	0	3965	271	0
2	B	3615	0	3535	210	0
2	D	3607	0	3529	306	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	0	0	0
4	B	9	0	0	0	0
4	C	8	0	0	0	0
4	D	7	0	0	1	0
All	All	15474	0	14994	1005	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (1005) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:307:LEU:HA	2:D:309:GLN:NE2	1.64	1.12
2:B:345:GLU:OE2	2:B:369:LYS:NZ	1.83	1.12
1:A:470:GLN:HE21	1:A:471:GLN:HG3	1.06	1.12
2:D:307:LEU:HA	2:D:309:GLN:HE21	1.13	1.09
2:B:272:LEU:HD13	2:B:273:GLY:H	0.92	1.07
2:D:2:ILE:HG21	2:D:189:LEU:HD12	1.36	1.07
1:A:438:ASN:HB3	1:A:476:HIS:HB3	1.35	1.06
2:B:216:ASP:HB2	2:B:243:THR:HG22	1.35	1.05
2:B:320:MSE:HB3	2:B:324:LEU:HD21	1.37	1.03
2:D:169:PRO:O	2:D:171:ARG:NH1	1.91	1.03
1:A:363:GLU:HB2	1:A:366:LEU:HB2	1.35	1.02
1:A:470:GLN:NE2	1:A:471:GLN:HG3	1.74	1.01
2:D:297:ILE:HB	2:D:300:LEU:HD23	1.37	1.00
1:C:329:LEU:HA	1:C:333:LYS:HE3	1.42	0.99
1:A:467:GLN:NE2	1:A:469:ARG:HH12	1.60	0.99
2:B:272:LEU:HD13	2:B:273:GLY:N	1.78	0.98
1:C:494:THR:HG22	1:C:498:LYS:HZ1	1.26	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:272:LEU:CD1	2:B:273:GLY:H	1.76	0.97
2:B:16:HIS:NE2	2:B:40:ASP:OD2	1.97	0.96
1:A:449:VAL:HG13	1:A:452:GLN:NE2	1.82	0.95
1:C:417:GLY:HA2	1:C:478:TYR:HE1	1.31	0.95
1:A:304:PRO:HG3	1:A:488:ARG:NH2	1.82	0.94
2:D:307:LEU:CA	2:D:309:GLN:HE21	1.82	0.93
1:A:464:LEU:C	1:A:469:ARG:NH2	2.23	0.92
1:C:12:TRP:NE1	1:C:46:ASP:OD1	2.02	0.91
1:A:464:LEU:CA	1:A:469:ARG:HH21	1.84	0.89
1:C:328:ARG:HH22	1:C:359:LYS:H	1.19	0.89
2:B:258:MSE:O	2:B:266:GLN:NE2	2.05	0.89
2:D:272:LEU:HD23	2:D:436:LEU:HD22	1.50	0.89
2:B:193:HIS:NE2	2:B:446:GLY:O	2.06	0.88
1:C:328:ARG:NH2	1:C:359:LYS:O	2.06	0.88
1:C:437:LYS:HZ3	1:C:476:HIS:CG	1.90	0.88
2:B:251:LEU:HD21	2:B:271:HIS:CE1	2.09	0.88
1:C:85:LEU:HD11	1:C:104:TYR:HE2	1.39	0.87
2:B:362:GLN:HE21	2:B:365:GLN:HA	1.38	0.87
1:C:335:ILE:HA	1:C:338:LEU:HD23	1.54	0.87
1:C:494:THR:HG22	1:C:498:LYS:NZ	1.89	0.86
1:A:369:ARG:O	1:A:369:ARG:NE	2.08	0.86
1:A:369:ARG:HH12	1:A:373:ALA:CB	1.89	0.86
2:B:270:LEU:HD21	2:B:440:THR:CG2	2.05	0.86
2:B:1:MSE:HE3	2:B:445:LEU:HD11	1.56	0.86
2:D:220:TRP:HE1	2:D:224:LEU:HD21	1.41	0.85
1:A:369:ARG:HH12	1:A:373:ALA:HB3	1.42	0.85
2:D:11:GLU:OE2	2:D:388:HIS:HE1	1.60	0.85
1:C:417:GLY:HA2	1:C:478:TYR:CE1	2.12	0.84
2:D:125:ARG:NH2	2:D:144:TYR:O	2.10	0.84
2:D:362:GLN:HB3	2:D:384:LEU:HD21	1.59	0.84
1:A:359:LYS:NZ	1:A:384:HIS:H	1.75	0.84
2:B:376:LEU:HB2	2:B:422:LEU:HD21	1.59	0.84
2:B:285:ARG:NH2	2:B:349:LEU:O	2.11	0.83
1:C:335:ILE:HD11	1:C:366:LEU:HD21	1.61	0.83
1:A:449:VAL:O	1:A:452:GLN:NE2	2.12	0.83
2:D:2:ILE:HG21	2:D:189:LEU:CD1	2.09	0.83
2:D:145:SER:OG	2:D:147:ASP:OD2	1.95	0.83
2:D:220:TRP:NE1	2:D:224:LEU:HD21	1.94	0.82
1:A:462:ILE:O	1:A:466:SER:N	2.10	0.82
1:A:464:LEU:CA	1:A:469:ARG:NH2	2.42	0.82
1:C:349:LEU:HB3	1:C:352:LEU:HD13	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LYS:NZ	1:A:384:HIS:O	2.12	0.81
1:C:26:GLN:HA	1:C:29:ARG:NH1	1.95	0.81
2:D:353:ILE:HG22	2:D:376:LEU:HB3	1.62	0.81
1:A:295:ASP:OD2	1:A:297:GLN:NE2	2.13	0.81
2:B:380:PHE:HD2	2:B:396:PHE:HB2	1.44	0.81
1:C:23:TYR:OH	1:C:307:SER:HB2	1.81	0.81
2:D:168:GLU:OE1	2:D:171:ARG:NH2	2.14	0.81
1:C:108:GLN:CD	1:C:109:ASP:H	1.85	0.80
1:C:338:LEU:HD21	1:C:400:ALA:HB2	1.63	0.80
1:C:219:ASP:OD2	1:C:240:VAL:HG21	1.80	0.80
1:C:338:LEU:HD12	1:C:398:LEU:HB3	1.64	0.80
2:D:2:ILE:CG2	2:D:189:LEU:HD12	2.10	0.80
1:C:494:THR:CG2	1:C:498:LYS:HZ1	1.94	0.80
1:C:18:GLU:N	1:C:18:GLU:OE2	2.13	0.80
2:D:272:LEU:CD2	2:D:436:LEU:HD22	2.10	0.80
2:B:436:LEU:O	2:B:440:THR:OG1	1.99	0.79
2:D:376:LEU:HG	2:D:418:MSE:HE1	1.64	0.79
1:C:437:LYS:NZ	1:C:476:HIS:CG	2.51	0.79
1:A:334:HIS:CE1	1:A:337:TRP:CZ2	2.72	0.79
1:A:440:TYR:CD1	1:A:460:LYS:HD2	2.17	0.78
2:D:290:ILE:HD11	2:D:355:LEU:HB2	1.63	0.78
2:B:1:MSE:HE2	2:B:195:LEU:HD11	1.65	0.78
1:C:252:SER:O	1:C:293:TYR:OH	2.01	0.78
2:D:251:LEU:H	2:D:430:ASN:HD21	1.30	0.78
1:A:359:LYS:HZ2	1:A:384:HIS:N	1.82	0.78
2:B:100:ARG:NH1	1:C:257:LEU:HD11	1.99	0.78
1:C:453:ILE:HD12	1:C:454:ILE:N	1.98	0.78
2:D:184:LEU:HA	2:D:189:LEU:HD21	1.64	0.77
1:A:338:LEU:HD12	1:A:338:LEU:H	1.47	0.77
1:A:30:ARG:NH1	1:A:486:THR:HG21	1.98	0.77
2:B:291:LEU:O	2:B:358:ASN:ND2	2.18	0.77
2:B:310:LEU:HB3	2:B:312:PHE:HE2	1.49	0.77
1:A:338:LEU:HD11	1:A:400:ALA:HB2	1.67	0.77
1:A:463:ALA:C	1:A:469:ARG:HH21	1.88	0.77
1:A:465:PHE:N	1:A:469:ARG:NH2	2.33	0.77
2:B:321:SER:O	2:B:324:LEU:HD23	1.85	0.77
2:D:307:LEU:CD1	2:D:310:LEU:HD22	2.14	0.77
2:D:381:GLU:HB3	2:D:398:SER:HB2	1.66	0.76
2:D:244:GLN:O	2:D:268:LYS:HG2	1.83	0.76
1:A:466:SER:HA	1:A:467:GLN:HE21	1.51	0.76
1:C:453:ILE:HA	1:C:456:ALA:HB3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ASP:O	1:C:297:GLN:NE2	2.18	0.76
2:B:288:ALA:HB3	2:B:312:PHE:HA	1.68	0.75
1:C:354:LEU:O	1:C:380:ARG:HG2	1.86	0.75
1:C:395:GLU:O	1:C:419:PRO:HD2	1.86	0.75
2:D:300:LEU:HA	2:D:303:LEU:HD23	1.68	0.75
1:A:464:LEU:HA	1:A:469:ARG:HH21	1.52	0.74
1:A:30:ARG:HH12	1:A:486:THR:HG21	1.52	0.74
2:B:270:LEU:HD23	2:B:271:HIS:N	2.02	0.74
1:C:435:ASP:CG	1:C:441:LEU:H	1.89	0.74
2:D:297:ILE:CB	2:D:300:LEU:HD23	2.16	0.74
2:D:412:LEU:HD12	2:D:417:GLN:HB2	1.68	0.74
1:C:17:VAL:HG22	1:C:242:HIS:HD2	1.50	0.74
1:C:245:HIS:HE1	1:C:289:GLN:NE2	1.85	0.74
1:C:85:LEU:HD21	1:C:104:TYR:HD2	1.52	0.74
2:D:227:GLU:HA	2:D:260:LEU:HD13	1.67	0.74
1:A:473:MSE:O	1:A:476:HIS:N	2.20	0.74
1:A:342:THR:HG21	1:A:354:LEU:HD23	1.70	0.74
2:D:362:GLN:HB3	2:D:384:LEU:CD2	2.18	0.73
1:C:453:ILE:HD12	1:C:454:ILE:H	1.51	0.73
1:A:304:PRO:HG3	1:A:488:ARG:HH22	1.53	0.73
2:B:285:ARG:HG2	2:B:352:ASP:OD2	1.88	0.73
2:D:423:GLN:O	2:D:427:ARG:N	2.21	0.73
2:B:251:LEU:HD21	2:B:271:HIS:NE2	2.02	0.73
1:C:328:ARG:NH2	1:C:359:LYS:H	1.84	0.73
1:A:338:LEU:HD12	1:A:338:LEU:N	2.02	0.72
1:C:181:ASP:HB2	1:C:183:GLN:HE21	1.54	0.72
1:C:167:TYR:OH	2:D:150:GLU:OE2	2.01	0.72
2:D:263:ALA:O	2:D:266:GLN:HB2	1.88	0.72
1:A:94:ARG:HG3	1:A:105:PHE:HB2	1.72	0.72
2:B:397:ASP:HB2	2:B:401:PRO:HD3	1.69	0.72
2:D:362:GLN:NE2	2:D:365:GLN:HA	2.05	0.72
1:A:382:LYS:HD3	1:A:383:GLY:N	2.05	0.72
2:B:418:MSE:O	2:B:421:ALA:N	2.23	0.72
1:C:342:THR:HG21	1:C:354:LEU:HD23	1.70	0.71
1:C:414:VAL:HG12	1:C:481:ALA:HB2	1.73	0.71
2:B:251:LEU:H	2:B:430:ASN:HD21	1.37	0.71
1:C:496:LEU:HD12	1:C:499:GLU:OE1	1.89	0.71
2:D:412:LEU:HD12	2:D:417:GLN:CB	2.20	0.71
2:D:397:ASP:OD2	2:D:400:GLN:OE1	2.08	0.71
1:A:461:ILE:O	1:A:465:PHE:N	2.23	0.71
2:B:270:LEU:HD21	2:B:440:THR:HG21	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:LYS:H	1:C:498:LYS:HD2	1.56	0.70
2:B:362:GLN:NE2	2:B:365:GLN:HA	2.06	0.70
1:C:335:ILE:HD11	1:C:366:LEU:CD2	2.20	0.70
1:C:421:ILE:HD12	1:C:440:TYR:HB2	1.74	0.70
1:A:465:PHE:C	1:A:467:GLN:HE21	1.94	0.70
1:A:465:PHE:N	1:A:469:ARG:HH22	1.86	0.70
1:C:453:ILE:O	1:C:457:PHE:N	2.24	0.70
2:D:168:GLU:HB3	2:D:171:ARG:HH12	1.55	0.70
1:A:382:LYS:NZ	1:A:384:HIS:C	2.45	0.70
1:C:329:LEU:HD11	1:C:363:GLU:HB2	1.72	0.70
1:A:449:VAL:C	1:A:452:GLN:HE22	1.95	0.69
1:C:338:LEU:HD12	1:C:398:LEU:HD13	1.73	0.69
2:D:189:LEU:HD23	2:D:189:LEU:H	1.57	0.69
1:A:465:PHE:C	1:A:467:GLN:NE2	2.46	0.69
1:A:387:LEU:HA	1:A:390:ILE:HD13	1.75	0.69
2:D:397:ASP:CG	2:D:400:GLN:OE1	2.30	0.69
1:A:470:GLN:HE21	1:A:471:GLN:CG	1.95	0.69
2:B:100:ARG:HH11	1:C:257:LEU:HD11	1.57	0.69
2:B:359:HIS:HD2	2:B:382:GLN:HE21	1.40	0.69
2:D:401:PRO:HB2	2:D:403:GLN:OE1	1.91	0.69
2:B:376:LEU:HD11	2:B:394:HIS:CD2	2.28	0.69
1:C:397:TYR:HB3	1:C:420:LEU:CD1	2.23	0.69
2:B:4:LEU:CD2	2:B:205:VAL:HG21	2.23	0.69
1:C:321:TYR:N	1:C:395:GLU:OE1	2.26	0.69
2:D:295:ASP:OD1	2:D:321:SER:OG	2.11	0.69
1:C:437:LYS:NZ	1:C:476:HIS:CD2	2.61	0.68
2:D:287:ASP:HB2	2:D:351:SER:HA	1.76	0.68
1:A:464:LEU:HA	1:A:469:ARG:NH2	2.06	0.68
1:A:464:LEU:HD13	1:A:473:MSE:HE3	1.75	0.68
2:D:218:LEU:HD11	2:D:220:TRP:HB2	1.75	0.68
1:C:363:GLU:HG3	1:C:367:ARG:HE	1.58	0.68
2:D:286:LYS:HD2	2:D:310:LEU:HA	1.75	0.68
2:B:405:ALA:O	2:B:409:GLU:N	2.18	0.68
2:B:79:ALA:HB3	2:B:91:ILE:HB	1.74	0.68
1:C:492:ALA:HA	1:C:495:GLN:HB3	1.76	0.68
2:B:362:GLN:HA	2:B:384:LEU:HD23	1.74	0.68
2:D:412:LEU:CD1	2:D:417:GLN:HB2	2.24	0.68
1:A:485:LEU:O	1:A:488:ARG:HG3	1.94	0.68
2:D:292:THR:HA	2:D:358:ASN:HD22	1.57	0.68
2:B:320:MSE:CB	2:B:324:LEU:HD21	2.20	0.67
2:D:307:LEU:HD13	2:D:310:LEU:HD22	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:LYS:HZ3	1:C:476:HIS:C	1.97	0.67
1:C:495:GLN:HA	1:C:498:LYS:HZ2	1.59	0.67
2:D:295:ASP:OD2	2:D:323:LYS:HG2	1.92	0.67
2:B:338:ASN:O	1:C:249:ASN:ND2	2.24	0.67
2:B:399:SER:HA	2:B:402:ALA:HA	1.75	0.67
1:C:434:ASP:OD1	1:C:434:ASP:N	2.27	0.67
1:C:494:THR:C	1:C:498:LYS:HZ1	1.97	0.67
2:D:184:LEU:HD22	2:D:189:LEU:HD11	1.75	0.67
2:D:255:GLU:N	2:D:255:GLU:OE1	2.28	0.67
1:C:323:MSE:HB3	1:C:354:LEU:HA	1.75	0.67
2:B:322:PRO:HA	2:B:325:LEU:HB2	1.75	0.67
1:C:323:MSE:HB3	1:C:354:LEU:CA	2.25	0.67
2:D:45:TYR:O	2:D:49:LEU:HD11	1.95	0.67
1:C:180:GLU:O	1:C:183:GLN:HG3	1.95	0.66
2:B:407:ILE:HA	2:B:410:GLU:HB2	1.77	0.66
1:C:364:ASP:O	1:C:368:ARG:HG3	1.95	0.66
2:D:233:GLN:HA	2:D:236:LEU:HG	1.77	0.66
2:D:417:GLN:OE1	2:D:417:GLN:N	2.27	0.66
2:B:359:HIS:HD2	2:B:382:GLN:NE2	1.94	0.66
2:D:224:LEU:HB3	2:D:256:LYS:CE	2.25	0.66
2:D:236:LEU:O	2:D:268:LYS:NZ	2.23	0.66
2:D:254:TYR:O	2:D:257:ALA:N	2.28	0.66
1:C:240:VAL:HG12	1:C:276:ILE:HB	1.78	0.66
1:C:362:GLU:O	1:C:366:LEU:HD12	1.96	0.66
1:C:3:VAL:HG22	1:C:215:VAL:HB	1.78	0.66
2:D:220:TRP:HE1	2:D:224:LEU:CD2	2.07	0.66
2:B:125:ARG:NH1	2:B:146:THR:HA	2.11	0.66
2:B:272:LEU:HD11	2:B:437:TYR:CE1	2.30	0.66
2:D:219:PHE:CD1	2:D:247:VAL:CG1	2.79	0.66
2:D:295:ASP:HB2	2:D:296:GLN:HA	1.78	0.66
2:D:381:GLU:OE2	2:D:387:ARG:NH2	2.28	0.66
1:C:85:LEU:HD11	1:C:104:TYR:CE2	2.28	0.66
2:D:227:GLU:OE2	2:D:228:LEU:N	2.27	0.66
2:D:224:LEU:HB3	2:D:256:LYS:HE2	1.77	0.66
2:D:418:MSE:HG3	2:D:422:LEU:HD11	1.78	0.66
2:B:1:MSE:HE3	2:B:445:LEU:CD1	2.26	0.65
1:C:85:LEU:HD21	1:C:104:TYR:CD2	2.30	0.65
1:C:27:ILE:HG23	1:C:490:GLU:HG2	1.77	0.65
1:A:363:GLU:HB2	1:A:366:LEU:CB	2.20	0.65
1:A:321:TYR:CD2	1:A:349:LEU:HD11	2.32	0.65
2:B:282:ASN:HD21	2:B:418:MSE:HE3	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:412:LEU:HA	2:D:417:GLN:HG3	1.78	0.65
2:D:220:TRP:CE2	2:D:224:LEU:HD21	2.32	0.65
2:D:219:PHE:CD1	2:D:247:VAL:HG11	2.30	0.65
1:A:3:VAL:HG22	1:A:215:VAL:HB	1.79	0.65
1:C:244:GLU:OE2	1:C:427:TYR:OH	2.08	0.65
1:C:329:LEU:CA	1:C:333:LYS:HE3	2.25	0.65
1:C:440:TYR:CD1	1:C:460:LYS:HD2	2.32	0.65
2:D:190:ASP:OD1	2:D:192:ASP:OD2	2.14	0.65
1:C:23:TYR:CE2	1:C:27:ILE:HD11	2.32	0.65
2:D:218:LEU:CD1	2:D:220:TRP:HB2	2.26	0.65
2:B:264:ASP:O	2:B:267:GLN:NE2	2.30	0.64
2:D:224:LEU:HB2	2:D:256:LYS:HZ3	1.62	0.64
2:D:286:LYS:NZ	2:D:310:LEU:CD1	2.60	0.64
2:B:270:LEU:HD21	2:B:440:THR:HG22	1.80	0.64
2:D:238:ASN:ND2	2:D:241:LEU:HB2	2.12	0.64
2:D:384:LEU:C	2:D:384:LEU:HD23	2.18	0.64
1:C:434:ASP:HB2	1:C:437:LYS:HB3	1.78	0.64
2:B:125:ARG:HH11	2:B:146:THR:HA	1.62	0.64
2:B:4:LEU:HD12	2:B:29:ILE:HB	1.79	0.64
2:B:393:GLN:OE1	2:B:424:ALA:HB1	1.98	0.64
1:C:435:ASP:OD1	1:C:441:LEU:N	2.31	0.64
2:D:216:ASP:OD1	2:D:242:ARG:HG3	1.98	0.64
2:D:320:MSE:SE	2:D:324:LEU:HD22	2.48	0.64
2:D:417:GLN:H	2:D:417:GLN:CD	2.00	0.64
1:A:259:ASN:HD22	1:A:260:ASN:N	1.95	0.63
1:C:342:THR:HG21	1:C:354:LEU:CD2	2.29	0.63
1:A:440:TYR:CZ	1:A:473:MSE:HE1	2.33	0.63
2:B:194:ILE:O	2:B:216:ASP:HB3	1.98	0.63
2:D:286:LYS:NZ	2:D:310:LEU:HD12	2.13	0.63
2:D:287:ASP:HA	2:D:311:VAL:HG13	1.80	0.63
1:C:199:GLU:OE2	1:C:202:ARG:NH1	2.32	0.63
1:C:7:ASN:OD1	1:C:8:LEU:N	2.30	0.63
2:D:298:GLU:OE2	2:D:359:HIS:NE2	2.24	0.63
1:A:11:GLY:H	1:A:14:SER:HB2	1.64	0.63
2:B:251:LEU:CD2	2:B:271:HIS:CE1	2.82	0.62
1:C:459:GLU:OE1	1:C:460:LYS:HG2	2.00	0.62
2:D:194:ILE:O	2:D:216:ASP:HB2	2.00	0.62
2:D:224:LEU:C	2:D:256:LYS:HZ1	2.01	0.62
2:B:313:ARG:HA	2:B:334:VAL:O	1.99	0.62
1:C:397:TYR:HD1	1:C:420:LEU:HD11	1.65	0.62
2:D:397:ASP:OD2	2:D:400:GLN:CD	2.37	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ARG:HA	1:A:472:GLU:HB3	1.82	0.62
2:D:254:TYR:CZ	2:D:258:MSE:HG3	2.34	0.62
2:D:409:GLU:HA	2:D:412:LEU:HD22	1.81	0.62
1:C:440:TYR:CD2	1:C:460:LYS:HB3	2.35	0.62
2:B:377:ILE:O	2:B:378:LEU:HD23	2.00	0.62
1:A:397:TYR:HB3	1:A:420:LEU:CD1	2.30	0.62
2:D:419:ARG:C	2:D:423:GLN:HE22	2.01	0.62
1:A:449:VAL:HG13	1:A:452:GLN:HE22	1.65	0.61
2:B:314:ILE:HB	2:B:335:LEU:HD22	1.81	0.61
2:D:307:LEU:HD11	2:D:406:SER:HB2	1.82	0.61
2:B:250:ASP:HA	2:B:430:ASN:ND2	2.15	0.61
1:C:110:ASP:OD1	1:C:110:ASP:N	2.21	0.61
1:C:17:VAL:HG22	1:C:242:HIS:CD2	2.35	0.61
1:C:363:GLU:O	1:C:367:ARG:HG2	2.00	0.61
2:D:286:LYS:CE	2:D:310:LEU:HD12	2.31	0.61
2:D:79:ALA:HB3	2:D:91:ILE:HB	1.80	0.61
1:A:119:GLN:HB2	1:A:122:GLN:HG3	1.82	0.61
1:A:414:VAL:HG23	1:A:420:LEU:HD21	1.83	0.61
2:B:272:LEU:HD11	2:B:437:TYR:CZ	2.35	0.61
1:C:395:GLU:O	1:C:419:PRO:CD	2.48	0.61
1:C:476:HIS:ND1	1:C:476:HIS:O	2.34	0.61
2:B:6:ASP:OD2	2:B:198:SER:HB3	2.01	0.61
1:C:245:HIS:HB2	1:C:266:PHE:HE2	1.66	0.61
2:D:261:ALA:HB1	2:D:265:GLN:HG3	1.82	0.61
1:A:395:GLU:O	1:A:419:PRO:HD2	2.01	0.61
2:B:282:ASN:OD1	2:B:284:LEU:N	2.25	0.61
2:B:400:GLN:HB2	2:B:401:PRO:HD3	1.83	0.61
2:B:427:ARG:HG2	2:B:427:ARG:HH11	1.66	0.61
2:D:397:ASP:OD1	2:D:401:PRO:HD2	2.01	0.61
1:A:15:SER:HA	1:A:19:TYR:HD2	1.66	0.60
2:B:203:PHE:HE2	2:B:231:ASN:OD1	1.84	0.60
2:D:300:LEU:O	2:D:304:VAL:HG23	2.01	0.60
1:A:315:LYS:C	1:A:317:PRO:HD3	2.21	0.60
1:C:323:MSE:HE2	1:C:342:THR:HG22	1.84	0.60
2:D:246:ILE:HB	2:D:269:PHE:HB3	1.83	0.60
1:A:476:HIS:O	1:A:480:VAL:HG22	2.02	0.60
1:A:483:ASN:O	1:A:488:ARG:HD3	2.00	0.60
2:D:305:GLN:HG2	2:D:306:SER:N	2.16	0.60
2:D:416:GLU:N	2:D:417:GLN:OE1	2.35	0.60
2:D:7:TYR:O	2:D:12:THR:HG21	2.01	0.60
2:B:378:LEU:HD21	2:B:394:HIS:HD2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ARG:HG3	1:C:176:ASP:HB3	1.84	0.60
2:B:230:GLY:O	2:B:233:GLN:HB2	2.01	0.60
2:D:307:LEU:C	2:D:309:GLN:HE21	2.05	0.60
2:B:307:LEU:HD11	2:B:406:SER:HB2	1.83	0.59
2:B:332:ASN:O	2:B:332:ASN:ND2	2.35	0.59
1:C:245:HIS:HE1	1:C:289:GLN:HE22	1.47	0.59
1:C:343:VAL:HG21	1:C:373:ALA:HB1	1.83	0.59
2:D:195:LEU:HA	2:D:217:ILE:HD11	1.85	0.59
1:A:345:ALA:HB2	1:A:458:VAL:HG23	1.85	0.59
1:A:382:LYS:HZ1	1:A:384:HIS:C	2.04	0.59
2:D:396:PHE:CD2	2:D:405:ALA:HA	2.36	0.59
1:A:440:TYR:HD1	1:A:460:LYS:HB3	1.66	0.59
1:A:467:GLN:HA	1:A:469:ARG:NH1	2.18	0.59
2:D:234:LEU:HD12	2:D:235:ILE:HB	1.85	0.59
1:A:318:ARG:NH1	1:A:394:TYR:O	2.35	0.59
2:B:4:LEU:HD21	2:B:205:VAL:HG21	1.85	0.59
1:C:117:LEU:HD21	1:C:122:GLN:O	2.02	0.59
1:C:424:ASP:HB2	1:C:441:LEU:HB3	1.84	0.59
2:B:301:ASP:N	2:B:327:MSE:HE1	2.17	0.58
1:C:211:GLN:HG2	1:C:212:ALA:H	1.68	0.58
1:C:363:GLU:HA	1:C:366:LEU:HD13	1.84	0.58
2:D:234:LEU:HD12	2:D:235:ILE:N	2.17	0.58
1:A:310:GLN:OE1	1:A:310:GLN:N	2.36	0.58
1:A:464:LEU:N	1:A:469:ARG:HH21	1.99	0.58
1:C:47:ASN:HB3	1:C:50:HIS:CE1	2.39	0.58
2:D:249:PRO:O	2:D:430:ASN:ND2	2.35	0.58
1:C:101:ILE:O	1:C:101:ILE:HG13	2.02	0.58
1:C:27:ILE:HD12	1:C:27:ILE:H	1.68	0.58
2:D:319:GLU:HG2	2:D:338:ASN:HD21	1.69	0.58
1:A:189:PHE:HB2	1:A:192:ARG:HB2	1.85	0.58
1:A:323:MSE:HE3	1:A:352:LEU:HD11	1.86	0.58
2:B:341:LEU:O	2:B:344:ILE:HG22	2.04	0.58
1:A:337:TRP:CH2	1:A:453:ILE:HD13	2.39	0.58
1:A:363:GLU:CB	1:A:366:LEU:HB2	2.24	0.58
1:C:88:VAL:HG21	1:C:113:ILE:HD13	1.84	0.58
2:D:220:TRP:CZ2	2:D:224:LEU:HD21	2.38	0.58
1:A:359:LYS:HZ2	1:A:383:GLY:CA	2.16	0.58
1:A:440:TYR:CE1	1:A:460:LYS:HD2	2.38	0.58
1:C:494:THR:C	1:C:498:LYS:NZ	2.56	0.58
2:B:249:PRO:HA	2:B:272:LEU:O	2.03	0.58
1:C:422:GLY:O	1:C:441:LEU:HA	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:324:LEU:O	2:D:327:MSE:HG2	2.04	0.58
2:D:343:GLN:O	2:D:347:LEU:HD12	2.03	0.58
2:D:336:TYR:CD1	2:D:347:LEU:HD21	2.38	0.58
2:D:231:ASN:O	2:D:234:LEU:HG	2.03	0.58
1:C:354:LEU:HG	1:C:379:ILE:HG12	1.85	0.58
2:D:300:LEU:CD1	2:D:327:MSE:HE2	2.34	0.58
2:D:397:ASP:OD2	2:D:400:GLN:NE2	2.36	0.58
1:A:437:LYS:HB3	1:A:476:HIS:CD2	2.39	0.57
1:A:81:LEU:HD21	1:A:102:VAL:HG21	1.85	0.57
1:A:465:PHE:CA	1:A:469:ARG:HH22	2.16	0.57
1:C:437:LYS:HD3	1:C:476:HIS:CD2	2.39	0.57
2:B:401:PRO:HB2	2:B:404:LEU:HB2	1.85	0.57
2:D:386:ASP:HB3	2:D:388:HIS:HB2	1.86	0.57
1:A:143:SER:OG	1:A:144:TYR:N	2.37	0.57
1:A:7:ASN:OD1	1:A:8:LEU:N	2.36	0.57
1:C:111:GLN:OE1	2:D:174:LYS:NZ	2.36	0.57
1:C:161:LEU:HD21	1:C:164:ARG:HH12	1.69	0.57
2:D:296:GLN:HB2	2:D:323:LYS:HE2	1.85	0.57
2:D:290:ILE:CD1	2:D:355:LEU:HB2	2.33	0.57
2:D:412:LEU:HD12	2:D:417:GLN:C	2.24	0.57
1:C:437:LYS:HZ2	1:C:476:HIS:CD2	2.22	0.57
1:A:367:ARG:HB3	1:A:368:ARG:NH1	2.20	0.57
1:A:482:GLU:HA	1:A:485:LEU:HD13	1.86	0.57
1:A:488:ARG:CZ	1:A:489:VAL:HG22	2.35	0.57
1:C:474:SER:O	1:C:477:SER:HB3	2.05	0.57
2:B:58:PRO:HB2	2:B:101:LEU:HD12	1.86	0.57
2:B:386:ASP:HB3	2:B:388:HIS:ND1	2.20	0.57
1:C:27:ILE:HG22	1:C:31:ILE:HD11	1.87	0.57
1:C:397:TYR:HB3	1:C:420:LEU:HD13	1.87	0.57
1:A:476:HIS:HA	1:A:479:GLN:HB2	1.86	0.56
1:A:483:ASN:O	1:A:488:ARG:NH1	2.38	0.56
1:C:420:LEU:O	1:C:439:GLY:HA3	2.05	0.56
1:C:432:PHE:HE1	1:C:484:TYR:CD2	2.24	0.56
2:D:363:VAL:HG12	2:D:364:LEU:HG	1.87	0.56
1:A:466:SER:N	1:A:469:ARG:HH22	2.02	0.56
2:B:380:PHE:CD2	2:B:396:PHE:HB2	2.34	0.56
2:D:181:ARG:HE	2:D:209:LEU:HD21	1.69	0.56
2:B:193:HIS:ND1	2:B:215:GLN:O	2.37	0.56
1:A:369:ARG:HH12	1:A:373:ALA:HB2	1.68	0.56
1:C:316:GLU:HB3	1:C:317:PRO:HD2	1.87	0.56
1:A:370:ILE:HG22	1:A:371:GLU:CD	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:MSE:HE3	2:B:246:ILE:HG21	1.87	0.56
2:D:320:MSE:HE3	2:D:335:LEU:HD13	1.87	0.56
2:B:282:ASN:ND2	2:B:418:MSE:HE3	2.20	0.56
1:C:323:MSE:HE3	1:C:398:LEU:HD11	1.87	0.56
1:C:397:TYR:OH	1:C:409:THR:OG1	2.06	0.56
1:A:417:GLY:HA2	1:A:477:SER:HB2	1.87	0.56
1:C:202:ARG:NH2	1:C:230:GLU:OE1	2.39	0.56
2:D:195:LEU:HA	2:D:217:ILE:CD1	2.36	0.56
2:D:207:HIS:CD2	2:D:241:LEU:HD11	2.41	0.56
2:D:235:ILE:HD11	2:D:243:THR:O	2.05	0.56
2:D:254:TYR:CZ	2:D:271:HIS:NE2	2.74	0.56
1:A:284:ARG:O	1:A:288:GLN:NE2	2.39	0.56
1:A:80:THR:OG1	1:A:83:GLN:HG3	2.06	0.56
2:B:267:GLN:N	2:B:267:GLN:OE1	2.36	0.56
1:C:221:GLU:HG2	1:C:225:GLY:HA3	1.87	0.56
2:D:168:GLU:HB3	2:D:171:ARG:HH22	1.71	0.56
1:A:366:LEU:HD13	1:A:370:ILE:CD1	2.36	0.55
1:A:341:ALA:HA	1:A:454:ILE:HG23	1.88	0.55
1:C:437:LYS:NZ	1:C:476:HIS:C	2.59	0.55
2:D:240:GLN:HA	2:D:240:GLN:OE1	2.07	0.55
1:A:349:LEU:HD22	1:A:350:PRO:HD2	1.88	0.55
1:C:113:ILE:O	1:C:113:ILE:HG13	2.07	0.55
1:A:438:ASN:CB	1:A:476:HIS:HB3	2.24	0.55
2:B:164:THR:HG23	2:B:164:THR:O	2.06	0.55
1:C:335:ILE:O	1:C:339:VAL:N	2.37	0.55
1:A:327:SER:O	1:A:358:GLY:HA3	2.06	0.55
2:B:413:CYS:SG	2:B:417:GLN:NE2	2.80	0.55
1:C:338:LEU:CD1	1:C:398:LEU:HB3	2.35	0.55
2:D:196:PHE:CE2	2:D:218:LEU:HD23	2.41	0.55
2:B:270:LEU:HD11	2:B:440:THR:HG22	1.88	0.55
2:B:309:GLN:N	2:B:309:GLN:OE1	2.23	0.55
1:C:395:GLU:HG2	1:C:470:GLN:NE2	2.22	0.55
2:D:32:GLU:OE2	2:D:34:ASN:HB2	2.07	0.55
2:D:291:LEU:HD13	2:D:344:ILE:HD11	1.87	0.55
2:D:37:LEU:O	2:D:122:LYS:NZ	2.24	0.55
2:B:258:MSE:SE	2:B:266:GLN:HB3	2.55	0.55
1:A:366:LEU:CD1	1:A:370:ILE:HD11	2.36	0.55
1:C:24:ARG:NH1	1:C:219:ASP:OD1	2.40	0.55
2:B:297:ILE:H	2:B:297:ILE:HD12	1.71	0.55
1:C:173:VAL:HG21	2:D:144:TYR:HE2	1.71	0.55
2:D:217:ILE:C	2:D:217:ILE:HD12	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:287:ASP:OD1	2:D:311:VAL:HG11	2.07	0.55
2:B:125:ARG:HH12	2:B:145:SER:C	2.10	0.54
2:B:272:LEU:CD1	2:B:273:GLY:O	2.56	0.54
2:D:280:ARG:NH2	2:D:352:ASP:OD1	2.39	0.54
1:A:44:LEU:HB3	1:A:141:TYR:CE2	2.42	0.54
2:B:295:ASP:CB	2:B:296:GLN:HA	2.31	0.54
1:A:278:ALA:HB1	1:A:406:PHE:HB2	1.90	0.54
1:A:471:GLN:O	1:A:475:GLN:HG3	2.07	0.54
2:D:168:GLU:CB	2:D:171:ARG:HH12	2.18	0.54
2:D:362:GLN:HE22	2:D:365:GLN:HA	1.70	0.54
2:D:392:GLN:C	2:D:394:HIS:H	2.09	0.54
1:C:432:PHE:HE1	1:C:484:TYR:CE2	2.26	0.54
2:D:228:LEU:HD22	2:D:232:MSE:SE	2.57	0.54
1:A:359:LYS:HB2	1:A:384:HIS:NE2	2.23	0.54
1:C:355:ASP:OD2	1:C:380:ARG:HG3	2.07	0.54
2:D:250:ASP:OD2	2:D:253:THR:OG1	2.24	0.54
2:D:258:MSE:SE	2:D:266:GLN:OE1	2.76	0.54
2:B:84:MSE:HE2	1:C:199:GLU:OE2	2.07	0.54
2:D:408:LEU:O	2:D:411:ALA:HB3	2.08	0.54
1:A:414:VAL:HG12	1:A:481:ALA:HB2	1.88	0.54
2:B:362:GLN:CA	2:B:384:LEU:HD23	2.38	0.54
1:A:337:TRP:O	1:A:341:ALA:N	2.41	0.54
2:B:295:ASP:HB2	2:B:296:GLN:HA	1.90	0.54
1:C:437:LYS:HD3	1:C:476:HIS:NE2	2.23	0.54
1:C:449:VAL:O	1:C:452:GLN:HB2	2.08	0.54
2:D:227:GLU:CD	2:D:228:LEU:N	2.61	0.54
2:D:287:ASP:HA	2:D:311:VAL:CG1	2.38	0.54
1:C:424:ASP:HA	1:C:441:LEU:HD22	1.91	0.53
1:C:456:ALA:O	1:C:459:GLU:OE1	2.26	0.53
2:D:176:ARG:O	2:D:180:ILE:HG13	2.09	0.53
2:D:3:GLN:NE2	2:D:19:LEU:HD21	2.22	0.53
2:D:368:ARG:HB2	2:D:389:TYR:HE2	1.73	0.53
1:A:359:LYS:NZ	1:A:383:GLY:HA3	2.23	0.53
2:D:307:LEU:HD11	2:D:406:SER:CB	2.38	0.53
1:A:495:GLN:NE2	1:A:499:GLU:OE2	2.40	0.53
2:B:264:ASP:N	2:B:264:ASP:OD1	2.41	0.53
2:B:290:ILE:HG13	2:B:357:ILE:HD11	1.90	0.53
2:D:391:ALA:O	2:D:394:HIS:HB2	2.07	0.53
1:A:359:LYS:HG3	1:A:384:HIS:CG	2.44	0.53
2:B:125:ARG:NH1	2:B:145:SER:O	2.42	0.53
2:B:69:PHE:CZ	1:C:271:LYS:HD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:GLN:CD	2:D:174:LYS:HZ1	2.11	0.53
2:D:307:LEU:HD12	2:D:310:LEU:HD22	1.89	0.53
1:A:396:LEU:HD12	1:A:419:PRO:O	2.08	0.53
2:D:163:LEU:HD13	2:D:179:PHE:HE1	1.73	0.53
2:D:290:ILE:HD13	2:D:355:LEU:O	2.08	0.53
2:D:300:LEU:HD11	2:D:327:MSE:HE2	1.90	0.53
2:D:310:LEU:HD23	2:D:312:PHE:CZ	2.44	0.53
1:C:195:TYR:CE1	2:D:109:ASP:HA	2.44	0.53
1:C:24:ARG:HH12	1:C:219:ASP:CG	2.12	0.53
1:C:81:LEU:HD12	1:C:81:LEU:H	1.73	0.53
1:A:382:LYS:HZ1	1:A:385:ALA:HB2	1.74	0.53
2:B:196:PHE:CE2	2:B:218:LEU:HB2	2.44	0.53
1:C:378:TYR:O	1:C:379:ILE:HG13	2.09	0.53
1:C:338:LEU:CD2	1:C:400:ALA:HB2	2.38	0.53
2:D:297:ILE:HG22	2:D:357:ILE:HG22	1.91	0.53
2:D:1:MSE:N	2:D:190:ASP:O	2.30	0.53
1:A:244:GLU:OE2	1:A:427:TYR:CE1	2.62	0.52
2:B:18:SER:HB3	2:B:437:TYR:CZ	2.44	0.52
2:B:297:ILE:HG21	2:B:357:ILE:HD12	1.91	0.52
2:D:219:PHE:HD1	2:D:247:VAL:HG11	1.74	0.52
2:D:424:ALA:HA	2:D:427:ARG:HG2	1.89	0.52
1:A:339:VAL:O	1:A:343:VAL:HG13	2.09	0.52
1:A:363:GLU:CD	1:A:363:GLU:N	2.63	0.52
1:A:173:VAL:HG21	2:B:144:TYR:HE2	1.74	0.52
1:C:26:GLN:HA	1:C:29:ARG:HH12	1.74	0.52
2:D:286:LYS:CD	2:D:310:LEU:HD12	2.39	0.52
2:B:315:ALA:HA	2:B:336:TYR:O	2.09	0.52
1:C:329:LEU:HA	1:C:333:LYS:CE	2.27	0.52
1:C:459:GLU:CD	1:C:460:LYS:N	2.63	0.52
2:D:368:ARG:HD3	2:D:389:TYR:CE2	2.45	0.52
2:B:203:PHE:HE2	2:B:231:ASN:CG	2.13	0.52
2:B:403:GLN:HE21	2:B:404:LEU:HD12	1.74	0.52
1:A:15:SER:HA	1:A:19:TYR:CD2	2.44	0.52
2:D:423:GLN:CD	2:D:423:GLN:H	2.13	0.52
1:A:438:ASN:HA	1:A:473:MSE:HB3	1.91	0.52
1:A:467:GLN:HE22	1:A:469:ARG:HH12	1.49	0.52
1:C:245:HIS:HB2	1:C:266:PHE:CE2	2.43	0.52
1:C:321:TYR:H	1:C:395:GLU:CD	2.12	0.52
2:D:286:LYS:NZ	2:D:310:LEU:HD11	2.25	0.52
2:B:410:GLU:C	2:B:412:LEU:H	2.13	0.52
1:C:327:SER:O	1:C:333:LYS:NZ	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:306:SER:O	2:D:307:LEU:HD23	2.10	0.52
1:A:42:MSE:HE3	1:A:164:ARG:HH11	1.75	0.51
2:B:396:PHE:CZ	2:B:405:ALA:HA	2.45	0.51
2:D:11:GLU:OE2	2:D:388:HIS:CE1	2.52	0.51
1:A:144:TYR:CD1	1:A:145:VAL:HG23	2.45	0.51
2:B:271:HIS:CE1	2:B:272:LEU:O	2.64	0.51
2:B:320:MSE:SE	2:B:324:LEU:HD11	2.59	0.51
2:B:407:ILE:HA	2:B:410:GLU:CB	2.40	0.51
2:B:441:LEU:O	2:B:444:LEU:N	2.37	0.51
1:A:241:VAL:HA	1:A:262:TYR:CE1	2.45	0.51
1:A:270:ASP:OD2	1:A:271:LYS:HE3	2.10	0.51
1:A:369:ARG:O	1:A:369:ARG:CZ	2.58	0.51
1:C:437:LYS:O	1:C:473:MSE:SE	2.79	0.51
2:D:212:ARG:HG3	2:D:213:ALA:N	2.25	0.51
2:D:236:LEU:HD12	2:D:237:ASP:N	2.25	0.51
2:B:282:ASN:HD22	2:B:422:LEU:HD11	1.76	0.51
1:C:406:PHE:CZ	1:C:411:MSE:HE2	2.45	0.51
1:C:397:TYR:HB3	1:C:420:LEU:HD11	1.91	0.51
2:D:165:LEU:HD22	2:D:165:LEU:N	2.25	0.51
2:D:181:ARG:HH11	2:D:209:LEU:CD1	2.23	0.51
2:D:5:PHE:O	2:D:30:VAL:HA	2.11	0.51
1:A:420:LEU:HB2	1:A:433:ILE:HG12	1.92	0.51
2:D:6:ASP:HA	2:D:31:ILE:HG13	1.93	0.51
2:B:280:ARG:HH21	2:B:349:LEU:HA	1.76	0.51
2:B:368:ARG:NH1	2:B:389:TYR:OH	2.40	0.51
1:C:17:VAL:HG13	1:C:242:HIS:CD2	2.46	0.51
1:C:31:ILE:HG12	1:C:494:THR:OG1	2.11	0.51
1:C:81:LEU:O	1:C:85:LEU:HD12	2.10	0.51
2:D:254:TYR:CE2	2:D:258:MSE:HG3	2.46	0.51
2:B:247:VAL:HG12	2:B:249:PRO:HD3	1.93	0.51
1:C:495:GLN:CA	1:C:498:LYS:HZ2	2.21	0.51
2:D:196:PHE:HE2	2:D:218:LEU:HD23	1.75	0.51
1:A:404:GLU:O	1:A:427:TYR:N	2.34	0.51
2:B:289:LEU:HD13	2:B:347:LEU:HB3	1.93	0.51
1:C:323:MSE:HB3	1:C:354:LEU:HB3	1.92	0.51
2:D:254:TYR:CZ	2:D:258:MSE:HE3	2.45	0.51
2:D:307:LEU:HB3	2:D:310:LEU:HB2	1.93	0.51
1:A:85:LEU:HD11	1:A:104:TYR:CZ	2.46	0.51
2:D:409:GLU:HA	2:D:412:LEU:CD2	2.41	0.51
1:A:244:GLU:OE2	1:A:427:TYR:HE1	1.94	0.51
2:D:391:ALA:HB3	2:D:394:HIS:HD2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:392:GLN:O	2:B:395:ILE:HG22	2.11	0.50
2:B:396:PHE:CE2	2:B:405:ALA:HB2	2.46	0.50
1:C:397:TYR:CD1	1:C:420:LEU:HD11	2.46	0.50
2:B:346:GLN:O	2:B:350:GLU:HG3	2.11	0.50
2:B:304:VAL:HG13	2:B:330:TYR:HE2	1.77	0.50
1:C:24:ARG:HD2	1:C:493:TRP:CZ2	2.46	0.50
1:C:329:LEU:HB3	1:C:333:LYS:NZ	2.27	0.50
2:D:162:ILE:HG13	2:D:162:ILE:O	2.11	0.50
1:A:244:GLU:OE1	1:A:426:ARG:NE	2.42	0.50
1:A:377:ASP:O	1:A:380:ARG:NE	2.44	0.50
2:B:254:TYR:CD2	2:B:271:HIS:HB2	2.46	0.50
2:B:78:VAL:HG22	2:B:79:ALA:H	1.76	0.50
1:C:241:VAL:HA	1:C:262:TYR:CE2	2.47	0.50
1:A:202:ARG:NH1	2:D:84:MSE:HE2	2.27	0.50
2:D:168:GLU:HB3	2:D:171:ARG:NH1	2.26	0.50
2:D:190:ASP:OD1	2:D:192:ASP:CG	2.50	0.50
2:D:406:SER:HA	2:D:409:GLU:OE1	2.11	0.50
2:D:419:ARG:CG	2:D:423:GLN:NE2	2.75	0.50
2:B:300:LEU:O	2:B:304:VAL:HG12	2.12	0.50
2:B:84:MSE:HE1	1:C:227:VAL:HB	1.94	0.50
1:C:323:MSE:HB3	1:C:354:LEU:CB	2.42	0.50
1:C:435:ASP:HA	1:C:439:GLY:O	2.11	0.50
2:B:203:PHE:CE2	2:B:231:ASN:OD1	2.65	0.50
2:D:321:SER:O	2:D:325:LEU:HD12	2.12	0.50
1:A:390:ILE:N	1:A:390:ILE:HD12	2.27	0.49
1:C:138:ARG:NH2	1:C:146:ARG:NH1	2.59	0.49
1:C:321:TYR:N	1:C:395:GLU:CD	2.65	0.49
2:D:194:ILE:H	2:D:216:ASP:HB3	1.77	0.49
2:D:290:ILE:HB	2:D:314:ILE:HD13	1.93	0.49
2:D:320:MSE:HG2	2:D:337:GLN:CD	2.32	0.49
2:D:407:ILE:HA	2:D:410:GLU:HB3	1.93	0.49
1:C:75:ALA:HB3	1:C:143:SER:OG	2.12	0.49
1:C:318:ARG:O	1:C:320:PRO:HD3	2.12	0.49
2:D:286:LYS:HZ1	2:D:310:LEU:HD11	1.76	0.49
2:D:321:SER:C	2:D:325:LEU:HD12	2.32	0.49
1:A:363:GLU:H	1:A:363:GLU:CD	2.16	0.49
1:C:270:ASP:OD2	1:C:271:LYS:HE3	2.12	0.49
1:C:495:GLN:HA	1:C:498:LYS:NZ	2.24	0.49
1:A:449:VAL:HG13	1:A:452:GLN:CD	2.31	0.49
1:A:449:VAL:CG1	1:A:452:GLN:NE2	2.66	0.49
2:B:348:TYR:CZ	2:B:369:LYS:HG2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:VAL:O	1:C:342:THR:OG1	2.27	0.49
2:D:199:LEU:N	2:D:199:LEU:HD22	2.28	0.49
2:B:195:LEU:HB3	2:B:219:PHE:HE1	1.77	0.49
1:C:391:TYR:HB2	1:C:416:SER:OG	2.13	0.49
1:C:453:ILE:HD12	1:C:454:ILE:HG13	1.95	0.49
2:D:217:ILE:O	2:D:217:ILE:HD12	2.13	0.49
2:D:203:PHE:CZ	2:D:234:LEU:HD11	2.47	0.49
1:A:366:LEU:HD13	1:A:370:ILE:HD11	1.95	0.49
1:A:400:ALA:O	1:A:423:PHE:HE2	1.96	0.49
2:B:38:PRO:HG2	2:B:41:MSE:HE3	1.94	0.49
1:C:87:GLN:O	2:D:170:LEU:N	2.31	0.49
1:A:322:SER:HA	1:A:353:THR:O	2.12	0.49
2:B:363:VAL:HG12	2:B:364:LEU:HD12	1.94	0.49
2:D:15:LEU:HD11	2:D:219:PHE:CB	2.43	0.49
1:A:42:MSE:HE1	1:A:166:PHE:CZ	2.48	0.48
1:A:466:SER:CA	1:A:467:GLN:HE21	2.23	0.48
1:C:420:LEU:O	1:C:421:ILE:HD13	2.12	0.48
1:C:90:GLY:O	1:C:91:GLN:NE2	2.45	0.48
2:D:219:PHE:HD1	2:D:247:VAL:CG1	2.24	0.48
2:D:291:LEU:O	2:D:358:ASN:ND2	2.46	0.48
2:D:391:ALA:HB2	2:D:424:ALA:O	2.13	0.48
2:D:46:THR:O	2:D:49:LEU:HD12	2.13	0.48
1:A:145:VAL:HG12	1:A:146:ARG:N	2.28	0.48
1:A:111:GLN:HB3	2:B:174:LYS:NZ	2.28	0.48
2:B:291:LEU:CD1	2:B:344:ILE:HD11	2.43	0.48
1:C:283:LYS:O	1:C:287:GLU:HB2	2.13	0.48
2:D:286:LYS:HZ1	2:D:310:LEU:CD1	2.25	0.48
2:D:338:ASN:HD22	2:D:338:ASN:N	2.12	0.48
2:D:390:ILE:O	2:D:428:HIS:ND1	2.47	0.48
1:A:349:LEU:HD13	1:A:350:PRO:N	2.29	0.48
1:A:371:GLU:HB3	1:A:375:ALA:O	2.13	0.48
2:B:203:PHE:HE2	2:B:231:ASN:ND2	2.11	0.48
2:B:363:VAL:HG12	2:B:364:LEU:CD1	2.43	0.48
2:D:210:THR:CG2	2:D:241:LEU:HG	2.43	0.48
2:D:258:MSE:SE	2:D:266:GLN:CD	3.02	0.48
2:D:291:LEU:CD1	2:D:344:ILE:HD11	2.43	0.48
1:C:322:SER:N	1:C:395:GLU:OE1	2.47	0.48
1:C:349:LEU:HB3	1:C:352:LEU:CD1	2.38	0.48
1:C:44:LEU:HB3	1:C:141:TYR:CE1	2.49	0.48
1:C:461:ILE:O	1:C:464:LEU:HG	2.13	0.48
1:C:494:THR:CG2	1:C:498:LYS:NZ	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:309:GLN:H	2:D:309:GLN:NE2	2.11	0.48
1:A:481:ALA:O	1:A:484:TYR:N	2.38	0.48
1:C:161:LEU:HD21	1:C:164:ARG:NH1	2.27	0.48
1:C:423:PHE:HD2	1:C:442:LEU:HB2	1.79	0.48
2:D:227:GLU:CD	2:D:228:LEU:H	2.12	0.48
1:A:245:HIS:CD2	1:A:286:LEU:HD13	2.48	0.48
1:A:462:ILE:C	1:A:465:PHE:H	2.16	0.48
2:B:280:ARG:NH2	2:B:348:TYR:O	2.47	0.48
2:B:353:ILE:HD13	2:B:355:LEU:HG	1.95	0.48
2:B:403:GLN:NE2	2:B:404:LEU:HA	2.29	0.48
1:C:323:MSE:HG2	1:C:354:LEU:HB3	1.94	0.48
1:C:350:PRO:O	1:C:352:LEU:HD12	2.13	0.48
1:A:285:ILE:O	1:A:289:GLN:HG3	2.14	0.48
1:A:414:VAL:HA	1:A:477:SER:HB3	1.95	0.48
2:B:220:TRP:CZ2	2:B:222:GLU:HB2	2.48	0.48
2:B:262:ALA:O	2:B:266:GLN:HG3	2.14	0.48
2:B:427:ARG:CG	2:B:427:ARG:HH11	2.26	0.48
1:A:27:ILE:HG21	1:A:493:TRP:CD1	2.49	0.48
2:B:220:TRP:HE1	2:B:224:LEU:CD1	2.27	0.48
2:B:384:LEU:HD12	2:B:384:LEU:N	2.29	0.48
2:B:432:VAL:HB	2:B:436:LEU:HD23	1.96	0.48
2:D:164:THR:HG22	2:D:170:LEU:HB2	1.96	0.48
1:A:25:ALA:O	1:A:29:ARG:HG3	2.13	0.47
2:B:386:ASP:N	2:B:386:ASP:OD1	2.47	0.47
1:C:346:HIS:HD2	1:C:375:ALA:HB2	1.79	0.47
1:C:79:VAL:O	1:C:125:VAL:N	2.43	0.47
2:D:196:PHE:HZ	2:D:243:THR:HG21	1.79	0.47
1:A:338:LEU:CD1	1:A:400:ALA:HB2	2.39	0.47
1:C:81:LEU:HD12	1:C:123:ASP:O	2.15	0.47
2:D:224:LEU:CB	2:D:256:LYS:CE	2.93	0.47
2:D:5:PHE:HB2	2:D:30:VAL:HG12	1.96	0.47
1:A:361:SER:O	1:A:362:GLU:HB2	2.14	0.47
1:C:239:VAL:HG11	1:C:265:GLN:HG2	1.97	0.47
1:C:23:TYR:CZ	1:C:27:ILE:HD11	2.50	0.47
2:D:336:TYR:CE1	2:D:347:LEU:HD21	2.49	0.47
1:A:367:ARG:HA	1:A:370:ILE:HG12	1.96	0.47
1:A:440:TYR:CE2	1:A:473:MSE:HE1	2.48	0.47
2:B:2:ILE:HG22	2:B:27:PRO:HG2	1.96	0.47
1:C:426:ARG:HB3	1:C:427:TYR:CG	2.49	0.47
1:A:359:LYS:NZ	1:A:383:GLY:CA	2.77	0.47
2:D:419:ARG:HG3	2:D:423:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:HG12	1:A:146:ARG:H	1.78	0.47
1:A:470:GLN:HG3	1:A:471:GLN:H	1.80	0.47
2:B:118:GLU:HG2	2:B:129:LYS:HG2	1.96	0.47
2:B:203:PHE:O	2:B:206:SER:N	2.46	0.47
1:C:346:HIS:CD2	1:C:375:ALA:HB2	2.49	0.47
1:C:468:GLY:O	1:C:472:GLU:HG3	2.14	0.47
2:D:165:LEU:CD2	2:D:165:LEU:N	2.78	0.47
2:D:212:ARG:HG2	2:D:242:ARG:HH22	1.80	0.47
2:D:246:ILE:O	2:D:269:PHE:HA	2.14	0.47
1:C:80:THR:HA	1:C:123:ASP:O	2.15	0.47
1:C:23:TYR:O	1:C:27:ILE:HD12	2.14	0.47
1:C:492:ALA:O	1:C:496:LEU:N	2.46	0.47
2:D:217:ILE:HG22	2:D:245:THR:HB	1.97	0.47
1:C:117:LEU:HD11	1:C:124:PHE:N	2.29	0.47
2:D:216:ASP:OD1	2:D:243:THR:HG22	2.15	0.47
1:A:256:ILE:HD11	1:A:289:GLN:NE2	2.30	0.47
1:A:367:ARG:CZ	1:A:368:ARG:HH12	2.27	0.47
1:A:454:ILE:H	1:A:454:ILE:HD12	1.80	0.47
2:B:271:HIS:ND1	2:B:272:LEU:N	2.63	0.47
2:D:154:GLU:OE2	2:D:176:ARG:NH1	2.48	0.47
1:A:382:LYS:HD3	1:A:382:LYS:C	2.35	0.47
1:A:359:LYS:HB2	1:A:384:HIS:CE1	2.50	0.47
1:A:359:LYS:NZ	1:A:384:HIS:N	2.44	0.47
1:C:328:ARG:NH2	1:C:359:LYS:N	2.60	0.47
1:C:117:LEU:HD12	1:C:125:VAL:HA	1.96	0.46
1:C:129:GLU:HB3	1:C:136:LEU:CD1	2.45	0.46
2:D:286:LYS:HD2	2:D:310:LEU:HD12	1.97	0.46
2:B:254:TYR:OH	2:B:258:MSE:HE2	2.15	0.46
2:B:288:ALA:N	2:B:311:VAL:O	2.47	0.46
2:B:403:GLN:O	2:B:405:ALA:N	2.49	0.46
2:B:84:MSE:HE3	1:C:198:ALA:HB1	1.97	0.46
1:A:464:LEU:HG	1:A:464:LEU:O	2.16	0.46
1:C:81:LEU:HD21	1:C:102:VAL:HG11	1.98	0.46
1:C:321:TYR:HB3	1:C:352:LEU:CD1	2.44	0.46
2:B:317:LEU:HA	2:B:338:ASN:HA	1.97	0.46
2:B:70:TRP:CZ3	2:B:88:ARG:HG3	2.50	0.46
2:D:267:GLN:CD	2:D:267:GLN:H	2.19	0.46
2:D:302:THR:O	2:D:306:SER:OG	2.29	0.46
2:D:368:ARG:NH1	2:D:389:TYR:OH	2.49	0.46
1:A:370:ILE:HG22	1:A:371:GLU:OE1	2.16	0.46
1:A:397:TYR:HD2	1:A:420:LEU:HD12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:TRP:CZ3	1:A:453:ILE:HD13	2.51	0.46
2:B:295:ASP:HB2	2:B:296:GLN:CA	2.45	0.46
1:C:26:GLN:HA	1:C:29:ARG:HH11	1.78	0.46
2:D:315:ALA:HA	2:D:336:TYR:O	2.16	0.46
1:A:414:VAL:HG11	1:A:480:VAL:HG23	1.98	0.46
2:B:231:ASN:HA	2:B:234:LEU:HD13	1.97	0.46
2:B:37:LEU:O	2:B:122:LYS:NZ	2.39	0.46
1:C:311:LEU:H	1:C:311:LEU:HD12	1.79	0.46
1:C:12:TRP:CE2	1:C:46:ASP:OD1	2.66	0.46
2:D:254:TYR:HE2	2:D:269:PHE:HE1	1.63	0.46
1:A:283:LYS:O	1:A:287:GLU:HB2	2.15	0.46
2:B:257:ALA:HB1	2:B:269:PHE:CE2	2.51	0.46
2:D:224:LEU:HB2	2:D:256:LYS:NZ	2.29	0.46
2:B:378:LEU:CD2	2:B:394:HIS:HB3	2.46	0.45
2:B:378:LEU:HD21	2:B:394:HIS:CD2	2.47	0.45
1:C:117:LEU:HD11	1:C:123:ASP:C	2.36	0.45
1:C:352:LEU:HD21	1:C:465:PHE:CE2	2.51	0.45
2:D:28:THR:HG23	2:D:41:MSE:HA	1.98	0.45
1:A:334:HIS:CE1	1:A:337:TRP:CE2	3.04	0.45
1:A:376:GLN:O	1:A:379:ILE:HG22	2.16	0.45
1:C:407:GLY:HA3	1:C:410:LEU:HD22	1.98	0.45
2:D:35:GLY:HA3	2:D:121:ASN:HA	1.98	0.45
2:D:235:ILE:CD1	2:D:243:THR:O	2.65	0.45
2:D:264:ASP:C	2:D:266:GLN:H	2.19	0.45
2:D:412:LEU:HD12	2:D:417:GLN:CG	2.46	0.45
1:A:146:ARG:HD2	1:A:149:SER:OG	2.15	0.45
2:B:289:LEU:O	2:B:290:ILE:HD13	2.16	0.45
1:C:323:MSE:O	1:C:324:ILE:HB	2.16	0.45
1:A:473:MSE:C	1:A:475:GLN:N	2.69	0.45
1:C:130:TYR:CE1	1:C:140:ASP:OD1	2.70	0.45
1:C:303:ILE:HG21	1:C:493:TRP:NE1	2.31	0.45
2:D:163:LEU:HD21	2:D:165:LEU:CD2	2.46	0.45
1:A:366:LEU:HD13	1:A:370:ILE:HD13	1.98	0.45
1:A:463:ALA:O	1:A:469:ARG:NH2	2.48	0.45
2:B:299:GLY:O	2:B:302:THR:OG1	2.33	0.45
1:C:437:LYS:HD2	1:C:437:LYS:HA	1.71	0.45
2:B:292:THR:HA	2:B:358:ASN:HD22	1.81	0.45
1:C:499:GLU:OE2	1:C:499:GLU:N	2.44	0.45
2:D:286:LYS:HE2	2:D:286:LYS:HB2	1.83	0.45
1:A:472:GLU:HA	1:A:475:GLN:CD	2.37	0.45
2:B:251:LEU:H	2:B:430:ASN:ND2	2.10	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:TYR:CZ	2:B:347:LEU:HD21	2.51	0.45
1:C:494:THR:O	1:C:495:GLN:C	2.54	0.45
1:A:417:GLY:HA3	1:A:478:TYR:CZ	2.52	0.45
2:B:64:VAL:HG21	2:B:91:ILE:HG12	1.98	0.45
1:C:408:LEU:O	1:C:411:MSE:HB3	2.17	0.45
2:D:194:ILE:H	2:D:216:ASP:CB	2.29	0.45
1:A:1:SER:HB3	1:A:213:ASP:OD2	2.17	0.45
1:A:359:LYS:HG3	1:A:384:HIS:CD2	2.51	0.45
1:A:128:VAL:HG23	1:A:142:PHE:HE2	1.82	0.44
1:A:359:LYS:HZ2	1:A:383:GLY:C	2.20	0.44
1:A:464:LEU:HA	1:A:469:ARG:CZ	2.46	0.44
2:D:217:ILE:HD13	2:D:219:PHE:CE2	2.52	0.44
2:D:254:TYR:OH	2:D:258:MSE:SE	2.85	0.44
2:D:336:TYR:CD2	2:D:343:GLN:NE2	2.85	0.44
1:A:484:TYR:HA	1:A:488:ARG:CZ	2.47	0.44
1:C:245:HIS:CE1	1:C:289:GLN:HE22	2.30	0.44
2:D:209:LEU:O	2:D:212:ARG:N	2.49	0.44
2:D:196:PHE:CZ	2:D:243:THR:HG21	2.51	0.44
1:A:344:GLN:N	1:A:344:GLN:OE1	2.50	0.44
1:A:367:ARG:HB3	1:A:368:ARG:HH11	1.81	0.44
2:B:344:ILE:HA	2:B:347:LEU:HD12	1.99	0.44
1:C:263:ASP:O	1:C:267:THR:OG1	2.27	0.44
1:C:323:MSE:CG	1:C:354:LEU:HB3	2.47	0.44
2:B:441:LEU:HD23	2:B:441:LEU:HA	1.73	0.44
2:D:224:LEU:CB	2:D:256:LYS:NZ	2.81	0.44
2:D:290:ILE:HD11	2:D:355:LEU:CB	2.39	0.44
2:B:427:ARG:NH1	2:B:427:ARG:CG	2.81	0.44
1:C:117:LEU:HD23	1:C:119:GLN:O	2.18	0.44
1:C:327:SER:C	1:C:333:LYS:NZ	2.70	0.44
1:C:432:PHE:CE1	1:C:484:TYR:CE2	3.06	0.44
2:D:219:PHE:CD1	2:D:247:VAL:HG12	2.51	0.44
2:D:236:LEU:C	2:D:268:LYS:HZ1	2.14	0.44
1:A:369:ARG:O	1:A:370:ILE:C	2.55	0.44
2:B:7:TYR:O	2:B:12:THR:HG21	2.18	0.44
2:B:304:VAL:CG1	2:B:330:TYR:HE2	2.30	0.44
2:D:122:LYS:HG2	2:D:123:GLN:OE1	2.18	0.44
2:D:217:ILE:CD1	2:D:219:PHE:CE2	3.01	0.44
2:D:310:LEU:HB3	2:D:312:PHE:CE1	2.53	0.44
2:D:307:LEU:HD22	2:D:410:GLU:OE2	2.17	0.44
1:C:141:TYR:CB	1:C:147:TYR:HE1	2.31	0.44
1:C:324:ILE:HD11	1:C:357:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:LEU:HG	1:C:359:LYS:HA	1.99	0.44
2:D:108:LEU:HD23	2:D:114:LEU:HA	1.99	0.44
2:B:217:ILE:HG23	2:B:245:THR:HB	2.00	0.44
1:C:467:GLN:HB3	1:C:468:GLY:HA2	2.00	0.44
1:C:308:LEU:O	1:C:485:LEU:HB2	2.18	0.44
2:D:174:LYS:N	2:D:174:LYS:HD3	2.31	0.44
2:D:192:ASP:HB3	2:D:193:HIS:ND1	2.33	0.44
2:D:236:LEU:HA	2:D:268:LYS:NZ	2.33	0.44
1:A:256:ILE:HB	1:A:293:TYR:CD2	2.53	0.43
1:C:80:THR:OG1	1:C:82:ASP:HB2	2.18	0.43
2:D:151:ARG:NH1	4:D:501:HOH:O	2.49	0.43
2:D:301:ASP:O	2:D:305:GLN:OE1	2.36	0.43
1:A:462:ILE:CA	1:A:465:PHE:H	2.32	0.43
2:B:359:HIS:CD2	2:B:382:GLN:HE21	2.28	0.43
2:B:380:PHE:HB3	2:B:397:ASP:O	2.17	0.43
1:C:167:TYR:CE2	2:D:150:GLU:OE2	2.71	0.43
1:A:202:ARG:NH2	1:A:230:GLU:OE1	2.52	0.43
2:B:378:LEU:CD2	2:B:394:HIS:HD2	2.31	0.43
1:C:108:GLN:CD	1:C:109:ASP:N	2.63	0.43
1:C:130:TYR:HE1	1:C:140:ASP:OD1	2.01	0.43
2:D:297:ILE:HD12	2:D:358:ASN:HB3	2.00	0.43
2:D:251:LEU:N	2:D:430:ASN:HD21	2.05	0.43
1:A:338:LEU:H	1:A:338:LEU:CD1	2.23	0.43
2:B:235:ILE:HD12	2:B:243:THR:OG1	2.19	0.43
1:A:335:ILE:HD13	1:A:366:LEU:HD21	2.00	0.43
2:B:191:LEU:HD22	2:B:194:ILE:HD11	1.99	0.43
2:B:244:GLN:CD	2:B:268:LYS:HZ3	2.18	0.43
1:C:141:TYR:HB2	1:C:147:TYR:HE1	1.84	0.43
1:C:387:LEU:HB2	1:C:390:ILE:HG12	2.00	0.43
1:C:406:PHE:HZ	1:C:411:MSE:HE2	1.83	0.43
2:D:377:ILE:O	2:D:378:LEU:HD23	2.18	0.43
2:D:362:GLN:CB	2:D:384:LEU:HD21	2.40	0.43
1:A:382:LYS:NZ	1:A:385:ALA:HB2	2.32	0.43
1:C:408:LEU:HA	1:C:408:LEU:HD23	1.65	0.43
1:C:426:ARG:HA	1:C:427:TYR:HA	1.61	0.43
1:A:282:GLN:HG3	1:A:427:TYR:CZ	2.54	0.43
1:C:324:ILE:HG13	1:C:355:ASP:O	2.19	0.43
2:D:250:ASP:HA	2:D:430:ASN:ND2	2.33	0.43
1:A:151:TYR:CE1	2:B:153:VAL:HG11	2.53	0.43
1:A:370:ILE:HG23	1:A:370:ILE:HD12	1.70	0.43
1:A:404:GLU:OE2	1:A:406:PHE:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:VAL:CG2	1:A:420:LEU:HD21	2.47	0.43
1:A:440:TYR:CD1	1:A:460:LYS:HB3	2.52	0.43
2:B:196:PHE:CZ	2:B:243:THR:HG21	2.54	0.43
2:B:378:LEU:CD2	2:B:394:HIS:CD2	3.02	0.43
2:D:272:LEU:HD21	2:D:436:LEU:HD22	1.97	0.43
2:B:94:ALA:HB2	2:B:103:LYS:HB2	2.01	0.43
2:B:212:ARG:HD3	2:B:242:ARG:NH1	2.34	0.43
1:A:366:LEU:HD12	1:A:381:LEU:CD1	2.49	0.43
1:A:357:TYR:HD1	1:A:387:LEU:HD11	1.82	0.43
2:D:184:LEU:CA	2:D:189:LEU:HD21	2.41	0.43
2:D:298:GLU:N	2:D:357:ILE:HG22	2.33	0.43
1:A:188:ARG:NH1	1:A:189:PHE:O	2.52	0.42
1:A:192:ARG:NH1	1:A:203:TYR:CE1	2.87	0.42
1:A:250:ALA:HB3	1:A:257:LEU:HD23	2.01	0.42
1:A:465:PHE:O	1:A:467:GLN:NE2	2.52	0.42
1:A:469:ARG:O	1:A:473:MSE:N	2.52	0.42
2:B:5:PHE:HA	2:B:197:ASN:OD1	2.18	0.42
1:C:17:VAL:HG11	1:C:220:ARG:HE	1.83	0.42
1:C:181:ASP:CB	1:C:183:GLN:HE21	2.28	0.42
1:C:365:LYS:O	1:C:368:ARG:HB2	2.19	0.42
2:D:305:GLN:O	2:D:308:PRO:HD3	2.19	0.42
2:B:150:GLU:O	2:B:164:THR:HG23	2.18	0.42
2:B:3:GLN:OE1	2:B:28:THR:OG1	2.30	0.42
2:D:355:LEU:HB3	2:D:357:ILE:HG12	2.02	0.42
2:B:403:GLN:O	2:B:406:SER:N	2.42	0.42
1:C:478:TYR:N	1:C:478:TYR:CD1	2.86	0.42
2:D:220:TRP:O	2:D:249:PRO:HD2	2.19	0.42
2:D:244:GLN:N	2:D:244:GLN:CD	2.72	0.42
2:D:246:ILE:O	2:D:269:PHE:HB2	2.20	0.42
1:A:23:TYR:HD1	1:A:305:VAL:O	2.02	0.42
2:B:261:ALA:HB3	2:B:266:GLN:HG2	2.01	0.42
2:B:288:ALA:HA	2:B:353:ILE:HD11	2.01	0.42
1:C:81:LEU:HG	1:C:125:VAL:CG2	2.49	0.42
1:C:167:TYR:CZ	2:D:150:GLU:OE2	2.73	0.42
2:D:314:ILE:HG21	2:D:324:LEU:HD11	2.01	0.42
2:D:44:PRO:HB3	2:D:183:PHE:CG	2.55	0.42
2:B:195:LEU:HB3	2:B:219:PHE:CE1	2.55	0.42
2:B:314:ILE:HB	2:B:335:LEU:CD2	2.48	0.42
2:B:89:ALA:HB2	2:B:107:TRP:CE3	2.55	0.42
1:C:391:TYR:O	1:C:418:LEU:HD11	2.19	0.42
1:C:420:LEU:C	1:C:421:ILE:HD13	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:194:ILE:CD1	2:D:242:ARG:HH11	2.32	0.42
1:A:367:ARG:HA	1:A:370:ILE:CG1	2.50	0.42
1:A:464:LEU:HA	1:A:469:ARG:NE	2.35	0.42
2:B:44:PRO:HB3	2:B:183:PHE:CG	2.55	0.42
2:B:422:LEU:N	2:B:422:LEU:HD23	2.34	0.42
2:D:210:THR:HG22	2:D:241:LEU:HG	2.02	0.42
2:D:285:ARG:HB2	2:D:285:ARG:HE	1.21	0.42
2:D:324:LEU:C	2:D:324:LEU:HD23	2.40	0.42
1:A:354:LEU:C	1:A:354:LEU:HD12	2.40	0.42
1:A:464:LEU:HD12	1:A:469:ARG:NE	2.35	0.42
2:B:298:GLU:HB2	2:B:359:HIS:CE1	2.54	0.42
1:C:338:LEU:HD22	1:C:338:LEU:N	2.34	0.42
2:D:51:ASP:OD2	2:D:125:ARG:NH1	2.53	0.42
2:D:180:ILE:O	2:D:184:LEU:HG	2.19	0.42
2:D:19:LEU:HD12	2:D:20:LEU:N	2.35	0.42
2:D:236:LEU:HA	2:D:268:LYS:CE	2.50	0.42
2:D:377:ILE:HG13	2:D:425:GLN:HE22	1.84	0.42
1:A:334:HIS:CD2	1:A:336:ASP:OD2	2.73	0.42
1:A:366:LEU:CD1	1:A:370:ILE:CD1	2.97	0.42
1:C:66:TYR:CD2	1:C:177:MSE:HE1	2.54	0.42
1:C:329:LEU:HD21	1:C:363:GLU:OE1	2.19	0.42
1:C:362:GLU:HG3	1:C:365:LYS:CD	2.49	0.42
1:C:437:LYS:CD	1:C:476:HIS:CD2	3.02	0.42
2:D:263:ALA:HA	2:D:266:GLN:HG3	2.02	0.42
2:D:400:GLN:HB2	2:D:401:PRO:CD	2.50	0.42
2:D:419:ARG:CG	2:D:423:GLN:HE22	2.33	0.42
2:B:107:TRP:NE1	2:B:118:GLU:OE2	2.50	0.42
2:B:215:GLN:HA	2:B:242:ARG:O	2.20	0.42
1:C:111:GLN:CD	2:D:174:LYS:NZ	2.73	0.42
1:C:8:LEU:HD11	1:C:222:THR:HB	2.02	0.42
2:D:9:ASN:OD1	2:D:11:GLU:HG2	2.20	0.42
1:C:24:ARG:CD	1:C:493:TRP:CZ2	3.03	0.42
1:C:453:ILE:CD1	1:C:454:ILE:HG13	2.50	0.42
2:D:307:LEU:HD13	2:D:310:LEU:CD2	2.46	0.42
1:A:397:TYR:HB3	1:A:420:LEU:HD13	2.00	0.41
1:A:426:ARG:HA	1:A:427:TYR:HA	1.74	0.41
1:C:391:TYR:O	1:C:394:TYR:HB2	2.20	0.41
1:C:490:GLU:O	1:C:494:THR:HB	2.19	0.41
2:D:297:ILE:CG1	2:D:300:LEU:HD23	2.50	0.41
1:A:311:LEU:HD23	1:A:415:GLY:O	2.20	0.41
1:A:363:GLU:C	1:A:366:LEU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:SER:C	1:C:333:LYS:HZ1	2.23	0.41
1:C:483:ASN:HA	1:C:488:ARG:HD3	2.02	0.41
2:D:419:ARG:HG2	2:D:423:GLN:NE2	2.35	0.41
1:A:33:GLN:OE1	1:A:501:ARG:NH1	2.40	0.41
2:B:1:MSE:HE2	2:B:195:LEU:CD1	2.44	0.41
1:C:6:ILE:HB	1:C:218:LEU:HD12	2.02	0.41
1:C:29:ARG:HH21	1:C:58:LEU:HG	1.84	0.41
2:D:223:PRO:HG2	2:D:225:TYR:OH	2.21	0.41
1:A:157:ASP:OD1	1:A:157:ASP:O	2.38	0.41
1:A:202:ARG:O	1:A:206:GLN:HG3	2.21	0.41
2:B:59:LEU:HD23	2:B:59:LEU:HA	1.87	0.41
1:C:22:ALA:O	1:C:26:GLN:HG3	2.20	0.41
1:C:285:ILE:HA	1:C:288:GLN:OE1	2.21	0.41
1:C:282:GLN:HG3	1:C:427:TYR:CZ	2.55	0.41
2:D:64:VAL:HG11	2:D:105:VAL:HG21	2.01	0.41
2:D:272:LEU:HD23	2:D:272:LEU:HA	1.94	0.41
2:D:295:ASP:CB	2:D:296:GLN:HA	2.45	0.41
2:D:385:HIS:HA	2:D:386:ASP:C	2.40	0.41
1:A:357:TYR:OH	1:A:394:TYR:OH	2.37	0.41
2:B:238:ASN:OD1	2:B:240:GLN:N	2.44	0.41
2:B:397:ASP:HB2	2:B:400:GLN:HB2	2.03	0.41
1:C:1:SER:OG	1:C:213:ASP:OD2	2.24	0.41
1:C:31:ILE:O	1:C:32:GLN:HB2	2.21	0.41
1:C:497:LEU:HB3	1:C:501:ARG:NH1	2.36	0.41
1:A:21:GLN:NE2	1:A:219:ASP:OD2	2.54	0.41
1:C:335:ILE:HB	1:C:338:LEU:HB2	2.02	0.41
2:D:272:LEU:HD23	2:D:436:LEU:CD2	2.37	0.41
2:D:378:LEU:HD11	2:D:409:GLU:HB3	2.03	0.41
1:A:281:ALA:O	1:A:285:ILE:HG12	2.21	0.41
2:B:228:LEU:HD13	2:B:232:MSE:HG2	2.03	0.41
2:B:272:LEU:CD1	2:B:273:GLY:N	2.57	0.41
1:C:21:GLN:HG2	1:C:24:ARG:NH1	2.36	0.41
1:A:335:ILE:HD13	1:A:366:LEU:CD2	2.50	0.41
1:A:357:TYR:CE2	1:A:382:LYS:HB3	2.56	0.41
2:B:413:CYS:N	2:B:417:GLN:OE1	2.54	0.41
2:D:227:GLU:OE1	2:D:228:LEU:HB2	2.21	0.41
2:D:297:ILE:HG22	2:D:357:ILE:CG2	2.50	0.41
1:A:295:ASP:C	1:A:296:LYS:HG2	2.41	0.41
1:A:338:LEU:HA	1:A:341:ALA:HB3	2.02	0.41
1:A:488:ARG:NH2	1:A:489:VAL:HG22	2.35	0.41
2:B:348:TYR:CE1	2:B:369:LYS:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:LYS:HA	1:C:368:ARG:HG3	2.03	0.41
2:D:163:LEU:HD13	2:D:179:PHE:CE1	2.55	0.41
2:D:206:SER:HB2	2:D:216:ASP:OD2	2.20	0.41
2:D:235:ILE:HA	2:D:235:ILE:HD12	1.75	0.41
1:A:173:VAL:HG21	2:B:144:TYR:CE2	2.54	0.41
1:A:465:PHE:HA	1:A:467:GLN:HE22	1.85	0.41
2:B:253:THR:O	2:B:257:ALA:N	2.48	0.41
1:C:324:ILE:HD11	1:C:357:TYR:CD2	2.56	0.41
1:C:321:TYR:HB3	1:C:352:LEU:HD12	2.03	0.41
1:A:337:TRP:HZ3	1:A:423:PHE:CZ	2.39	0.41
1:A:321:TYR:N	1:A:395:GLU:OE2	2.51	0.41
1:A:397:TYR:CD2	1:A:420:LEU:HD12	2.56	0.41
2:B:123:GLN:N	2:B:123:GLN:OE1	2.51	0.41
2:B:354:TYR:O	2:B:377:ILE:HA	2.21	0.41
1:C:321:TYR:CD2	1:C:350:PRO:HG2	2.56	0.41
2:D:246:ILE:O	2:D:269:PHE:CB	2.69	0.41
2:D:291:LEU:CD2	2:D:315:ALA:HB3	2.51	0.41
2:D:392:GLN:C	2:D:394:HIS:N	2.74	0.41
1:A:352:LEU:HA	1:A:352:LEU:HD12	1.77	0.40
1:A:364:ASP:HB3	1:A:368:ARG:NH2	2.36	0.40
1:A:460:LYS:HD3	1:A:463:ALA:HB3	2.03	0.40
1:A:469:ARG:O	1:A:473:MSE:HG3	2.21	0.40
2:B:163:LEU:HD11	2:B:165:LEU:HD21	2.03	0.40
2:D:264:ASP:O	2:D:267:GLN:NE2	2.51	0.40
1:A:11:GLY:N	1:A:14:SER:HB2	2.34	0.40
1:A:470:GLN:CG	1:A:471:GLN:N	2.83	0.40
1:C:136:LEU:O	1:C:152:PHE:HB2	2.21	0.40
1:C:318:ARG:HH22	1:C:471:GLN:NE2	2.19	0.40
2:D:209:LEU:O	2:D:211:GLY:N	2.53	0.40
2:D:220:TRP:HD1	2:D:248:ILE:HG23	1.86	0.40
1:A:84:VAL:O	1:A:88:VAL:HG23	2.21	0.40
1:C:187:TYR:CD2	1:C:200:LEU:HD12	2.56	0.40
1:C:498:LYS:N	1:C:498:LYS:HD2	2.29	0.40
2:D:1:MSE:HE2	2:D:195:LEU:HD11	2.04	0.40
2:D:246:ILE:O	2:D:269:PHE:CA	2.69	0.40
2:D:341:LEU:HA	2:D:341:LEU:HD23	1.86	0.40
1:A:421:ILE:HD12	1:A:440:TYR:HB2	2.03	0.40
1:A:466:SER:N	1:A:467:GLN:HE21	2.20	0.40
2:D:373:ASN:HB2	2:D:375:LEU:HD23	2.03	0.40
1:A:449:VAL:CG1	1:A:452:GLN:HE22	2.32	0.40
1:A:195:TYR:CE2	2:B:109:ASP:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:HIS:CD2	2:B:382:GLN:NE2	2.83	0.40
1:C:28:LEU:HA	1:C:28:LEU:HD23	1.80	0.40
1:C:50:HIS:CE1	1:C:118:ARG:HD2	2.56	0.40
2:D:168:GLU:OE2	2:D:186:ARG:NH2	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	501/503 (100%)	482 (96%)	16 (3%)	3 (1%)	30	66
1	C	501/503 (100%)	480 (96%)	21 (4%)	0	100	100
2	B	445/447 (100%)	418 (94%)	26 (6%)	1 (0%)	52	83
2	D	443/447 (99%)	413 (93%)	30 (7%)	0	100	100
All	All	1890/1900 (100%)	1793 (95%)	93 (5%)	4 (0%)	52	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	GLU
1	A	474	SER
1	A	370	ILE
2	B	78	VAL

### 5.3.2 Protein sidechains [i](#)

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	435/429 (101%)	414 (95%)	21 (5%)	31	67
1	C	435/429 (101%)	421 (97%)	14 (3%)	46	81
2	B	392/384 (102%)	381 (97%)	11 (3%)	51	83
2	D	392/384 (102%)	379 (97%)	13 (3%)	45	80
All	All	1654/1626 (102%)	1595 (96%)	59 (4%)	42	77

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	GLU
1	A	95	SER
1	A	120	GLU
1	A	135	ARG
1	A	184	GLU
1	A	199	GLU
1	A	222	THR
1	A	230	GLU
1	A	249	ASN
1	A	253	ASP
1	A	259	ASN
1	A	283	LYS
1	A	290	PHE
1	A	296	LYS
1	A	334	HIS
1	A	363	GLU
1	A	377	ASP
1	A	380	ARG
1	A	386	ASP
1	A	469	ARG
1	A	488	ARG
2	B	12	THR
2	B	20	LEU
2	B	119	ARG
2	B	212	ARG
2	B	271	HIS
2	B	286	LYS
2	B	317	LEU
2	B	323	LYS
2	B	386	ASP

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Mol	Chain	Res	Type
2	B	387	ARG
2	B	406	SER
1	C	95	SER
1	C	118	ARG
1	C	147	TYR
1	C	157	ASP
1	C	233	GLN
1	C	318	ARG
1	C	323	MSE
1	C	355	ASP
1	C	387	LEU
1	C	434	ASP
1	C	457	PHE
1	C	476	HIS
1	C	485	LEU
1	C	493	TRP
2	D	10	GLN
2	D	47	TYR
2	D	49	LEU
2	D	60	PHE
2	D	136	GLN
2	D	171	ARG
2	D	189	LEU
2	D	242	ARG
2	D	272	LEU
2	D	280	ARG
2	D	306	SER
2	D	309	GLN
2	D	338	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	127	HIS
1	A	249	ASN
1	A	259	ASN
1	A	288	GLN
1	A	297	GLN
1	A	334	HIS
1	A	467	GLN
1	A	470	GLN

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Mol	Chain	Res	Type
2	B	231	ASN
2	B	359	HIS
2	B	362	GLN
2	B	382	GLN
2	B	430	ASN
1	C	163	GLN
1	C	183	GLN
1	C	209	GLN
1	C	211	GLN
1	C	242	HIS
1	C	245	HIS
1	C	289	GLN
1	C	310	GLN
1	C	476	HIS
1	C	495	GLN
2	D	309	GLN
2	D	338	ASN
2	D	388	HIS
2	D	430	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	497/503 (98%)	0.28	27 (5%) 29 24	11, 51, 121, 141	0
1	C	497/503 (98%)	0.53	37 (7%) 17 12	22, 71, 119, 141	0
2	B	439/447 (98%)	0.32	18 (4%) 41 35	14, 62, 105, 131	0
2	D	437/447 (97%)	0.48	39 (8%) 12 8	15, 77, 118, 161	0
All	All	1870/1900 (98%)	0.40	121 (6%) 22 16	11, 67, 117, 161	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	354	LEU	6.8
1	C	448	HIS	6.7
1	C	379	ILE	6.4
1	C	325	THR	5.4
2	B	401	PRO	4.9
1	A	354	LEU	4.8
2	B	406	SER	4.7
1	C	381	LEU	4.6
1	A	373	ALA	4.5
1	C	396	LEU	4.2
1	C	369	ARG	4.2
1	C	330	ALA	3.9
2	D	261	ALA	3.9
2	D	270	LEU	3.8
1	A	448	HIS	3.7
2	B	357	ILE	3.7
2	D	228	LEU	3.6
2	B	331	LYS	3.6
2	D	383	THR	3.6
1	C	440	TYR	3.6
2	D	395	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	338	LEU	3.4
2	D	213	ALA	3.4
1	A	352	LEU	3.4
1	A	453	ILE	3.3
2	D	385	HIS	3.3
1	C	90	GLY	3.2
1	C	449	VAL	3.2
2	B	288	ALA	3.1
1	C	365	LYS	3.1
2	D	264	ASP	3.1
2	D	211	GLY	3.1
1	A	380	ARG	3.1
2	D	357	ILE	3.1
2	D	234	LEU	3.0
2	B	271	HIS	3.0
1	C	398	LEU	3.0
2	B	380	PHE	3.0
1	C	356	ILE	3.0
2	B	407	ILE	3.0
1	C	351	GLU	3.0
2	D	365	GLN	3.0
1	C	391	TYR	2.9
2	D	260	LEU	2.9
2	D	226	ASP	2.9
2	D	243	THR	2.9
1	A	320	PRO	2.9
2	B	310	LEU	2.8
2	D	217	ILE	2.8
1	C	363	GLU	2.8
2	D	437	TYR	2.8
1	A	488	ARG	2.8
2	B	305	GLN	2.8
2	D	423	GLN	2.8
2	B	385	HIS	2.8
1	A	449	VAL	2.7
1	A	329	LEU	2.7
2	D	218	LEU	2.7
1	A	367	ARG	2.7
2	D	235	ILE	2.7
1	C	432	PHE	2.7
1	C	328	ARG	2.7
2	D	379	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	367	ARG	2.6
1	A	326	ALA	2.6
2	D	219	PHE	2.6
2	D	257	ALA	2.6
2	D	246	ILE	2.6
2	D	225	TYR	2.6
1	C	326	ALA	2.6
1	C	368	ARG	2.6
2	D	310	LEU	2.6
1	C	380	ARG	2.6
1	C	341	ALA	2.5
1	A	366	LEU	2.5
1	C	464	LEU	2.5
1	C	334	HIS	2.5
2	B	392	GLN	2.5
2	D	256	LYS	2.5
2	B	400	GLN	2.5
1	A	379	ILE	2.4
2	B	361	GLY	2.4
1	A	464	LEU	2.4
2	D	253	THR	2.4
1	A	360	GLY	2.4
1	A	372	GLU	2.4
2	B	303	LEU	2.4
1	C	371	GLU	2.4
2	D	269	PHE	2.4
2	B	213	ALA	2.4
1	A	465	PHE	2.4
2	D	267	GLN	2.4
2	D	265	GLN	2.3
1	A	370	ILE	2.3
2	B	300	LEU	2.3
2	D	398	SER	2.3
2	D	201	TYR	2.3
1	A	337	TRP	2.3
1	A	362	GLU	2.3
1	A	364	ASP	2.2
1	C	442	LEU	2.2
1	C	465	PHE	2.2
1	C	378	TYR	2.2
2	D	206	SER	2.2
2	D	413	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	466	SER	2.2
1	C	344	GLN	2.2
1	C	316	GLU	2.2
1	C	339	VAL	2.2
1	C	457	PHE	2.1
2	D	396	PHE	2.1
2	D	134	SER	2.1
1	A	420	LEU	2.1
1	A	330	ALA	2.1
2	D	268	LYS	2.1
1	A	339	VAL	2.1
1	C	87	GLN	2.1
1	C	455	ALA	2.0
2	B	393	GLN	2.0
1	C	407	GLY	2.0
2	D	415	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	A	601	1/1	0.92	0.31	-	14,14,14,14	0
3	MG	B	501	1/1	0.98	0.33	-	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.