



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:47 PM GMT

PDB ID : 4PW8
Title : Human tryptophan 2,3-dioxygenase
Authors : Meng, B.; Wu, D.; Gu, J.H.; Ouyang, S.Y.; Ding, W.; Liu, Z.J.
Deposited on : 2014-03-19
Resolution : 2.90 Å(reported)

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

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

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

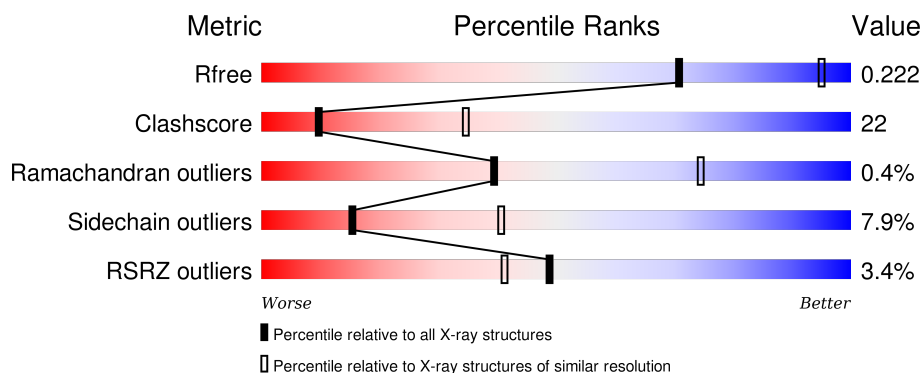
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	373	<div> <div>0%</div> <div> <div>57%</div> <div>23%</div> <div>•</div> <div>18%</div> </div> </div>
1	B	373	<div> <div>2%</div> <div> <div>59%</div> <div>15%</div> <div>5%</div> <div>•</div> <div>21%</div> </div> </div>
1	C	373	<div> <div>2%</div> <div> <div>60%</div> <div>20%</div> <div>•</div> <div>•</div> <div>16%</div> </div> </div>
1	D	373	<div> <div>5%</div> <div> <div>51%</div> <div>21%</div> <div>5%</div> <div>23%</div> </div> </div>
1	E	373	<div> <div>4%</div> <div> <div>52%</div> <div>22%</div> <div>•</div> <div>21%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	373	<div><div>%</div><div><div></div><div>56%</div><div>20%</div><div>5%</div><div>19%</div></div></div>
1	G	373	<div><div>3%</div><div><div></div><div>53%</div><div>21%</div><div>6%</div><div>18%</div></div></div>
1	H	373	<div><div>3%</div><div><div></div><div>62%</div><div>17%</div><div>•</div><div>19%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20451 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 Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2592	1669	447	466	10			
1	B	296	Total	C	N	O	S	0	0	0
			2510	1627	432	441	10			
1	C	313	Total	C	N	O	S	0	0	0
			2660	1711	463	475	11			
1	D	288	Total	C	N	O	S	0	0	0
			2449	1587	424	428	10			
1	E	293	Total	C	N	O	S	0	0	0
			2481	1604	428	439	10			
1	F	303	Total	C	N	O	S	0	0	0
			2564	1658	444	452	10			
1	G	304	Total	C	N	O	S	0	0	0
			2582	1668	446	458	10			
1	H	301	Total	C	N	O	S	0	0	0
			2557	1651	441	455	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	SER	-	EXPRESSION TAG	UNP P48775
A	17	ASN	-	EXPRESSION TAG	UNP P48775
A	18	ALA	-	EXPRESSION TAG	UNP P48775
B	16	SER	-	EXPRESSION TAG	UNP P48775
B	17	ASN	-	EXPRESSION TAG	UNP P48775
B	18	ALA	-	EXPRESSION TAG	UNP P48775
C	16	SER	-	EXPRESSION TAG	UNP P48775
C	17	ASN	-	EXPRESSION TAG	UNP P48775
C	18	ALA	-	EXPRESSION TAG	UNP P48775
D	16	SER	-	EXPRESSION TAG	UNP P48775
D	17	ASN	-	EXPRESSION TAG	UNP P48775
D	18	ALA	-	EXPRESSION TAG	UNP P48775
E	16	SER	-	EXPRESSION TAG	UNP P48775

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Chain	Residue	Modelled	Actual	Comment	Reference
E	17	ASN	-	EXPRESSION TAG	UNP P48775
E	18	ALA	-	EXPRESSION TAG	UNP P48775
F	16	SER	-	EXPRESSION TAG	UNP P48775
F	17	ASN	-	EXPRESSION TAG	UNP P48775
F	18	ALA	-	EXPRESSION TAG	UNP P48775
G	16	SER	-	EXPRESSION TAG	UNP P48775
G	17	ASN	-	EXPRESSION TAG	UNP P48775
G	18	ALA	-	EXPRESSION TAG	UNP P48775
H	16	SER	-	EXPRESSION TAG	UNP P48775
H	17	ASN	-	EXPRESSION TAG	UNP P48775
H	18	ALA	-	EXPRESSION TAG	UNP P48775

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Co 1 1	0	0

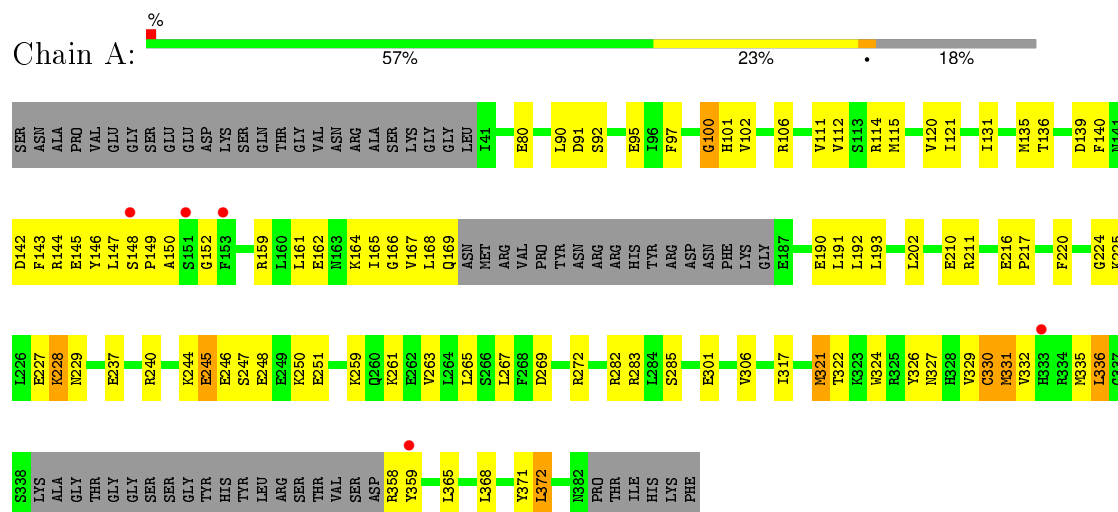
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	11	Total O 11 11	0	0
3	B	5	Total O 5 5	0	0
3	C	5	Total O 5 5	0	0
3	E	13	Total O 13 13	0	0
3	F	7	Total O 7 7	0	0
3	G	2	Total O 2 2	0	0
3	H	12	Total O 12 12	0	0

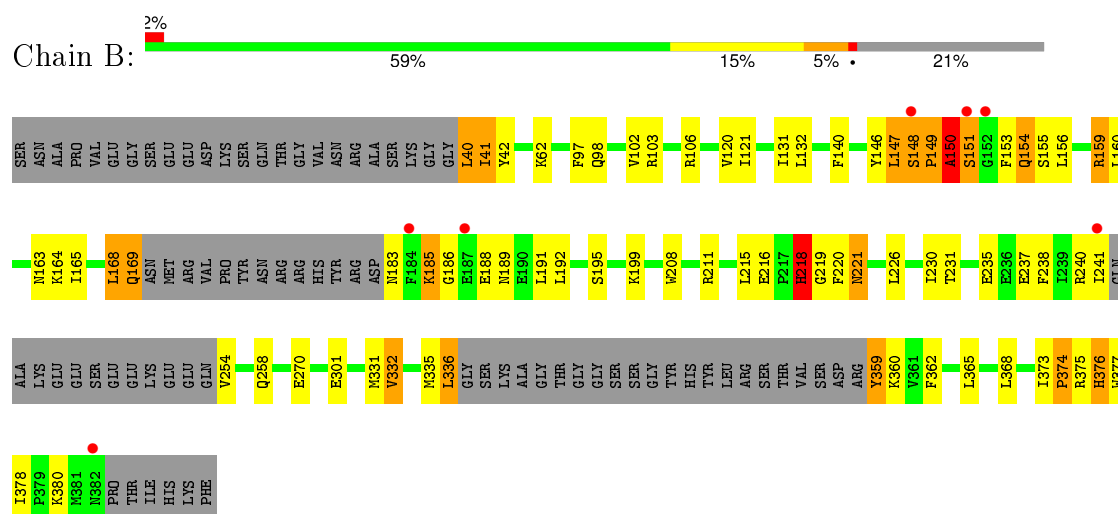
3 Residue-property plots

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: Tryptophan 2,3-dioxygenase

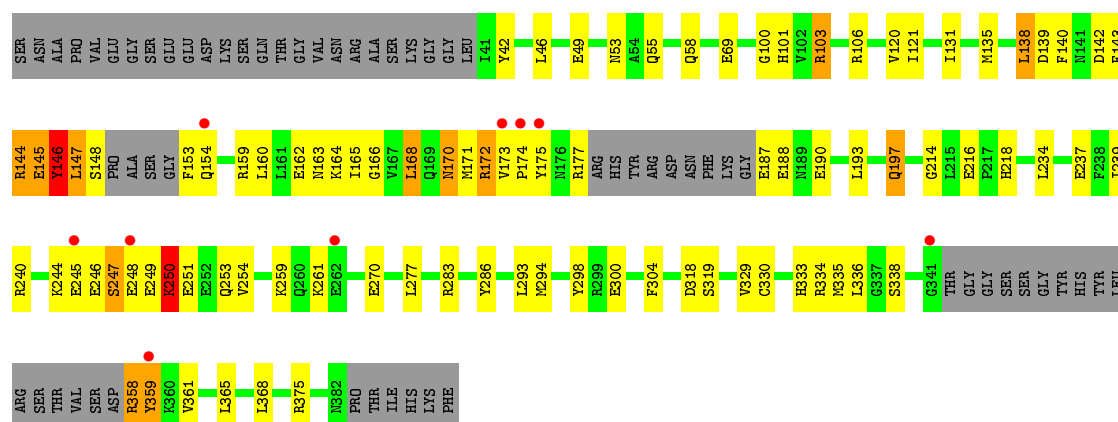


• Molecule 1: Tryptophan 2,3-dioxygenase

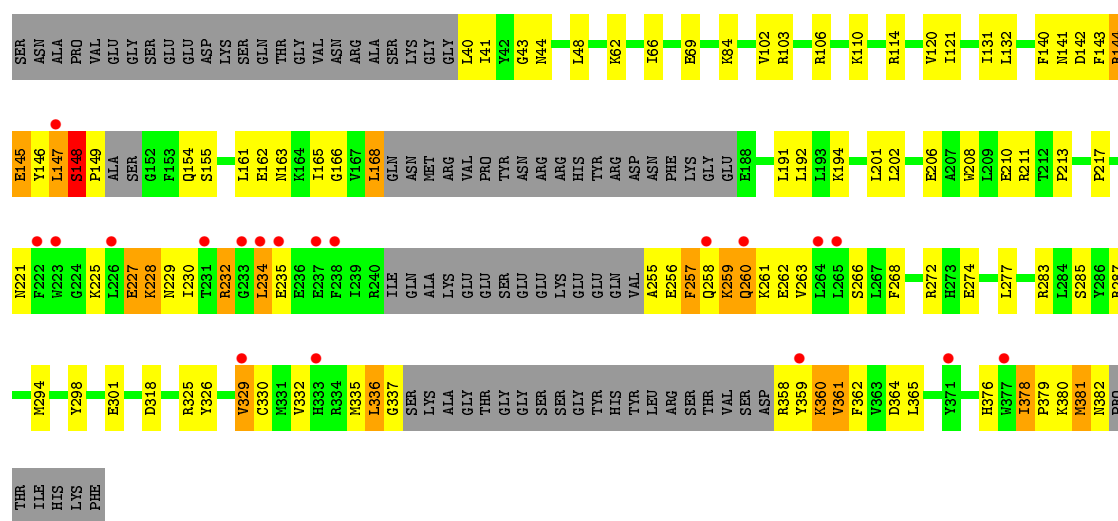


• Molecule 1: Tryptophan 2,3-dioxygenase

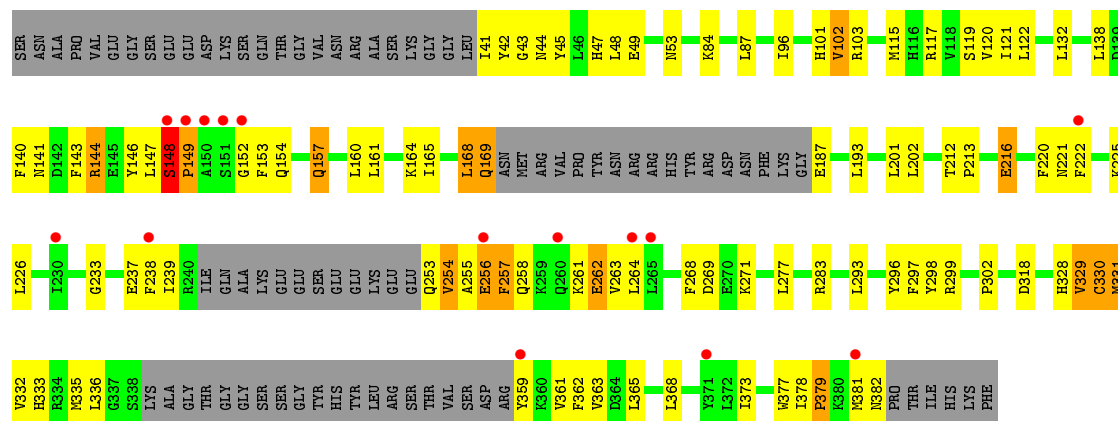




• Molecule 1: Tryptophan 2,3-dioxygenase



• Molecule 1: Tryptophan 2,3-dioxygenase



• Molecule 1: Tryptophan 2,3-dioxygenase

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.33Å 156.92Å 160.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 2.90 49.73 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.73-2.90) 96.0 (49.73-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.204 , 0.222 0.202 , 0.222	Depositor DCC
R_{free} test set	1927 reflections (2.66%)	DCC
Wilson B-factor (Å ²)	60.5	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.2	EDS
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 75388 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20451	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.81	1/2648 (0.0%)	0.69	2/3561 (0.1%)
1	B	0.65	2/2566 (0.1%)	0.70	5/3452 (0.1%)
1	C	0.63	0/2716	0.67	1/3649 (0.0%)
1	D	0.58	0/2503	0.65	2/3365 (0.1%)
1	E	0.61	2/2536 (0.1%)	0.64	3/3412 (0.1%)
1	F	0.58	1/2620 (0.0%)	0.66	2/3522 (0.1%)
1	G	0.63	1/2638 (0.0%)	0.66	2/3545 (0.1%)
1	H	0.53	0/2612	0.61	0/3513
All	All	0.63	7/20839 (0.0%)	0.66	17/28019 (0.1%)

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	C	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	379	PRO	N-CD	7.11	1.57	1.47
1	F	149	PRO	N-CD	5.71	1.55	1.47
1	A	324	TRP	CB-CG	-5.65	1.40	1.50
1	E	379	PRO	N-CD	-5.62	1.40	1.47
1	B	149	PRO	N-CD	5.37	1.55	1.47
1	E	149	PRO	N-CD	5.21	1.55	1.47
1	B	374	PRO	N-CD	5.11	1.55	1.47

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	ALA	N-CA-C	-8.30	88.59	111.00
1	G	148	SER	C-N-CD	6.41	141.85	128.40
1	F	166	GLY	N-CA-C	-6.09	97.86	113.10
1	E	216	GLU	C-N-CD	5.97	140.94	128.40
1	D	148	SER	C-N-CD	5.95	140.89	128.40
1	A	336	LEU	CA-CB-CG	5.88	128.82	115.30
1	B	373	ILE	C-N-CD	5.78	140.53	128.40
1	C	146	TYR	N-CA-CB	-5.72	100.31	110.60
1	E	148	SER	C-N-CD	5.71	140.40	128.40
1	A	100	GLY	N-CA-C	-5.71	98.83	113.10
1	D	378	ILE	C-N-CD	5.60	140.17	128.40
1	G	149	PRO	CA-N-CD	-5.51	103.78	111.50
1	B	153	PHE	N-CA-C	-5.38	96.47	111.00
1	E	379	PRO	N-CD-CG	5.21	111.01	103.20
1	B	218	HIS	N-CA-C	-5.07	97.31	111.00
1	F	149	PRO	CA-N-CD	-5.07	104.41	111.50
1	B	186	GLY	N-CA-C	5.01	125.63	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	146	TYR	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	2592	0	2588	83	0
1	B	2510	0	2520	94	0
1	C	2660	0	2660	125	0
1	D	2449	0	2460	141	0
1	E	2481	0	2483	130	0
1	F	2564	0	2575	136	0
1	G	2582	0	2587	187	0
1	H	2557	0	2560	66	0
2	H	1	0	0	0	0
3	A	11	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	5	0	0	3	0
3	E	13	0	0	4	0
3	F	7	0	0	2	0
3	G	2	0	0	1	0
3	H	12	0	0	1	0
All	All	20451	0	20433	909	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 22.

All (909) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:GLU:O	1:C:146:TYR:CD1	1.83	1.29
1:G:146:TYR:C	1:G:147:LEU:HD23	1.63	1.18
1:H:187:GLU:HG3	1:H:188:GLU:H	1.02	1.16
1:B:375:ARG:HA	1:B:378:ILE:HD12	1.15	1.13
1:E:144:ARG:NH1	1:E:336:LEU:HD11	1.65	1.11
1:D:336:LEU:HD23	1:D:337:GLY:H	0.98	1.10
1:G:194:LYS:HE3	1:G:198:GLU:OE2	1.48	1.07
1:C:187:GLU:OE1	1:C:187:GLU:N	1.88	1.06
1:F:184:PHE:O	1:F:185:LYS:HD2	1.56	1.05
1:A:159:ARG:HH22	1:A:169:GLN:HG3	1.14	1.04
1:E:144:ARG:HH12	1:E:336:LEU:CD1	1.71	1.03
1:D:144:ARG:HA	1:D:147:LEU:HD22	1.37	1.03
1:C:358:ARG:HA	1:C:359:TYR:CD1	1.93	1.02
1:D:168:LEU:HD12	1:D:168:LEU:H	1.19	1.02
1:E:144:ARG:HH12	1:E:336:LEU:HD11	0.88	1.02
1:G:191:LEU:H	1:G:191:LEU:HD12	1.22	1.02
1:C:247:SER:HB3	1:C:248:GLU:HA	1.40	1.02
1:D:260:GLN:HA	1:D:260:GLN:HE21	1.22	1.01
1:D:361:VAL:HG23	1:D:361:VAL:O	1.60	1.01
1:D:360:LYS:NZ	1:D:360:LYS:HB2	1.76	1.01
1:D:144:ARG:O	1:D:147:LEU:HB2	1.61	1.01
1:C:168:LEU:H	1:C:168:LEU:HD23	1.25	1.01
1:E:147:LEU:HB3	1:E:149:PRO:HD2	1.43	0.99
1:B:154:GLN:HE21	1:B:155:SER:H	1.10	0.99
1:G:40:LEU:HB2	1:G:41:ILE:HD12	1.41	0.99
1:F:358:ARG:HG2	1:F:358:ARG:HH11	1.28	0.97
1:G:140:PHE:CE2	1:G:335:MET:HB3	2.00	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LEU:HB2	1:B:148:SER:HA	1.47	0.95
1:D:336:LEU:HD23	1:D:337:GLY:N	1.80	0.95
1:D:360:LYS:NZ	1:D:360:LYS:CB	2.30	0.95
1:D:154:GLN:OE1	1:D:155:SER:N	1.99	0.95
1:B:375:ARG:HA	1:B:378:ILE:CD1	1.96	0.94
1:C:187:GLU:HG2	1:C:188:GLU:H	1.33	0.93
1:D:227:GLU:HG3	1:D:268:PHE:CE1	2.02	0.93
1:H:160:LEU:O	1:H:164:LYS:HG3	1.68	0.93
1:H:187:GLU:CG	1:H:188:GLU:H	1.81	0.92
1:E:138:LEU:HB3	1:G:375:ARG:NH1	1.85	0.91
1:D:255:ALA:HA	1:D:256:GLU:CG	2.00	0.91
1:G:146:TYR:O	1:G:147:LEU:HD23	1.70	0.90
1:D:260:GLN:O	1:D:263:VAL:HG12	1.68	0.90
1:F:162:GLU:O	1:F:166:GLY:HA2	1.70	0.90
1:H:358:ARG:HH21	1:H:358:ARG:HG2	1.34	0.89
1:G:380:LYS:HD2	1:G:380:LYS:H	1.36	0.89
1:F:328:HIS:O	1:F:329:VAL:HG22	1.72	0.89
1:G:190:GLU:OE1	1:G:190:GLU:N	2.05	0.89
1:B:156:LEU:CD2	1:B:188:GLU:HG2	2.02	0.89
1:D:227:GLU:HG3	1:D:268:PHE:CD1	2.07	0.89
1:H:187:GLU:HG3	1:H:188:GLU:N	1.86	0.88
1:D:232:ARG:NH1	1:D:232:ARG:HB3	1.89	0.87
1:E:216:GLU:N	1:E:216:GLU:OE1	2.07	0.87
1:F:300:GLU:HG3	1:G:106:ARG:HH12	1.39	0.87
1:G:217:PRO:HA	1:G:221:ASN:HB3	1.56	0.87
1:E:152:GLY:HA2	1:E:153:PHE:HB3	1.55	0.86
1:D:259:LYS:NZ	1:D:260:GLN:HG2	1.89	0.86
1:B:154:GLN:HE21	1:B:155:SER:N	1.71	0.86
1:F:147:LEU:H	1:F:147:LEU:HD12	1.40	0.86
1:E:148:SER:HB3	1:F:40:LEU:N	1.90	0.86
1:C:103:ARG:HG2	3:C:404:HOH:O	1.75	0.86
1:E:149:PRO:CB	1:E:153:PHE:HB2	2.05	0.86
1:A:372:LEU:O	1:A:372:LEU:HD13	1.75	0.85
1:B:159:ARG:NH2	1:B:169:GLN:HE22	1.73	0.85
1:D:362:PHE:HB3	1:D:365:LEU:HD12	1.58	0.85
1:D:255:ALA:HA	1:D:256:GLU:CB	2.05	0.85
1:F:147:LEU:O	1:F:148:SER:OG	1.95	0.85
1:D:360:LYS:HZ3	1:D:360:LYS:CB	1.89	0.85
1:F:42:TYR:O	1:F:42:TYR:CD1	2.30	0.85
1:C:249:GLU:O	1:C:250:LYS:HB2	1.75	0.84
1:G:358:ARG:HH11	1:G:358:ARG:CB	1.90	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:LYS:HZ2	1:D:360:LYS:HB2	1.38	0.84
1:D:168:LEU:HD11	1:D:283:ARG:NH1	1.93	0.84
1:A:159:ARG:NH2	1:A:169:GLN:HG3	1.93	0.83
1:F:329:VAL:HA	1:F:332:VAL:HB	1.61	0.83
1:D:230:ILE:O	1:D:234:LEU:HD23	1.78	0.82
1:C:246:GLU:O	1:C:247:SER:OG	1.95	0.82
1:F:193:LEU:HA	1:F:196:GLU:HG3	1.61	0.82
1:D:255:ALA:HA	1:D:256:GLU:HG3	1.62	0.82
1:B:185:LYS:HB2	1:B:188:GLU:OE1	1.78	0.82
1:G:221:ASN:OD1	1:G:221:ASN:O	1.96	0.81
1:B:98:GLN:HE21	1:B:199:LYS:HD2	1.45	0.81
1:F:162:GLU:O	1:F:166:GLY:CA	2.28	0.81
1:F:184:PHE:O	1:F:185:LYS:CD	2.29	0.81
1:F:62:LYS:HD2	1:F:146:TYR:HD1	1.46	0.81
1:D:336:LEU:CD2	1:D:337:GLY:H	1.87	0.81
1:G:251:GLU:O	1:G:254:VAL:HG12	1.80	0.81
1:G:190:GLU:HA	1:G:192:LEU:N	1.96	0.81
1:D:260:GLN:O	1:D:263:VAL:CG1	2.28	0.80
1:B:374:PRO:HD2	1:B:377:TRP:CD2	2.17	0.80
1:E:144:ARG:NH1	1:E:336:LEU:HD21	1.96	0.80
1:G:190:GLU:CB	1:G:194:LYS:H	1.95	0.80
1:E:149:PRO:HB3	1:E:153:PHE:CB	2.12	0.80
1:C:170:ASN:H	1:C:170:ASN:HD22	1.29	0.80
1:D:259:LYS:C	1:D:259:LYS:HE2	2.02	0.80
1:A:372:LEU:O	1:A:372:LEU:CD1	2.29	0.80
1:D:163:ASN:O	1:D:166:GLY:HA3	1.82	0.80
1:E:149:PRO:HB3	1:E:153:PHE:HB2	1.64	0.79
1:C:42:TYR:CE1	1:C:46:LEU:HD11	2.17	0.79
1:G:154:GLN:HA	1:G:154:GLN:HE21	1.47	0.79
1:B:154:GLN:NE2	1:B:155:SER:H	1.80	0.79
1:F:144:ARG:HA	1:F:147:LEU:HD11	1.65	0.79
1:D:361:VAL:HG22	1:D:362:PHE:CD2	2.18	0.78
1:G:140:PHE:CE2	1:G:335:MET:CB	2.66	0.78
1:D:234:LEU:HD12	1:D:261:LYS:HG3	1.66	0.78
1:G:190:GLU:HA	1:G:193:LEU:H	1.47	0.78
1:B:168:LEU:HD12	1:B:168:LEU:H	1.49	0.78
1:G:188:GLU:OE2	1:G:188:GLU:HA	1.84	0.77
1:F:186:GLY:HA2	1:F:189:ASN:H	1.49	0.77
1:C:247:SER:HB3	1:C:248:GLU:CA	2.14	0.77
1:G:161:LEU:O	1:G:165:ILE:HG12	1.84	0.77
1:C:334:ARG:HH21	1:C:335:MET:CE	1.96	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:VAL:CG2	1:D:361:VAL:O	2.30	0.77
1:F:163:ASN:O	1:F:166:GLY:HA3	1.85	0.77
1:D:232:ARG:HH11	1:D:232:ARG:HB3	1.50	0.77
1:E:168:LEU:HD12	1:E:168:LEU:O	1.85	0.77
1:E:148:SER:CB	1:F:40:LEU:N	2.46	0.77
1:A:224:GLY:O	1:A:228:LYS:HE2	1.83	0.77
1:H:187:GLU:HG3	1:H:189:ASN:H	1.48	0.77
1:B:149:PRO:HG2	1:B:150:ALA:O	1.85	0.77
1:F:148:SER:HB3	1:F:149:PRO:CA	2.14	0.77
1:D:260:GLN:HA	1:D:260:GLN:NE2	1.97	0.76
1:F:185:LYS:O	1:F:189:ASN:HB2	1.85	0.76
1:E:149:PRO:CG	1:E:153:PHE:HD1	1.97	0.76
1:E:144:ARG:NH1	1:E:336:LEU:CD1	2.39	0.76
1:F:336:LEU:N	1:F:336:LEU:HD22	1.99	0.76
1:H:319:SER:OG	1:H:359:TYR:CE1	2.38	0.76
1:E:144:ARG:O	1:E:144:ARG:HD2	1.86	0.76
1:H:358:ARG:HG2	1:H:358:ARG:NH2	1.96	0.76
1:E:141:ASN:HA	1:E:144:ARG:HB3	1.66	0.76
1:C:358:ARG:HA	1:C:359:TYR:CG	2.21	0.75
1:G:154:GLN:NE2	1:G:155:SER:H	1.85	0.75
1:A:224:GLY:O	1:A:228:LYS:CE	2.33	0.75
1:F:140:PHE:CD2	1:F:335:MET:HG3	2.21	0.75
1:F:318:ASP:OD2	1:F:360:LYS:HB3	1.87	0.74
1:C:172:ARG:HG3	1:C:172:ARG:HH11	1.52	0.74
1:C:187:GLU:N	1:C:190:GLU:OE1	2.20	0.74
1:E:41:ILE:HG21	1:F:148:SER:O	1.87	0.74
1:F:329:VAL:O	1:F:333:HIS:N	2.20	0.74
1:F:62:LYS:CD	1:F:146:TYR:HD1	2.00	0.74
1:B:147:LEU:CB	1:B:148:SER:HA	2.17	0.74
1:D:148:SER:OG	1:D:149:PRO:HD2	1.87	0.74
1:G:40:LEU:HD23	1:G:40:LEU:N	2.02	0.74
1:F:193:LEU:HD12	1:F:196:GLU:HG3	1.69	0.74
1:A:372:LEU:N	1:A:372:LEU:HD12	2.02	0.73
1:C:154:GLN:OE1	1:C:173:VAL:HB	1.88	0.73
1:B:148:SER:HB3	1:B:150:ALA:N	2.03	0.73
1:G:332:VAL:O	1:G:335:MET:HG2	1.89	0.73
1:G:194:LYS:CE	1:G:198:GLU:OE2	2.34	0.73
1:B:154:GLN:HA	1:B:154:GLN:NE2	2.03	0.73
1:G:380:LYS:N	1:G:380:LYS:HD2	2.04	0.73
1:C:168:LEU:CD2	1:C:168:LEU:H	2.02	0.72
1:C:248:GLU:HG2	1:C:249:GLU:H	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:PRO:HG2	1:E:153:PHE:CD1	2.23	0.72
1:G:190:GLU:HB3	1:G:194:LYS:H	1.54	0.72
1:D:360:LYS:HZ3	1:D:360:LYS:HB2	1.50	0.72
1:G:41:ILE:N	1:G:41:ILE:HD12	2.05	0.72
1:G:189:ASN:HA	1:G:192:LEU:HB2	1.71	0.72
1:G:149:PRO:O	1:G:152:GLY:N	2.23	0.72
1:C:244:LYS:HB3	1:C:244:LYS:HZ2	1.55	0.71
1:C:145:GLU:O	1:C:146:TYR:CG	2.43	0.71
1:G:332:VAL:O	1:G:335:MET:CG	2.38	0.71
1:G:358:ARG:HH11	1:G:358:ARG:HB3	1.54	0.71
1:F:217:PRO:O	1:F:221:ASN:HB2	1.90	0.71
1:C:145:GLU:C	1:C:146:TYR:CG	2.63	0.71
1:E:120:VAL:HG12	1:F:131:ILE:HD13	1.71	0.71
1:C:170:ASN:N	1:C:170:ASN:HD22	1.89	0.71
1:G:150:ALA:HA	1:G:152:GLY:N	2.04	0.71
1:E:149:PRO:CB	1:E:153:PHE:CD1	2.73	0.71
1:G:331:MET:HE2	1:G:332:VAL:N	2.06	0.71
1:B:41:ILE:N	1:B:41:ILE:HD13	2.04	0.71
1:D:259:LYS:HZ2	1:D:260:GLN:HG2	1.53	0.71
1:G:140:PHE:HE2	1:G:335:MET:CB	2.02	0.71
1:B:147:LEU:HD13	1:B:147:LEU:N	2.05	0.71
1:C:153:PHE:N	1:C:154:GLN:HA	2.05	0.71
1:C:103:ARG:NH1	3:C:404:HOH:O	2.24	0.71
1:E:263:VAL:HG13	1:E:264:LEU:N	2.06	0.71
1:C:160:LEU:O	1:C:164:LYS:HG3	1.91	0.70
1:F:161:LEU:O	1:F:165:ILE:HG12	1.90	0.70
1:B:301:GLU:OE2	1:C:106:ARG:NH2	2.23	0.70
1:E:138:LEU:HD13	1:G:375:ARG:HH12	1.56	0.70
1:B:376:HIS:H	1:B:376:HIS:CD2	2.10	0.70
1:D:143:PHE:O	1:D:144:ARG:C	2.30	0.70
1:E:43:GLY:HA2	1:E:48:LEU:HD12	1.72	0.70
1:D:332:VAL:O	1:D:336:LEU:HB2	1.92	0.70
1:F:184:PHE:C	1:F:185:LYS:HD2	2.10	0.70
1:G:155:SER:OG	1:G:158:PHE:CB	2.40	0.70
1:A:106:ARG:NH2	1:D:301:GLU:OE2	2.22	0.70
1:B:219:GLY:O	1:B:220:PHE:C	2.30	0.70
1:B:156:LEU:HD11	1:B:192:LEU:HD13	1.74	0.70
1:A:161:LEU:O	1:A:165:ILE:HG12	1.91	0.70
1:E:152:GLY:HA2	1:E:153:PHE:CB	2.22	0.70
1:F:140:PHE:CG	1:F:335:MET:HG3	2.27	0.70
1:D:62:LYS:HB2	1:D:146:TYR:CE2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:GLU:HG3	1:C:143:PHE:CD2	2.27	0.69
1:F:300:GLU:HG3	1:G:106:ARG:NH1	2.05	0.69
1:C:145:GLU:O	1:C:146:TYR:CE1	2.44	0.69
1:A:322:THR:HB	1:A:359:TYR:CD1	2.28	0.69
1:B:150:ALA:HB1	1:B:151:SER:HA	1.74	0.69
1:A:301:GLU:OE1	1:D:106:ARG:NH2	2.25	0.69
1:E:138:LEU:HD22	1:G:375:ARG:HH11	1.58	0.69
1:F:148:SER:HB3	1:F:149:PRO:HA	1.74	0.69
1:F:147:LEU:N	1:F:147:LEU:HD12	2.01	0.69
1:D:255:ALA:HA	1:D:256:GLU:HB2	1.72	0.69
1:G:147:LEU:HD23	1:G:147:LEU:N	2.04	0.68
1:F:358:ARG:HG2	1:F:358:ARG:NH1	2.05	0.68
1:B:188:GLU:O	1:B:191:LEU:N	2.26	0.68
1:E:149:PRO:HB2	1:E:153:PHE:HB2	1.76	0.68
1:G:162:GLU:O	1:G:166:GLY:HA2	1.92	0.68
1:G:216:GLU:C	1:G:218:HIS:H	1.94	0.68
1:F:328:HIS:O	1:F:329:VAL:CG2	2.40	0.68
1:E:149:PRO:CB	1:E:153:PHE:HD1	2.07	0.68
1:C:145:GLU:C	1:C:146:TYR:CD1	2.66	0.67
1:G:214:GLY:O	1:G:220:PHE:HD2	1.78	0.67
1:A:144:ARG:O	1:A:147:LEU:N	2.28	0.67
1:G:140:PHE:HE2	1:G:335:MET:HB3	1.56	0.67
1:G:358:ARG:O	1:G:359:TYR:HB2	1.95	0.67
1:A:149:PRO:HD2	1:B:40:LEU:HG	1.76	0.67
1:D:259:LYS:HE2	1:D:260:GLN:N	2.10	0.67
1:G:220:PHE:CE1	1:G:225:LYS:HE3	2.30	0.67
1:F:372:LEU:HD21	1:H:141:ASN:HD21	1.60	0.67
1:D:255:ALA:CA	1:D:256:GLU:HG3	2.25	0.67
1:D:259:LYS:HZ1	1:D:260:GLN:HG2	1.58	0.66
1:F:99:ASN:ND2	1:F:99:ASN:O	2.24	0.66
1:E:147:LEU:HB3	1:E:149:PRO:CD	2.21	0.66
1:G:216:GLU:C	1:G:218:HIS:N	2.48	0.66
1:G:190:GLU:HA	1:G:193:LEU:N	2.09	0.66
1:H:154:GLN:OE1	1:H:154:GLN:HA	1.96	0.66
1:E:258:GLN:O	1:E:262:GLU:N	2.29	0.66
1:E:149:PRO:CG	1:E:153:PHE:CD1	2.78	0.66
1:G:191:LEU:N	1:G:191:LEU:HD12	2.04	0.66
1:G:219:GLY:O	1:G:220:PHE:HB3	1.96	0.66
1:C:131:ILE:HD13	1:D:120:VAL:HG12	1.78	0.66
1:G:190:GLU:HB2	1:G:194:LYS:H	1.61	0.65
1:C:172:ARG:CG	1:C:172:ARG:HH11	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:ILE:O	1:F:43:GLY:N	2.30	0.65
1:C:214:GLY:N	1:C:216:GLU:OE2	2.30	0.65
1:C:103:ARG:CG	1:C:103:ARG:HH11	2.09	0.65
1:D:143:PHE:O	1:D:145:GLU:N	2.30	0.65
1:D:168:LEU:CD1	1:D:168:LEU:H	1.96	0.65
1:G:216:GLU:O	1:G:218:HIS:N	2.30	0.65
1:G:161:LEU:O	1:G:165:ILE:CG1	2.44	0.65
1:C:172:ARG:HG3	1:C:172:ARG:NH1	2.09	0.64
1:A:144:ARG:O	1:A:147:LEU:HB2	1.95	0.64
1:A:244:LYS:HB2	1:A:250:LYS:HD2	1.79	0.64
1:A:259:LYS:O	1:A:263:VAL:HG23	1.97	0.64
1:G:225:LYS:O	1:G:229:ASN:ND2	2.23	0.64
1:E:144:ARG:C	1:E:144:ARG:HD2	2.17	0.64
1:H:234:LEU:HD13	1:H:261:LYS:HG3	1.79	0.64
1:E:302:PRO:HB2	3:E:406:HOH:O	1.97	0.64
1:E:160:LEU:O	1:E:164:LYS:HG3	1.98	0.64
1:D:266:SER:OG	1:D:272:ARG:NH1	2.30	0.64
1:C:193:LEU:O	1:C:197:GLN:HG2	1.97	0.64
1:C:334:ARG:HH21	1:C:335:MET:HE1	1.61	0.64
1:E:144:ARG:NH1	1:E:336:LEU:CD2	2.61	0.64
1:D:168:LEU:CD1	1:D:283:ARG:NH1	2.61	0.64
1:G:163:ASN:O	1:G:166:GLY:HA3	1.97	0.64
1:G:103:ARG:NH1	3:G:401:HOH:O	2.30	0.64
1:G:223:TRP:CZ3	1:G:290:GLN:HG2	2.32	0.64
1:A:331:MET:HG3	1:A:332:VAL:N	2.13	0.64
1:A:247:SER:OG	1:A:248:GLU:N	2.26	0.64
1:C:250:LYS:O	1:C:254:VAL:N	2.26	0.63
1:G:331:MET:CE	1:G:332:VAL:HA	2.28	0.63
1:D:259:LYS:HZ1	1:D:260:GLN:N	1.96	0.63
1:G:239:ILE:O	1:G:242:GLN:NE2	2.30	0.63
1:F:184:PHE:C	1:F:185:LYS:CD	2.67	0.63
1:E:84:LYS:NZ	1:F:52:LEU:O	2.31	0.63
1:D:227:GLU:HG3	1:D:268:PHE:CZ	2.33	0.63
1:E:138:LEU:HB3	1:G:375:ARG:HH12	1.63	0.63
1:G:189:ASN:HA	1:G:192:LEU:CB	2.28	0.63
1:C:187:GLU:CG	1:C:188:GLU:H	2.06	0.62
1:C:168:LEU:HD22	1:C:283:ARG:NH1	2.14	0.62
1:E:329:VAL:O	1:E:332:VAL:HB	2.00	0.62
1:E:335:MET:O	1:E:336:LEU:HG	1.99	0.62
1:D:258:GLN:O	1:D:261:LYS:HB3	2.00	0.62
1:H:359:TYR:HB3	1:H:366:PHE:CE2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:LEU:CD1	1:E:157:GLN:HG2	2.29	0.62
1:G:214:GLY:O	1:G:220:PHE:CD2	2.52	0.62
1:B:374:PRO:O	1:B:375:ARG:HB3	1.98	0.62
1:D:144:ARG:HA	1:D:147:LEU:CD2	2.21	0.62
1:D:217:PRO:O	1:D:221:ASN:HB2	2.00	0.62
1:C:120:VAL:HG12	1:D:131:ILE:HD13	1.80	0.62
1:E:147:LEU:CB	1:E:149:PRO:HD2	2.25	0.62
1:G:331:MET:HE2	1:G:332:VAL:HG23	1.81	0.62
1:F:62:LYS:HG3	1:F:146:TYR:CD1	2.33	0.62
1:G:223:TRP:CH2	1:G:290:GLN:HG2	2.34	0.62
1:B:160:LEU:HD23	1:B:192:LEU:HD12	1.81	0.62
1:F:242:GLN:O	1:F:242:GLN:HG3	1.99	0.62
1:H:367:ASN:O	1:H:370:THR:HG23	1.99	0.61
1:A:251:GLU:HA	1:A:251:GLU:OE1	1.97	0.61
1:G:150:ALA:HA	1:G:151:SER:C	2.18	0.61
1:D:325:ARG:O	1:D:329:VAL:HG22	2.00	0.61
1:E:253:GLN:O	1:E:254:VAL:HG22	2.01	0.61
1:G:254:VAL:O	1:G:257:PHE:HB3	2.00	0.61
1:G:155:SER:HG	1:G:158:PHE:H	1.48	0.61
1:F:40:LEU:HD22	1:F:41:ILE:H	1.65	0.61
1:F:238:PHE:O	1:F:241:ILE:HB	2.00	0.61
1:B:150:ALA:CB	1:B:151:SER:HA	2.29	0.61
1:G:334:ARG:O	1:G:335:MET:HB3	1.98	0.61
1:B:156:LEU:HD22	1:B:188:GLU:HG2	1.81	0.61
1:F:193:LEU:HA	1:F:196:GLU:CG	2.29	0.61
1:A:327:ASN:O	1:A:330:CYS:HB2	2.01	0.61
1:C:237:GLU:OE2	1:C:240:ARG:NH2	2.21	0.61
1:A:228:LYS:HD3	1:A:228:LYS:N	2.16	0.61
1:C:358:ARG:CA	1:C:359:TYR:CG	2.84	0.61
1:F:165:ILE:HB	1:F:166:GLY:HA2	1.83	0.60
1:A:372:LEU:C	1:A:372:LEU:CD1	2.67	0.60
1:E:161:LEU:O	1:E:165:ILE:HG12	2.01	0.60
1:G:190:GLU:HB3	1:G:194:LYS:N	2.15	0.60
1:G:162:GLU:HG2	1:G:167:VAL:HG21	1.83	0.60
1:H:162:GLU:O	1:H:166:GLY:HA2	2.01	0.60
1:H:40:LEU:O	1:H:40:LEU:HD12	2.00	0.60
1:C:42:TYR:CE1	1:C:46:LEU:CD1	2.84	0.60
1:G:150:ALA:HA	1:G:153:PHE:H	1.65	0.60
1:D:234:LEU:CD1	1:D:261:LYS:HG3	2.31	0.60
1:G:380:LYS:H	1:G:380:LYS:CD	2.12	0.60
1:B:219:GLY:C	1:B:220:PHE:O	2.39	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:LEU:CD1	1:G:191:LEU:H	1.94	0.60
1:E:138:LEU:HD22	1:G:375:ARG:NH1	2.15	0.60
1:A:372:LEU:C	1:A:372:LEU:HD13	2.22	0.60
1:C:162:GLU:O	1:C:166:GLY:HA2	2.02	0.60
1:C:244:LYS:HB2	1:C:250:LYS:HE3	1.84	0.60
1:E:220:PHE:O	1:E:225:LYS:NZ	2.31	0.60
1:B:163:ASN:ND2	1:B:195:SER:OG	2.31	0.60
1:E:149:PRO:HG2	1:E:153:PHE:HD1	1.60	0.59
1:F:148:SER:HB3	1:F:149:PRO:HB3	1.84	0.59
1:A:120:VAL:HG12	1:B:131:ILE:HD13	1.83	0.59
1:C:187:GLU:HG2	1:C:188:GLU:N	2.13	0.59
1:C:216:GLU:CD	1:C:216:GLU:H	2.06	0.59
1:F:144:ARG:O	1:F:147:LEU:CD1	2.50	0.59
1:E:381:MET:O	1:E:382:ASN:HB2	2.01	0.59
1:E:169:GLN:HG2	1:E:169:GLN:O	2.01	0.59
1:G:358:ARG:HG2	1:G:359:TYR:H	1.67	0.59
1:B:154:GLN:HA	1:B:154:GLN:HE21	1.67	0.59
1:E:101:HIS:HB2	3:E:405:HOH:O	2.01	0.59
1:G:331:MET:HE3	1:G:332:VAL:HA	1.84	0.59
1:D:257:PHE:CD1	1:D:258:GLN:HA	2.38	0.59
1:E:149:PRO:HB3	1:E:153:PHE:CA	2.33	0.59
1:G:154:GLN:HG3	1:G:155:SER:N	2.18	0.59
1:D:257:PHE:HD1	1:D:258:GLN:N	2.00	0.58
1:E:138:LEU:CB	1:G:375:ARG:HH12	2.16	0.58
1:D:232:ARG:HH11	1:D:232:ARG:CB	2.15	0.58
1:F:62:LYS:HD2	1:F:146:TYR:CD1	2.34	0.58
1:B:160:LEU:CD2	1:B:192:LEU:HD12	2.34	0.58
1:F:42:TYR:C	1:F:42:TYR:CD1	2.76	0.58
1:H:282:ARG:NH1	3:H:507:HOH:O	2.33	0.58
1:D:257:PHE:CD1	1:D:258:GLN:N	2.71	0.58
1:A:147:LEU:O	1:A:148:SER:C	2.41	0.58
1:B:160:LEU:O	1:B:164:LYS:HG3	2.03	0.58
1:D:232:ARG:HA	1:D:235:GLU:HG2	1.84	0.58
1:A:372:LEU:HD12	1:A:372:LEU:H	1.68	0.58
1:G:154:GLN:CA	1:G:154:GLN:HE21	2.15	0.58
1:G:246:GLU:OE1	1:G:246:GLU:N	2.30	0.58
1:D:168:LEU:HD12	1:D:168:LEU:N	2.04	0.58
1:D:362:PHE:O	1:D:365:LEU:HB2	2.04	0.58
1:B:168:LEU:HD12	1:B:168:LEU:N	2.18	0.58
1:G:239:ILE:HD12	1:G:242:GLN:NE2	2.19	0.58
1:C:135:MET:CE	1:C:143:PHE:HE1	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:PHE:HZ	1:B:380:LYS:O	1.87	0.57
1:F:329:VAL:O	1:F:332:VAL:N	2.37	0.57
1:F:148:SER:HB3	1:F:149:PRO:CB	2.33	0.57
1:F:42:TYR:O	1:F:42:TYR:CG	2.56	0.57
1:A:322:THR:CB	1:A:359:TYR:HD1	2.18	0.57
1:G:189:ASN:OD1	1:G:189:ASN:N	2.32	0.57
1:C:170:ASN:H	1:C:170:ASN:ND2	2.01	0.57
1:G:223:TRP:O	1:G:226:LEU:HB3	2.05	0.57
1:D:165:ILE:N	1:D:166:GLY:HA2	2.20	0.57
1:E:138:LEU:CB	1:G:375:ARG:NH1	2.63	0.57
1:A:144:ARG:NE	3:A:410:HOH:O	2.37	0.57
1:F:144:ARG:O	1:F:147:LEU:HD12	2.05	0.57
1:B:159:ARG:HH22	1:B:169:GLN:HE22	1.49	0.57
1:F:140:PHE:CG	1:F:335:MET:CG	2.88	0.57
1:B:359:TYR:N	1:B:359:TYR:CD1	2.72	0.57
1:G:254:VAL:O	1:G:257:PHE:N	2.38	0.57
1:C:358:ARG:N	1:C:359:TYR:CG	2.73	0.57
1:C:248:GLU:HG2	1:C:249:GLU:N	2.19	0.57
1:D:261:LYS:O	1:D:262:GLU:C	2.42	0.57
1:C:103:ARG:HH11	1:C:103:ARG:HG3	1.70	0.57
1:F:193:LEU:O	1:F:196:GLU:HG3	2.05	0.57
1:H:140:PHE:CE2	1:H:335:MET:HB3	2.40	0.56
1:B:216:GLU:O	1:B:220:PHE:O	2.23	0.56
1:G:331:MET:HE2	1:G:332:VAL:CG2	2.35	0.56
1:F:372:LEU:HD11	1:H:141:ASN:ND2	2.21	0.56
1:G:234:LEU:HD13	1:G:261:LYS:HG3	1.87	0.56
1:F:141:ASN:HD21	1:H:372:LEU:HD21	1.69	0.56
1:B:148:SER:N	1:B:149:PRO:HA	2.21	0.56
1:G:270:GLU:HG2	1:G:286:TYR:CE2	2.40	0.56
1:F:332:VAL:HG13	1:F:336:LEU:HD23	1.86	0.56
1:B:376:HIS:N	1:B:376:HIS:CD2	2.73	0.56
1:H:220:PHE:CZ	1:H:381:MET:HA	2.41	0.56
1:B:62:LYS:HD2	1:B:146:TYR:HD1	1.69	0.56
1:F:162:GLU:O	1:F:167:VAL:N	2.38	0.56
1:F:140:PHE:CD2	1:F:335:MET:CG	2.88	0.55
1:G:377:TRP:N	1:G:377:TRP:CD1	2.73	0.55
1:A:139:ASP:O	1:A:142:ASP:HB2	2.06	0.55
1:C:249:GLU:O	1:C:250:LYS:CB	2.47	0.55
1:B:150:ALA:CB	1:B:151:SER:CA	2.85	0.55
1:E:331:MET:HG3	1:E:332:VAL:N	2.21	0.55
1:A:167:VAL:CG1	1:A:168:LEU:N	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:358:ARG:CG	1:G:358:ARG:HH11	2.18	0.55
1:E:87:LEU:HD11	1:E:157:GLN:HG2	1.88	0.55
1:A:131:ILE:HD13	1:B:120:VAL:HG12	1.86	0.55
1:G:190:GLU:CA	1:G:193:LEU:H	2.17	0.55
1:D:227:GLU:HG3	1:D:268:PHE:CG	2.41	0.55
1:F:193:LEU:CA	1:F:196:GLU:HG3	2.35	0.55
1:H:40:LEU:C	1:H:40:LEU:HD12	2.27	0.55
1:F:302:PRO:HG3	1:G:105:GLU:OE1	2.06	0.55
1:G:155:SER:OG	1:G:158:PHE:HB2	2.06	0.55
1:G:332:VAL:C	1:G:335:MET:HG2	2.28	0.54
1:F:163:ASN:ND2	1:F:195:SER:OG	2.35	0.54
1:E:302:PRO:HB3	1:H:105:GLU:OE1	2.06	0.54
1:C:135:MET:CE	1:C:143:PHE:CE1	2.90	0.54
1:G:188:GLU:HG3	1:G:191:LEU:CD1	2.37	0.54
1:C:244:LYS:HB3	1:C:244:LYS:NZ	2.17	0.54
1:A:90:LEU:HD22	1:A:165:ILE:HD11	1.88	0.54
1:D:326:TYR:O	1:D:329:VAL:HG23	2.08	0.54
1:G:363:VAL:HG13	1:G:364:ASP:N	2.22	0.54
1:H:215:LEU:O	1:H:217:PRO:HD3	2.06	0.54
1:B:150:ALA:HB1	1:B:151:SER:CA	2.38	0.54
1:A:169:GLN:NE2	1:A:169:GLN:HA	2.23	0.54
1:A:167:VAL:HG12	1:A:168:LEU:N	2.21	0.54
1:F:184:PHE:O	1:F:185:LYS:CG	2.55	0.54
1:G:219:GLY:O	1:G:220:PHE:CB	2.55	0.54
1:A:322:THR:HB	1:A:359:TYR:HD1	1.72	0.54
1:E:101:HIS:CA	3:E:405:HOH:O	2.56	0.54
1:B:218:HIS:H	1:B:218:HIS:CD2	2.24	0.54
1:C:247:SER:HA	1:C:249:GLU:O	2.08	0.54
1:G:331:MET:CE	1:G:332:VAL:CA	2.86	0.54
1:E:328:HIS:O	1:E:332:VAL:HG23	2.07	0.54
1:E:299:ARG:HH12	1:G:138:LEU:H	1.56	0.54
1:B:237:GLU:O	1:B:241:ILE:HG12	2.08	0.54
1:C:100:GLY:O	1:C:101:HIS:HB2	2.07	0.54
1:G:332:VAL:O	1:G:335:MET:HG3	2.08	0.54
1:G:141:ASN:OD1	1:G:144:ARG:HD3	2.08	0.54
1:B:97:PHE:HA	1:B:102:VAL:CG2	2.38	0.54
1:E:149:PRO:HB3	1:E:153:PHE:CD1	2.41	0.53
1:H:322:THR:HG21	1:H:358:ARG:HA	1.90	0.53
1:F:62:LYS:CD	1:F:146:TYR:CD1	2.87	0.53
1:D:360:LYS:HZ3	1:D:360:LYS:HB3	1.67	0.53
1:H:41:ILE:HG12	1:H:44:ASN:ND2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ARG:O	1:B:240:ARG:HG2	2.09	0.53
1:A:372:LEU:O	1:A:372:LEU:HD12	2.07	0.53
1:E:373:ILE:HD12	1:E:377:TRP:HB2	1.91	0.53
1:C:135:MET:HE3	1:C:143:PHE:CE1	2.44	0.53
1:B:147:LEU:HB2	1:B:148:SER:CA	2.28	0.53
1:D:43:GLY:HA3	1:D:48:LEU:HG	1.90	0.53
1:F:144:ARG:CZ	1:F:336:LEU:HD12	2.38	0.53
1:H:148:SER:HA	1:H:149:PRO:C	2.28	0.53
1:C:247:SER:CB	1:C:248:GLU:HA	2.26	0.53
1:D:361:VAL:HG22	1:D:362:PHE:CE2	2.43	0.53
1:C:154:GLN:HB2	1:C:174:PRO:O	2.08	0.53
1:E:335:MET:O	1:E:336:LEU:HD23	2.08	0.53
1:C:247:SER:HA	1:C:250:LYS:HB2	1.90	0.53
1:E:263:VAL:HG13	1:E:264:LEU:H	1.70	0.53
1:A:121:ILE:HG12	1:B:131:ILE:HD12	1.91	0.53
1:B:154:GLN:CA	1:B:154:GLN:HE21	2.22	0.53
1:G:331:MET:HE2	1:G:332:VAL:CA	2.39	0.53
1:F:193:LEU:HG	1:F:197:GLN:HG3	1.90	0.53
1:H:359:TYR:CG	1:H:366:PHE:CZ	2.96	0.53
1:E:258:GLN:O	1:E:261:LYS:HB3	2.09	0.53
1:E:318:ASP:OD2	1:E:361:VAL:N	2.36	0.53
1:F:334:ARG:HH11	1:F:335:MET:CE	2.22	0.52
1:E:233:GLY:O	1:E:237:GLU:HG2	2.08	0.52
1:B:148:SER:N	1:B:149:PRO:CA	2.72	0.52
1:D:162:GLU:O	1:D:166:GLY:HA2	2.09	0.52
1:H:246:GLU:OE1	1:H:246:GLU:N	2.42	0.52
1:C:58:GLN:HB3	1:C:146:TYR:CE2	2.45	0.52
1:G:154:GLN:CG	1:G:155:SER:N	2.73	0.52
1:G:162:GLU:O	1:G:167:VAL:HG23	2.09	0.52
1:G:150:ALA:CA	1:G:152:GLY:N	2.73	0.52
1:C:214:GLY:CA	1:C:216:GLU:OE2	2.57	0.52
1:G:227:GLU:O	1:G:231:THR:HG23	2.10	0.52
1:D:298:TYR:CD1	1:D:381:MET:HG3	2.43	0.52
1:E:138:LEU:CD1	1:G:375:ARG:HH12	2.22	0.52
1:B:154:GLN:CA	1:B:154:GLN:NE2	2.73	0.52
1:E:41:ILE:CG2	1:F:148:SER:O	2.56	0.52
1:E:49:GLU:O	1:E:53:ASN:ND2	2.42	0.52
1:C:147:LEU:HD23	1:D:40:LEU:HD21	1.92	0.52
1:G:190:GLU:HB2	1:G:191:LEU:HA	1.92	0.52
1:C:168:LEU:N	1:C:168:LEU:HD23	2.07	0.52
1:E:263:VAL:CG1	1:E:264:LEU:N	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:ARG:HH12	1:C:253:GLN:HE22	1.57	0.52
1:E:148:SER:N	1:E:149:PRO:CD	2.73	0.52
1:F:165:ILE:N	1:F:166:GLY:HA2	2.24	0.52
1:A:92:SER:OG	1:A:114:ARG:NH1	2.43	0.52
1:C:187:GLU:CG	1:C:188:GLU:N	2.73	0.52
1:E:335:MET:O	1:E:336:LEU:CG	2.58	0.52
1:F:144:ARG:NH2	1:F:336:LEU:HD12	2.24	0.52
1:F:148:SER:CB	1:F:149:PRO:HA	2.35	0.52
1:G:120:VAL:HG12	1:H:131:ILE:HD13	1.92	0.52
1:B:374:PRO:HD2	1:B:377:TRP:CE2	2.44	0.52
1:B:159:ARG:HH22	1:B:169:GLN:NE2	2.07	0.52
1:A:162:GLU:O	1:A:166:GLY:HA2	2.10	0.52
1:E:47:HIS:ND1	1:E:49:GLU:OE2	2.30	0.52
1:C:334:ARG:HH21	1:C:335:MET:HE3	1.74	0.51
1:B:332:VAL:HG13	1:B:336:LEU:HD22	1.92	0.51
1:A:80:GLU:OE2	1:B:42:TYR:OH	2.22	0.51
1:C:138:LEU:HD12	1:C:139:ASP:H	1.74	0.51
1:H:187:GLU:CG	1:H:189:ASN:H	2.19	0.51
1:C:175:TYR:OH	1:C:188:GLU:OE2	2.28	0.51
1:D:257:PHE:CD1	1:D:258:GLN:CA	2.93	0.51
1:E:299:ARG:NH1	1:G:138:LEU:HB2	2.25	0.51
1:H:41:ILE:O	1:H:41:ILE:HG13	2.10	0.51
1:C:359:TYR:C	1:C:359:TYR:HD1	2.14	0.51
1:E:257:PHE:CD1	1:E:258:GLN:N	2.79	0.51
1:B:103:ARG:NH2	1:B:208:TRP:O	2.43	0.51
1:E:140:PHE:CG	1:E:335:MET:SD	3.04	0.51
1:D:336:LEU:CD2	1:D:337:GLY:N	2.61	0.51
1:C:358:ARG:CD	1:C:358:ARG:N	2.72	0.51
1:D:259:LYS:CE	1:D:260:GLN:N	2.73	0.51
1:G:254:VAL:HG13	1:G:255:ALA:N	2.25	0.51
1:G:154:GLN:NE2	1:G:154:GLN:HA	2.21	0.51
1:G:332:VAL:HA	1:G:335:MET:CG	2.41	0.51
1:F:333:HIS:HB2	3:F:402:HOH:O	2.11	0.51
1:G:216:GLU:O	1:G:220:PHE:O	2.29	0.51
1:E:101:HIS:N	3:E:405:HOH:O	2.31	0.51
1:D:140:PHE:CD2	1:D:335:MET:HB3	2.46	0.51
1:B:147:LEU:N	1:B:147:LEU:CD1	2.73	0.51
1:A:322:THR:CG2	1:A:359:TYR:HD1	2.24	0.51
1:F:372:LEU:HD11	1:H:141:ASN:HD21	1.75	0.51
1:G:190:GLU:HA	1:G:191:LEU:C	2.31	0.51
1:A:322:THR:HG21	1:A:359:TYR:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:331:MET:HE3	1:G:335:MET:SD	2.51	0.50
1:D:255:ALA:CA	1:D:256:GLU:CB	2.84	0.50
1:A:322:THR:HG21	1:A:359:TYR:HD1	1.76	0.50
1:G:331:MET:CE	1:G:332:VAL:N	2.74	0.50
1:F:193:LEU:O	1:F:196:GLU:N	2.44	0.50
1:C:147:LEU:O	1:C:148:SER:O	2.29	0.50
1:H:187:GLU:CG	1:H:188:GLU:N	2.55	0.50
1:G:221:ASN:O	1:G:225:LYS:HG3	2.10	0.50
1:G:245:GLU:O	1:G:246:GLU:O	2.30	0.50
1:E:226:LEU:HD23	1:E:268:PHE:HZ	1.76	0.50
1:F:162:GLU:HB3	1:F:167:VAL:HG22	1.92	0.50
1:A:90:LEU:CD2	1:A:165:ILE:HD11	2.42	0.50
1:C:294:MET:HG3	1:C:298:TYR:HD2	1.76	0.50
1:D:257:PHE:CD1	1:D:257:PHE:C	2.85	0.50
1:H:322:THR:HG21	1:H:358:ARG:O	2.11	0.50
1:H:303:ARG:NH2	1:H:381:MET:HG2	2.26	0.50
1:B:97:PHE:HA	1:B:102:VAL:HG21	1.94	0.50
1:E:117:ARG:HD3	1:F:71:LEU:HD22	1.94	0.50
1:B:221:ASN:O	1:B:221:ASN:OD1	2.30	0.50
1:G:139:ASP:O	1:G:142:ASP:HB2	2.12	0.50
1:G:189:ASN:HB3	1:G:192:LEU:HD23	1.94	0.50
1:A:245:GLU:HG3	1:A:246:GLU:O	2.12	0.50
1:G:189:ASN:CB	1:G:192:LEU:HB3	2.42	0.50
1:G:155:SER:OG	1:G:158:PHE:N	2.38	0.50
1:D:103:ARG:NH2	1:D:208:TRP:O	2.45	0.50
1:G:376:HIS:CD2	1:G:377:TRP:CD1	3.00	0.50
1:E:149:PRO:CB	1:E:153:PHE:CB	2.77	0.49
1:F:165:ILE:N	1:F:166:GLY:CA	2.75	0.49
1:B:156:LEU:HD21	1:B:188:GLU:HG2	1.91	0.49
1:D:62:LYS:HB2	1:D:146:TYR:CD2	2.47	0.49
1:E:138:LEU:HD13	1:G:375:ARG:NH1	2.26	0.49
1:D:161:LEU:O	1:D:165:ILE:HG12	2.11	0.49
1:H:41:ILE:O	1:H:42:TYR:C	2.50	0.49
1:G:97:PHE:HA	1:G:102:VAL:HG22	1.93	0.49
1:G:190:GLU:CD	1:G:190:GLU:H	2.13	0.49
1:G:190:GLU:HB3	1:G:193:LEU:HB2	1.93	0.49
1:G:332:VAL:HA	1:G:335:MET:SD	2.52	0.49
1:A:322:THR:CG2	1:A:359:TYR:CD1	2.95	0.49
1:E:253:GLN:NE2	1:E:253:GLN:N	2.60	0.49
1:F:327:ASN:ND2	3:F:403:HOH:O	2.42	0.49
1:G:362:PHE:HB3	1:G:365:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:TYR:CD1	1:C:359:TYR:C	2.85	0.49
1:D:257:PHE:CD1	1:D:258:GLN:HG2	2.48	0.49
1:D:154:GLN:CD	1:D:155:SER:H	2.06	0.49
1:E:87:LEU:HD12	1:E:157:GLN:HG2	1.93	0.49
1:D:168:LEU:HD11	1:D:283:ARG:HH11	1.74	0.49
1:G:331:MET:CE	1:G:332:VAL:CG2	2.90	0.49
1:G:154:GLN:HE21	1:G:155:SER:N	2.10	0.49
1:C:144:ARG:O	1:C:144:ARG:HD3	2.11	0.49
1:H:115:MET:HE2	1:H:201:LEU:HD21	1.94	0.49
1:A:112:VAL:HG21	1:A:306:VAL:HG13	1.92	0.49
1:G:189:ASN:HB3	1:G:192:LEU:CB	2.43	0.49
1:F:184:PHE:CD1	1:F:184:PHE:C	2.85	0.49
1:D:259:LYS:NZ	1:D:260:GLN:N	2.60	0.49
1:G:165:ILE:N	1:G:166:GLY:HA2	2.27	0.49
1:B:219:GLY:O	1:B:220:PHE:O	2.30	0.49
1:D:298:TYR:CE1	1:D:381:MET:HG3	2.48	0.49
1:A:143:PHE:O	1:A:146:TYR:HD1	1.96	0.49
1:A:150:ALA:C	1:A:152:GLY:N	2.64	0.49
1:D:144:ARG:O	1:D:147:LEU:N	2.40	0.49
1:B:62:LYS:HD2	1:B:146:TYR:CD1	2.47	0.49
1:G:358:ARG:CG	1:G:358:ARG:NH1	2.73	0.49
1:D:232:ARG:CA	1:D:235:GLU:HG2	2.43	0.49
1:G:220:PHE:CD1	1:G:225:LYS:HE3	2.48	0.49
1:G:154:GLN:HE21	1:G:155:SER:H	1.55	0.49
1:H:140:PHE:HA	1:H:143:PHE:CE1	2.48	0.49
1:G:190:GLU:CA	1:G:192:LEU:N	2.73	0.48
1:F:334:ARG:NH1	1:F:335:MET:CE	2.75	0.48
1:G:160:LEU:O	1:G:164:LYS:HG3	2.13	0.48
1:A:227:GLU:HB3	1:A:228:LYS:HE2	1.94	0.48
1:A:97:PHE:HA	1:A:102:VAL:HG22	1.94	0.48
1:E:335:MET:O	1:E:336:LEU:CD2	2.61	0.48
1:G:331:MET:CE	1:G:335:MET:SD	3.02	0.48
1:H:258:GLN:HE22	1:H:261:LYS:HD3	1.77	0.48
1:C:334:ARG:NH2	1:C:335:MET:CE	2.73	0.48
1:B:375:ARG:O	1:B:375:ARG:HG2	2.12	0.48
1:F:149:PRO:O	1:F:152:GLY:HA3	2.13	0.48
1:G:155:SER:OG	1:G:158:PHE:HB3	2.11	0.48
1:A:224:GLY:O	1:A:228:LYS:HE3	2.10	0.48
1:A:322:THR:HB	1:A:359:TYR:CE1	2.48	0.48
1:G:141:ASN:HA	1:G:144:ARG:HD2	1.95	0.48
1:C:294:MET:HG3	1:C:298:TYR:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:234:LEU:HD13	1:F:261:LYS:HG3	1.96	0.48
1:C:154:GLN:CD	1:C:173:VAL:HG21	2.33	0.48
1:G:140:PHE:HE2	1:G:335:MET:HB2	1.77	0.48
1:F:328:HIS:O	1:F:330:CYS:N	2.43	0.48
1:G:40:LEU:CB	1:G:41:ILE:HD12	2.30	0.48
1:C:139:ASP:O	1:C:142:ASP:HB2	2.14	0.48
1:G:189:ASN:CB	1:G:192:LEU:CB	2.91	0.48
1:E:149:PRO:HB3	1:E:153:PHE:HD1	1.78	0.48
1:G:140:PHE:CE2	1:G:335:MET:HB2	2.48	0.48
1:A:131:ILE:HD12	1:B:121:ILE:HG12	1.96	0.48
1:E:140:PHE:CD2	1:E:335:MET:HB3	2.49	0.48
1:C:234:LEU:HD13	1:C:261:LYS:HG3	1.96	0.48
1:D:259:LYS:HZ1	1:D:260:GLN:CG	2.25	0.47
1:G:218:HIS:HA	1:G:219:GLY:HA2	1.56	0.47
1:G:190:GLU:HB2	1:G:191:LEU:CA	2.44	0.47
1:G:41:ILE:N	1:G:41:ILE:CD1	2.73	0.47
1:A:147:LEU:CD1	1:A:147:LEU:N	2.77	0.47
1:C:175:TYR:CD1	1:C:175:TYR:C	2.87	0.47
1:B:156:LEU:CD1	1:B:192:LEU:HD13	2.44	0.47
1:D:298:TYR:OH	1:D:379:PRO:HG2	2.15	0.47
1:D:103:ARG:NH2	1:D:208:TRP:CD1	2.83	0.47
1:A:91:ASP:OD1	1:A:164:LYS:NZ	2.40	0.47
1:E:202:LEU:HD21	1:E:283:ARG:HB3	1.95	0.47
1:E:41:ILE:HA	1:E:41:ILE:HD12	1.80	0.47
1:B:215:LEU:O	1:B:216:GLU:C	2.52	0.47
1:B:221:ASN:OD1	1:B:221:ASN:C	2.50	0.47
1:D:41:ILE:O	1:D:44:ASN:HB2	2.14	0.47
1:F:151:SER:HA	1:F:152:GLY:HA3	1.48	0.47
1:D:165:ILE:O	1:D:201:LEU:HB3	2.13	0.47
1:E:258:GLN:O	1:E:261:LYS:CB	2.61	0.47
1:A:332:VAL:O	1:A:336:LEU:HB2	2.13	0.47
1:E:103:ARG:HH22	1:E:212:THR:HA	1.78	0.47
1:A:282:ARG:NH2	3:A:406:HOH:O	2.47	0.47
1:D:140:PHE:HA	1:D:143:PHE:CE2	2.49	0.47
1:B:188:GLU:O	1:B:191:LEU:CB	2.63	0.47
1:G:223:TRP:O	1:G:227:GLU:N	2.38	0.47
1:G:121:ILE:HG12	1:H:131:ILE:HD12	1.97	0.47
1:A:317:ILE:O	1:A:321:MET:HB2	2.15	0.47
1:E:42:TYR:HD1	1:F:153:PHE:CD1	2.33	0.47
1:A:237:GLU:OE2	1:A:240:ARG:NH2	2.43	0.47
1:B:140:PHE:CE2	1:B:335:MET:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:362:PHE:O	1:E:365:LEU:N	2.47	0.47
1:A:225:LYS:O	1:A:229:ASN:OD1	2.33	0.47
1:D:69:GLU:HG3	1:D:143:PHE:CD1	2.50	0.47
1:E:148:SER:N	1:E:149:PRO:HD3	2.29	0.47
1:G:154:GLN:CD	1:G:155:SER:H	2.18	0.47
1:F:242:GLN:HA	1:F:243:ALA:HA	1.71	0.47
1:C:49:GLU:O	1:C:53:ASN:ND2	2.46	0.47
1:D:144:ARG:HG2	1:D:145:GLU:N	2.29	0.46
1:G:239:ILE:HA	1:G:239:ILE:HD12	1.78	0.46
1:A:220:PHE:O	1:A:225:LYS:HE3	2.15	0.46
1:G:318:ASP:OD2	1:G:361:VAL:N	2.48	0.46
1:C:250:LYS:O	1:C:253:GLN:HB2	2.15	0.46
1:F:241:ILE:O	1:F:243:ALA:HA	2.16	0.46
1:F:367:ASN:O	1:F:370:THR:OG1	2.32	0.46
1:H:270:GLU:HG2	1:H:286:TYR:CE2	2.50	0.46
1:F:189:ASN:O	1:F:189:ASN:ND2	2.44	0.46
1:F:62:LYS:CG	1:F:146:TYR:CD1	2.99	0.46
1:C:165:ILE:HG22	1:C:361:VAL:HG21	1.96	0.46
1:E:269:ASP:OD1	1:E:271:LYS:HG2	2.15	0.46
1:D:258:GLN:OE1	1:D:261:LYS:HD3	2.16	0.46
1:F:358:ARG:CG	1:F:358:ARG:NH1	2.71	0.46
1:D:232:ARG:O	1:D:235:GLU:HG2	2.16	0.46
1:H:66:ILE:HG13	1:H:143:PHE:HB3	1.97	0.46
1:D:228:LYS:HD2	1:D:228:LYS:HA	1.54	0.46
1:F:336:LEU:HD22	1:F:336:LEU:H	1.79	0.46
1:F:216:GLU:O	1:F:221:ASN:N	2.46	0.46
1:E:96:ILE:HG22	1:E:102:VAL:HG13	1.98	0.46
1:B:226:LEU:HG	1:B:230:ILE:HD12	1.98	0.46
1:F:237:GLU:O	1:F:241:ILE:HG13	2.15	0.46
1:D:206:GLU:OE2	1:D:285:SER:N	2.47	0.46
1:C:336:LEU:N	1:C:336:LEU:HD12	2.31	0.46
1:B:235:GLU:O	1:B:238:PHE:HB3	2.15	0.46
1:G:332:VAL:HA	1:G:335:MET:HG2	1.97	0.46
1:C:175:TYR:HD1	1:C:175:TYR:O	2.00	0.46
1:F:150:ALA:HA	1:F:151:SER:HA	1.65	0.46
1:H:381:MET:HG3	1:H:382:ASN:H	1.80	0.46
1:E:298:TYR:OH	1:E:379:PRO:HG2	2.15	0.46
1:H:187:GLU:OE2	1:H:189:ASN:HB2	2.16	0.45
1:C:240:ARG:HH12	1:C:253:GLN:NE2	2.14	0.45
1:F:40:LEU:HD23	1:F:40:LEU:HA	1.65	0.45
1:F:318:ASP:CG	1:F:360:LYS:HB3	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ARG:NH1	1:C:103:ARG:CG	2.72	0.45
1:F:235:GLU:O	1:F:239:ILE:HG13	2.15	0.45
1:C:163:ASN:O	1:C:166:GLY:HA3	2.16	0.45
1:H:140:PHE:CD2	1:H:335:MET:HB3	2.51	0.45
1:F:244:LYS:HA	1:F:245:GLU:C	2.36	0.45
1:B:374:PRO:HA	1:D:141:ASN:HD21	1.81	0.45
1:B:156:LEU:HD22	1:B:188:GLU:CG	2.44	0.45
1:F:358:ARG:CD	1:F:360:LYS:NZ	2.79	0.45
1:E:257:PHE:C	1:E:257:PHE:CD1	2.89	0.45
1:H:115:MET:HE3	1:H:317:ILE:HD12	1.98	0.45
1:F:115:MET:HE2	1:F:201:LEU:HD21	1.98	0.45
1:C:135:MET:O	1:C:334:ARG:NH2	2.50	0.45
1:D:257:PHE:HD1	1:D:258:GLN:HG2	1.81	0.45
1:C:154:GLN:NE2	1:C:173:VAL:HG21	2.32	0.45
1:G:190:GLU:CA	1:G:191:LEU:C	2.84	0.45
1:F:336:LEU:N	1:F:336:LEU:CD2	2.73	0.45
1:C:121:ILE:HG12	1:D:131:ILE:HD12	1.96	0.45
1:G:245:GLU:HG3	1:G:245:GLU:O	2.17	0.45
1:A:267:LEU:HD13	1:A:371:TYR:CE1	2.52	0.45
1:D:66:ILE:HG13	1:D:142:ASP:O	2.17	0.45
1:H:360:LYS:HE3	1:H:360:LYS:HB2	1.41	0.45
1:D:140:PHE:CE2	1:D:335:MET:HB3	2.51	0.45
1:C:168:LEU:CD2	1:C:168:LEU:N	2.73	0.45
1:F:148:SER:CB	1:F:149:PRO:CA	2.85	0.45
1:F:326:TYR:O	1:F:326:TYR:CD1	2.70	0.45
1:A:322:THR:CB	1:A:359:TYR:CD1	2.94	0.45
1:E:103:ARG:HH12	1:E:213:PRO:HD2	1.82	0.45
1:G:84:LYS:NZ	1:H:52:LEU:O	2.43	0.45
1:B:132:LEU:HD23	1:B:132:LEU:HA	1.79	0.45
1:E:41:ILE:HD12	1:E:44:ASN:HB2	1.98	0.45
1:D:259:LYS:HZ1	1:D:260:GLN:CA	2.30	0.45
1:D:376:HIS:C	1:D:378:ILE:H	2.20	0.45
1:E:140:PHE:HA	1:E:143:PHE:CE2	2.52	0.45
1:B:149:PRO:O	1:B:150:ALA:HB2	2.17	0.45
1:C:153:PHE:O	1:C:153:PHE:CD1	2.70	0.45
1:H:151:SER:N	1:H:152:GLY:HA3	2.31	0.45
1:H:64:ASN:HB3	1:H:146:TYR:OH	2.17	0.45
1:H:269:ASP:OD2	1:H:272:ARG:HB2	2.16	0.45
1:C:135:MET:HE3	1:C:143:PHE:HE1	1.78	0.44
1:E:153:PHE:CD2	1:E:153:PHE:O	2.70	0.44
1:B:148:SER:CB	1:B:149:PRO:C	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:GLN:CG	1:G:155:SER:H	2.30	0.44
1:A:136:THR:HG23	1:A:139:ASP:HB2	1.97	0.44
1:E:121:ILE:HG12	1:F:131:ILE:HD12	1.99	0.44
1:A:150:ALA:O	1:A:152:GLY:N	2.50	0.44
1:G:298:TYR:OH	1:G:379:PRO:O	2.24	0.44
1:D:361:VAL:CG2	1:D:362:PHE:CE2	3.00	0.44
1:D:232:ARG:HA	1:D:235:GLU:CG	2.47	0.44
1:H:359:TYR:CD2	1:H:366:PHE:CE1	3.06	0.44
1:C:154:GLN:CB	1:C:174:PRO:O	2.65	0.44
1:G:153:PHE:O	1:G:153:PHE:CD1	2.71	0.44
1:A:261:LYS:HE3	1:A:265:LEU:CD1	2.48	0.44
1:F:332:VAL:O	1:F:336:LEU:HD23	2.17	0.44
1:F:239:ILE:O	1:F:242:GLN:N	2.49	0.44
1:G:298:TYR:OH	1:G:379:PRO:HG2	2.17	0.44
1:C:175:TYR:CD1	1:C:175:TYR:O	2.70	0.44
1:D:260:GLN:O	1:D:263:VAL:HG13	2.13	0.44
1:D:165:ILE:N	1:D:166:GLY:CA	2.81	0.44
1:G:233:GLY:O	1:G:237:GLU:HG2	2.18	0.44
1:A:140:PHE:CE1	1:A:335:MET:HB3	2.53	0.44
1:G:254:VAL:CG1	1:G:255:ALA:N	2.81	0.44
1:G:132:LEU:HD12	1:G:132:LEU:HA	1.80	0.44
1:A:210:GLU:OE2	1:A:285:SER:OG	2.26	0.44
1:F:329:VAL:HG23	1:F:330:CYS:N	2.33	0.44
1:C:172:ARG:HG2	1:C:172:ARG:H	1.56	0.44
1:B:220:PHE:CZ	1:B:380:LYS:O	2.69	0.44
1:A:165:ILE:HG23	1:A:165:ILE:HD12	1.60	0.44
1:F:363:VAL:HG13	1:F:364:ASP:N	2.32	0.44
1:C:154:GLN:CD	1:C:173:VAL:CG2	2.86	0.44
1:A:165:ILE:N	1:A:166:GLY:HA2	2.33	0.44
1:B:140:PHE:CD2	1:B:335:MET:HB3	2.53	0.44
1:H:326:TYR:CZ	1:H:330:CYS:SG	3.10	0.44
1:H:265:LEU:HD23	1:H:265:LEU:HA	1.84	0.44
1:B:159:ARG:NH2	1:B:169:GLN:NE2	2.51	0.43
1:F:293:LEU:HG	1:F:368:LEU:HD22	2.00	0.43
1:G:146:TYR:O	1:G:147:LEU:CD2	2.53	0.43
1:D:260:GLN:C	1:D:263:VAL:HG12	2.37	0.43
1:E:140:PHE:CE2	1:E:335:MET:HB3	2.53	0.43
1:G:141:ASN:HA	1:G:144:ARG:CD	2.48	0.43
1:D:298:TYR:CE1	1:D:381:MET:CG	3.01	0.43
1:C:239:ILE:HD13	1:C:239:ILE:HA	1.85	0.43
1:H:381:MET:HG3	1:H:382:ASN:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:377:TRP:N	1:G:377:TRP:HD1	2.17	0.43
1:C:334:ARG:NH2	1:C:335:MET:HE1	2.30	0.43
1:D:140:PHE:CD1	1:D:143:PHE:CZ	3.07	0.43
1:D:360:LYS:HZ2	1:D:360:LYS:CB	2.08	0.43
1:B:377:TRP:N	1:B:377:TRP:CD1	2.87	0.43
1:F:184:PHE:O	1:F:185:LYS:HG3	2.19	0.43
1:H:358:ARG:HH21	1:H:358:ARG:CG	2.14	0.43
1:A:149:PRO:HD2	1:B:40:LEU:CG	2.44	0.43
1:E:103:ARG:NH1	1:E:213:PRO:CD	2.81	0.43
1:F:210:GLU:HG2	1:F:287:ARG:HB3	2.00	0.43
1:G:203:GLU:O	1:G:206:GLU:HB3	2.19	0.43
1:C:153:PHE:O	1:C:153:PHE:HD1	2.02	0.43
1:D:211:ARG:O	1:D:213:PRO:HD3	2.19	0.43
1:E:330:CYS:O	1:E:333:HIS:HB3	2.18	0.43
1:D:143:PHE:C	1:D:145:GLU:N	2.69	0.43
1:B:221:ASN:O	1:B:221:ASN:CG	2.56	0.43
1:G:294:MET:HG3	1:G:298:TYR:CD2	2.54	0.43
1:F:296:TYR:HB2	1:F:368:LEU:HD13	2.00	0.43
1:A:100:GLY:O	1:A:101:HIS:HB2	2.18	0.43
1:A:111:VAL:O	1:A:115:MET:HG2	2.19	0.43
1:H:380:LYS:HB2	1:H:380:LYS:HE2	1.77	0.43
1:E:140:PHE:CE2	1:E:144:ARG:HB2	2.54	0.43
1:G:329:VAL:O	1:G:332:VAL:N	2.52	0.43
1:D:41:ILE:O	1:D:44:ASN:N	2.51	0.43
1:G:293:LEU:HD13	1:G:368:LEU:HD22	2.00	0.43
1:E:144:ARG:CD	1:E:144:ARG:C	2.85	0.42
1:B:148:SER:N	1:B:149:PRO:C	2.72	0.42
1:C:162:GLU:O	1:C:166:GLY:CA	2.66	0.42
1:E:152:GLY:CA	1:E:153:PHE:CB	2.96	0.42
1:B:148:SER:CA	1:B:149:PRO:C	2.88	0.42
1:G:358:ARG:HB2	1:G:360:LYS:HZ3	1.84	0.42
1:F:58:GLN:O	1:F:62:LYS:HG2	2.19	0.42
1:E:253:GLN:C	1:E:254:VAL:CG2	2.88	0.42
1:H:286:TYR:O	1:H:289:LEU:HB3	2.19	0.42
1:E:293:LEU:HD22	1:E:297:PHE:CE2	2.55	0.42
1:C:131:ILE:HD12	1:D:121:ILE:HG12	2.01	0.42
1:A:229:ASN:OD1	1:A:229:ASN:N	2.52	0.42
1:D:194:LYS:HB2	1:D:194:LYS:HE3	1.72	0.42
1:F:132:LEU:HD12	1:F:132:LEU:HA	1.76	0.42
1:D:259:LYS:NZ	1:D:260:GLN:CG	2.73	0.42
1:G:358:ARG:HG2	1:G:359:TYR:N	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:LEU:O	1:C:197:GLN:CG	2.66	0.42
1:E:253:GLN:CD	1:E:253:GLN:N	2.73	0.42
1:H:220:PHE:CZ	1:H:381:MET:SD	3.12	0.42
1:E:373:ILE:HD11	1:E:378:ILE:HG12	2.02	0.42
1:E:293:LEU:HG	1:E:368:LEU:HD22	2.02	0.42
1:C:55:GLN:OE1	1:D:84:LYS:NZ	2.45	0.42
1:E:148:SER:OG	1:F:40:LEU:O	2.30	0.42
1:F:332:VAL:O	1:F:336:LEU:CD2	2.67	0.42
1:D:274:GLU:O	1:D:277:LEU:HB3	2.20	0.42
1:E:144:ARG:C	1:E:146:TYR:H	2.22	0.42
1:E:41:ILE:O	1:E:45:TYR:N	2.46	0.42
1:E:256:GLU:H	1:E:256:GLU:HG2	1.57	0.42
1:E:144:ARG:HH11	1:E:336:LEU:HD21	1.79	0.42
1:C:244:LYS:HB2	1:C:250:LYS:CE	2.50	0.42
1:F:41:ILE:C	1:F:43:GLY:H	2.23	0.42
1:F:217:PRO:HA	1:F:221:ASN:OD1	2.19	0.42
1:E:221:ASN:O	1:E:222:PHE:C	2.58	0.42
1:E:193:LEU:HD23	1:E:193:LEU:HA	1.91	0.42
1:D:141:ASN:C	1:D:143:PHE:N	2.71	0.42
1:D:144:ARG:O	1:D:147:LEU:CB	2.50	0.42
1:E:140:PHE:CD1	1:E:335:MET:SD	3.12	0.42
1:C:298:TYR:O	1:C:304:PHE:HB2	2.20	0.42
1:B:106:ARG:NH2	1:C:300:GLU:OE1	2.53	0.42
1:C:246:GLU:C	1:C:247:SER:HG	2.08	0.42
1:E:361:VAL:O	1:E:361:VAL:HG12	2.19	0.42
1:G:331:MET:HE1	1:G:332:VAL:HG22	2.02	0.41
1:B:156:LEU:CD2	1:B:188:GLU:CG	2.88	0.41
1:H:362:PHE:O	1:H:366:PHE:HD2	2.03	0.41
1:F:141:ASN:HD21	1:H:372:LEU:CD2	2.30	0.41
1:G:138:LEU:HA	1:G:138:LEU:HD12	1.84	0.41
1:C:140:PHE:HA	1:C:143:PHE:CE1	2.54	0.41
1:C:153:PHE:N	1:C:154:GLN:CA	2.81	0.41
1:C:270:GLU:HG2	1:C:286:TYR:CE2	2.56	0.41
1:C:365:LEU:HA	1:C:368:LEU:HG	2.02	0.41
1:E:122:LEU:HD23	1:E:122:LEU:HA	1.92	0.41
1:H:358:ARG:HH21	1:H:358:ARG:N	2.18	0.41
1:F:147:LEU:CD1	1:F:147:LEU:C	2.88	0.41
1:H:106:ARG:HG3	1:H:107:ASN:N	2.35	0.41
1:E:132:LEU:HA	1:E:132:LEU:HD23	1.78	0.41
1:F:109:LEU:HD11	1:G:305:GLN:NE2	2.36	0.41
1:C:103:ARG:HA	1:C:103:ARG:HD3	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:VAL:HG12	1:E:255:ALA:H	1.85	0.41
1:G:148:SER:HB2	1:H:40:LEU:HD13	2.01	0.41
1:C:259:LYS:HD2	1:C:259:LYS:HA	1.94	0.41
1:F:186:GLY:HA2	1:F:189:ASN:HB2	2.03	0.41
1:D:261:LYS:C	1:D:263:VAL:N	2.70	0.41
1:E:263:VAL:CG1	1:E:264:LEU:H	2.31	0.41
1:H:41:ILE:HG13	1:H:44:ASN:H	1.86	0.41
1:E:103:ARG:NH1	1:E:213:PRO:HD2	2.34	0.41
1:D:362:PHE:O	1:D:365:LEU:N	2.54	0.41
1:F:144:ARG:CA	1:F:147:LEU:HD11	2.43	0.41
1:G:189:ASN:HB3	1:G:192:LEU:HB2	2.03	0.41
1:B:146:TYR:C	1:B:147:LEU:HD13	2.41	0.41
1:D:210:GLU:HG2	1:D:287:ARG:HB3	2.02	0.41
1:A:190:GLU:HG3	1:A:191:LEU:N	2.34	0.41
1:B:362:PHE:HB3	1:B:365:LEU:HD12	2.03	0.41
1:C:358:ARG:N	1:C:359:TYR:CD2	2.89	0.41
1:D:202:LEU:HD21	1:D:283:ARG:HB3	2.03	0.41
1:E:153:PHE:CG	1:E:153:PHE:O	2.70	0.41
1:F:358:ARG:HD2	1:F:360:LYS:NZ	2.35	0.41
1:G:163:ASN:O	1:G:166:GLY:CA	2.69	0.41
1:B:218:HIS:N	1:B:218:HIS:CD2	2.88	0.41
1:E:296:TYR:HB2	1:E:368:LEU:HD13	2.01	0.41
1:B:365:LEU:HA	1:B:368:LEU:HG	2.03	0.41
1:D:110:LYS:HD3	1:D:114:ARG:NH2	2.36	0.41
1:A:216:GLU:HA	1:A:217:PRO:HD3	1.93	0.41
1:D:225:LYS:O	1:D:229:ASN:ND2	2.53	0.41
1:C:358:ARG:N	1:C:358:ARG:HD2	2.35	0.41
1:D:259:LYS:HE2	1:D:260:GLN:CA	2.50	0.41
1:D:154:GLN:HA	1:D:154:GLN:OE1	2.20	0.41
1:F:334:ARG:HH11	1:F:335:MET:HE1	1.86	0.41
1:F:245:GLU:HG2	1:F:245:GLU:H	1.56	0.41
1:F:85:GLN:O	1:F:88:TRP:HB3	2.20	0.41
1:C:293:LEU:HA	1:C:293:LEU:HD23	1.95	0.41
1:A:269:ASP:OD2	1:A:272:ARG:HB2	2.21	0.41
1:G:185:LYS:HE2	1:G:192:LEU:HD21	2.02	0.41
1:F:326:TYR:O	1:F:328:HIS:O	2.39	0.41
1:E:115:MET:HE2	1:E:201:LEU:HD21	2.02	0.41
1:A:326:TYR:O	1:A:329:VAL:HG22	2.21	0.41
1:G:332:VAL:CA	1:G:335:MET:HG2	2.51	0.40
1:A:165:ILE:HD13	1:A:165:ILE:HA	1.85	0.40
1:A:365:LEU:HA	1:A:368:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:HD21	1:A:283:ARG:HB3	2.03	0.40
1:D:140:PHE:CG	1:D:335:MET:SD	3.15	0.40
1:G:194:LYS:HE3	1:G:198:GLU:CD	2.34	0.40
1:G:162:GLU:CA	1:G:167:VAL:HG23	2.51	0.40
1:D:132:LEU:HD23	1:D:132:LEU:HA	1.81	0.40
1:D:147:LEU:HD12	1:D:147:LEU:HA	1.80	0.40
1:G:189:ASN:CA	1:G:192:LEU:HB2	2.44	0.40
1:C:103:ARG:CG	3:C:404:HOH:O	2.49	0.40
1:D:294:MET:HG3	1:D:298:TYR:CD2	2.56	0.40
1:G:168:LEU:O	1:G:169:GLN:CB	2.70	0.40
1:F:149:PRO:CD	1:F:149:PRO:O	2.69	0.40
1:C:159:ARG:NH1	1:C:172:ARG:NH2	2.69	0.40
1:G:149:PRO:O	1:G:152:GLY:CA	2.70	0.40
1:C:144:ARG:O	1:C:144:ARG:CG	2.69	0.40
1:C:143:PHE:O	1:C:145:GLU:N	2.54	0.40
1:D:257:PHE:CE1	1:D:258:GLN:HA	2.57	0.40
1:D:259:LYS:HZ1	1:D:260:GLN:CB	2.35	0.40
1:F:149:PRO:O	1:F:152:GLY:CA	2.69	0.40
1:H:332:VAL:O	1:H:336:LEU:HB2	2.22	0.40
1:A:192:LEU:HA	1:A:192:LEU:HD12	1.91	0.40
1:F:202:LEU:HD22	1:F:361:VAL:HG13	2.03	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	300/373 (80%)	294 (98%)	6 (2%)	0	100	100
1	B	288/373 (77%)	279 (97%)	8 (3%)	1 (0%)	46	79
1	C	305/373 (82%)	297 (97%)	6 (2%)	2 (1%)	26	63
1	D	278/373 (74%)	269 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	285/373 (76%)	278 (98%)	7 (2%)	0	100	100
1	F	295/373 (79%)	287 (97%)	5 (2%)	3 (1%)	19	54
1	G	296/373 (79%)	285 (96%)	8 (3%)	3 (1%)	19	54
1	H	293/373 (79%)	287 (98%)	6 (2%)	0	100	100
All	All	2340/2984 (78%)	2276 (97%)	55 (2%)	9 (0%)	39	74

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	150	ALA
1	C	247	SER
1	C	250	LYS
1	F	42	TYR
1	F	148	SER
1	G	149	PRO
1	G	220	PHE
1	G	217	PRO
1	F	149	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	285/340 (84%)	273 (96%)	12 (4%)	36	73
1	B	276/340 (81%)	250 (91%)	26 (9%)	11	32
1	C	292/340 (86%)	267 (91%)	25 (9%)	13	36
1	D	269/340 (79%)	242 (90%)	27 (10%)	9	28
1	E	273/340 (80%)	252 (92%)	21 (8%)	16	42
1	F	281/340 (83%)	254 (90%)	27 (10%)	10	31
1	G	283/340 (83%)	258 (91%)	25 (9%)	12	35
1	H	281/340 (83%)	268 (95%)	13 (5%)	33	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2240/2720 (82%)	2064 (92%)	176 (8%)	15	41

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	GLU
1	A	135	MET
1	A	145	GLU
1	A	193	LEU
1	A	211	ARG
1	A	228	LYS
1	A	245	GLU
1	A	321	MET
1	A	330	CYS
1	A	331	MET
1	A	358	ARG
1	A	372	LEU
1	B	40	LEU
1	B	41	ILE
1	B	147	LEU
1	B	148	SER
1	B	151	SER
1	B	154	GLN
1	B	159	ARG
1	B	165	ILE
1	B	168	LEU
1	B	169	GLN
1	B	183	ASN
1	B	185	LYS
1	B	189	ASN
1	B	211	ARG
1	B	218	HIS
1	B	221	ASN
1	B	231	THR
1	B	254	VAL
1	B	258	GLN
1	B	270	GLU
1	B	331	MET
1	B	332	VAL
1	B	336	LEU
1	B	359	TYR
1	B	360	LYS

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Mol	Chain	Res	Type
1	B	376	HIS
1	C	103	ARG
1	C	138	LEU
1	C	144	ARG
1	C	145	GLU
1	C	147	LEU
1	C	168	LEU
1	C	170	ASN
1	C	171	MET
1	C	172	ARG
1	C	177	ARG
1	C	197	GLN
1	C	218	HIS
1	C	245	GLU
1	C	250	LYS
1	C	251	GLU
1	C	277	LEU
1	C	318	ASP
1	C	319	SER
1	C	329	VAL
1	C	330	CYS
1	C	333	HIS
1	C	338	SER
1	C	358	ARG
1	C	359	TYR
1	C	375	ARG
1	D	102	VAL
1	D	144	ARG
1	D	145	GLU
1	D	147	LEU
1	D	148	SER
1	D	168	LEU
1	D	191	LEU
1	D	192	LEU
1	D	227	GLU
1	D	228	LYS
1	D	232	ARG
1	D	234	LEU
1	D	257	PHE
1	D	259	LYS
1	D	260	GLN
1	D	318	ASP

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Mol	Chain	Res	Type
1	D	329	VAL
1	D	330	CYS
1	D	336	LEU
1	D	358	ARG
1	D	359	TYR
1	D	360	LYS
1	D	361	VAL
1	D	364	ASP
1	D	380	LYS
1	D	381	MET
1	D	382	ASN
1	E	102	VAL
1	E	119	SER
1	E	144	ARG
1	E	148	SER
1	E	154	GLN
1	E	157	GLN
1	E	168	LEU
1	E	169	GLN
1	E	187	GLU
1	E	238	PHE
1	E	239	ILE
1	E	254	VAL
1	E	256	GLU
1	E	257	PHE
1	E	262	GLU
1	E	277	LEU
1	E	329	VAL
1	E	330	CYS
1	E	331	MET
1	E	359	TYR
1	E	363	VAL
1	F	40	LEU
1	F	99	ASN
1	F	102	VAL
1	F	110	LYS
1	F	113	SER
1	F	145	GLU
1	F	147	LEU
1	F	149	PRO
1	F	153	PHE
1	F	168	LEU

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Mol	Chain	Res	Type
1	F	184	PHE
1	F	187	GLU
1	F	189	ASN
1	F	190	GLU
1	F	195	SER
1	F	196	GLU
1	F	216	GLU
1	F	236	GLU
1	F	244	LYS
1	F	274	GLU
1	F	305	GLN
1	F	331	MET
1	F	334	ARG
1	F	335	MET
1	F	358	ARG
1	F	370	THR
1	F	372	LEU
1	G	40	LEU
1	G	41	ILE
1	G	102	VAL
1	G	138	LEU
1	G	145	GLU
1	G	149	PRO
1	G	154	GLN
1	G	155	SER
1	G	165	ILE
1	G	185	LYS
1	G	188	GLU
1	G	189	ASN
1	G	190	GLU
1	G	191	LEU
1	G	192	LEU
1	G	250	LYS
1	G	251	GLU
1	G	253	GLN
1	G	293	LEU
1	G	323	LYS
1	G	331	MET
1	G	358	ARG
1	G	360	LYS
1	G	375	ARG
1	G	376	HIS

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Mol	Chain	Res	Type
1	H	41	ILE
1	H	102	VAL
1	H	106	ARG
1	H	145	GLU
1	H	147	LEU
1	H	151	SER
1	H	189	ASN
1	H	237	GLU
1	H	331	MET
1	H	358	ARG
1	H	360	LYS
1	H	363	VAL
1	H	370	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	A	382	ASN
1	B	98	GLN
1	B	154	GLN
1	B	169	GLN
1	B	183	ASN
1	B	218	HIS
1	B	260	GLN
1	B	328	HIS
1	B	376	HIS
1	C	170	ASN
1	C	253	GLN
1	D	99	ASN
1	D	260	GLN
1	D	273	HIS
1	E	169	GLN
1	E	253	GLN
1	E	333	HIS
1	F	189	ASN
1	F	260	GLN
1	F	382	ASN
1	G	154	GLN
1	G	221	ASN
1	H	141	ASN
1	H	218	HIS

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Mol	Chain	Res	Type
1	H	258	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q < 0.9
1	A	306/373 (82%)	-0.00	5 (1%)	74	72	24, 44, 97, 131	0
1	B	296/373 (79%)	0.13	7 (2%)	62	57	29, 65, 129, 148	0
1	C	313/373 (83%)	0.13	9 (2%)	55	49	36, 59, 101, 138	0
1	D	288/373 (77%)	0.43	19 (6%)	22	16	42, 76, 129, 147	0
1	E	293/373 (78%)	0.30	15 (5%)	32	25	33, 67, 125, 155	0
1	F	303/373 (81%)	0.14	5 (1%)	73	70	31, 66, 119, 143	0
1	G	304/373 (81%)	0.21	10 (3%)	50	42	32, 74, 126, 140	0
1	H	301/373 (80%)	0.05	11 (3%)	45	38	27, 51, 103, 142	0
All	All	2404/2984 (80%)	0.17	81 (3%)	49	41	24, 62, 120, 155	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	151	SER	7.2
1	H	359	TYR	5.7
1	D	238	PHE	5.1
1	G	359	TYR	4.9
1	C	154	GLN	4.8
1	F	242	GLN	4.8
1	D	234	LEU	4.8
1	D	237	GLU	4.5
1	H	151	SER	4.4
1	H	245	GLU	4.4
1	D	235	GLU	4.4
1	F	169	GLN	4.2
1	C	248	GLU	4.1
1	E	238	PHE	4.1
1	E	152	GLY	4.0
1	G	151	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	151	SER	3.7
1	B	187	GLU	3.6
1	D	231	THR	3.6
1	E	371	TYR	3.5
1	H	335	MET	3.5
1	E	264	LEU	3.4
1	D	222	PHE	3.3
1	C	175	TYR	3.2
1	D	226	LEU	3.2
1	E	222	PHE	3.1
1	E	148	SER	3.1
1	A	151	SER	3.1
1	F	359	TYR	3.0
1	F	168	LEU	3.0
1	G	152	GLY	3.0
1	D	260	GLN	3.0
1	D	371	TYR	3.0
1	C	341	GLY	2.9
1	B	241	ILE	2.9
1	E	256	GLU	2.8
1	E	359	TYR	2.8
1	H	193	LEU	2.8
1	E	381	MET	2.8
1	C	359	TYR	2.8
1	E	150	ALA	2.8
1	A	333	HIS	2.7
1	D	333	HIS	2.7
1	E	260	GLN	2.7
1	C	262	GLU	2.7
1	E	265	LEU	2.6
1	D	377	TRP	2.6
1	F	153	PHE	2.5
1	C	173	VAL	2.5
1	H	218	HIS	2.5
1	H	252	GLU	2.5
1	C	174	PRO	2.5
1	D	223	TRP	2.5
1	G	150	ALA	2.5
1	H	244	LYS	2.4
1	C	245	GLU	2.4
1	H	148	SER	2.4
1	G	333	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	147	LEU	2.4
1	B	152	GLY	2.4
1	E	149	PRO	2.4
1	D	258	GLN	2.3
1	D	264	LEU	2.3
1	D	233	GLY	2.3
1	B	148	SER	2.3
1	G	246	GLU	2.2
1	A	359	TYR	2.2
1	E	230	ILE	2.2
1	H	241	ILE	2.2
1	B	382	ASN	2.2
1	D	329	VAL	2.2
1	G	271	LYS	2.2
1	D	265	LEU	2.1
1	G	287	ARG	2.1
1	G	245	GLU	2.1
1	G	335	MET	2.1
1	A	153	PHE	2.1
1	B	184	PHE	2.0
1	D	359	TYR	2.0
1	H	358	ARG	2.0
1	A	148	SER	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, 95th 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(\AA^2)	Q<0.9
2	CO	H	401	1/1	0.98	0.26	1.28	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.