



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:31 am BST

PDB ID : 2VRT
Title : Crystal Structure of E. coli RNase E possessing M1 RNA fragments - Catalytic Domain
Authors : Koslover, D.J.; Callaghan, A.J.; Marcaida, M.J.; Garman, E.F.; Martick, M.; Scott, W.G.; Luisi, B.F.
Deposited on : 2008-04-14
Resolution : 3.50 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

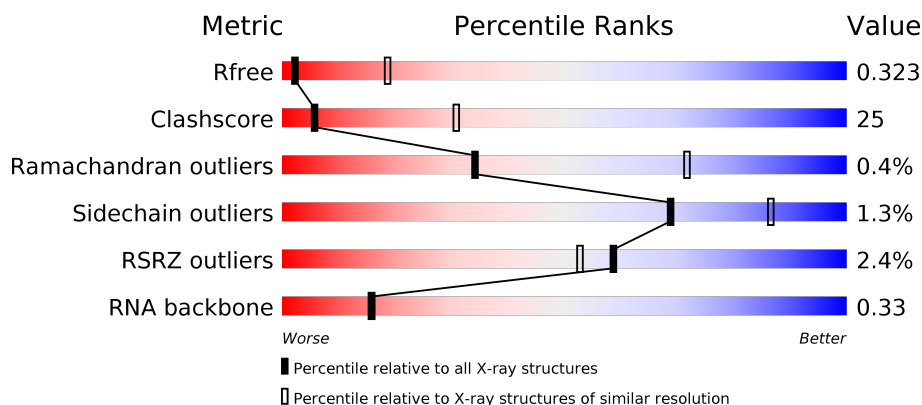
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



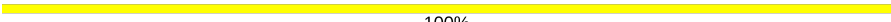
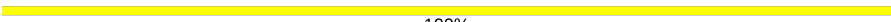
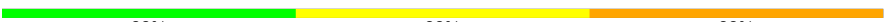
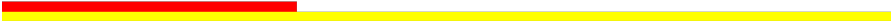
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	509	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>34%</div> <div>8%</div> </div> </div>
1	B	509	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>21%</div> <div>22%</div> </div> </div>
1	C	509	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>16%</div> <div>19%</div> </div> </div>
1	D	509	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	E	2	 100%
2	F	2	 100%
3	G	3	 33% 33% 33%
3	H	3	 33% 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ZN	D	1509	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13186 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 RIBONUCLEASE E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3465	2178	613	663	11			
1	B	398	Total	C	N	O	S	0	0	0
			2915	1825	522	557	11			
1	C	411	Total	C	N	O	S	0	0	0
			2966	1859	521	575	11			
1	D	487	Total	C	N	O	S	0	0	0
			3628	2273	648	696	11			

- Molecule 2 is a RNA chain called 5'-R(*UP*UP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	P	0	0	0
			41	18	4	17	2			
2	F	2	Total	C	N	O	P	0	0	0
			41	18	4	17	2			

- Molecule 3 is a RNA chain called 5'-R(*UP*UP*GP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O	P	0	0	0
			64	28	9	24	3			
3	H	3	Total	C	N	O	P	0	0	0
			64	28	9	24	3			

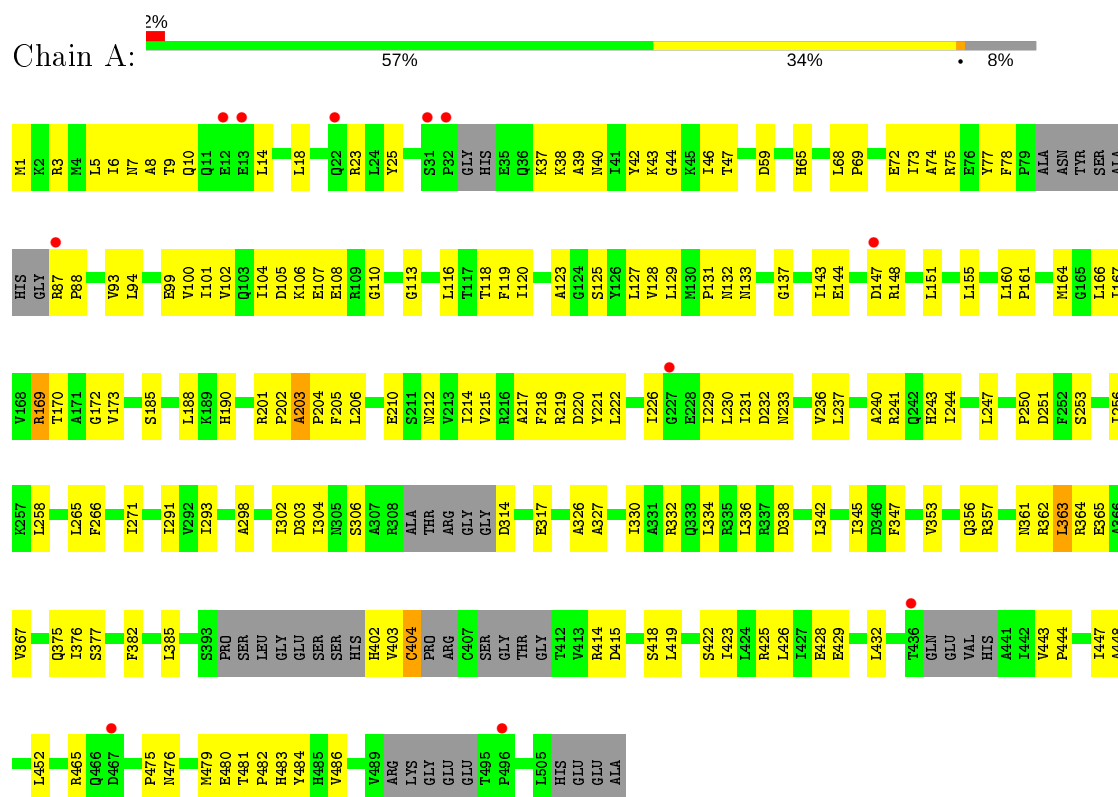
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

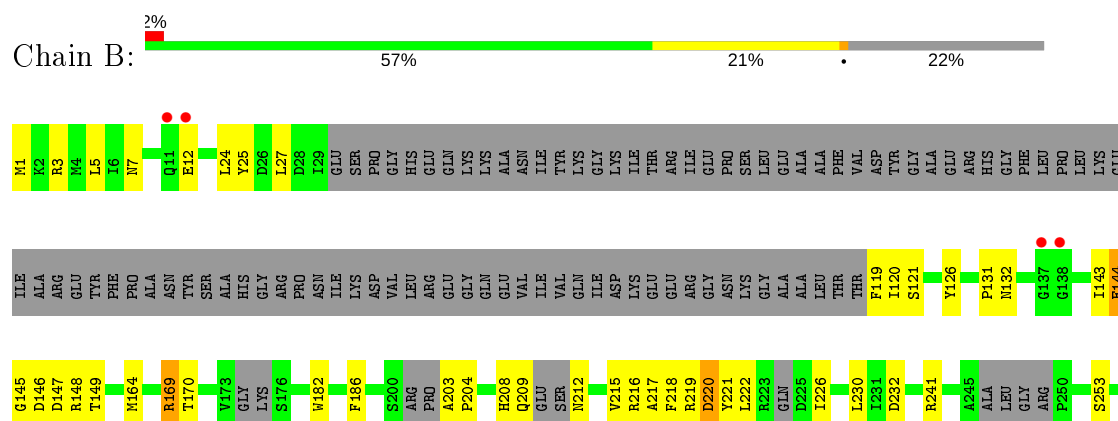
3 Residue-property plots [i](#)

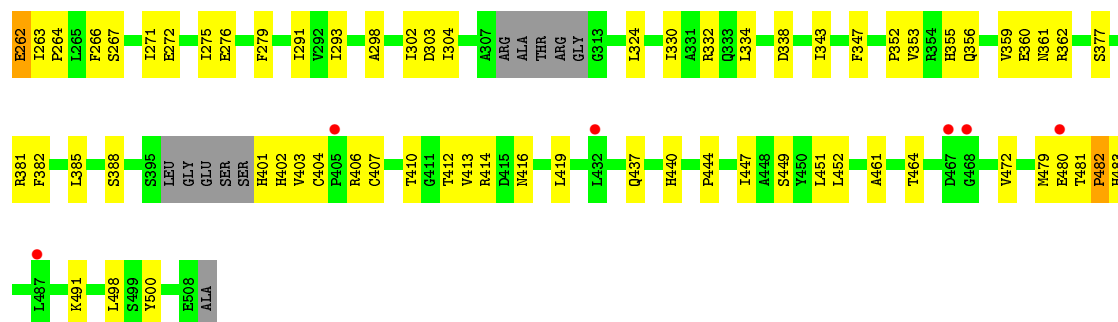
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: RIBONUCLEASE E

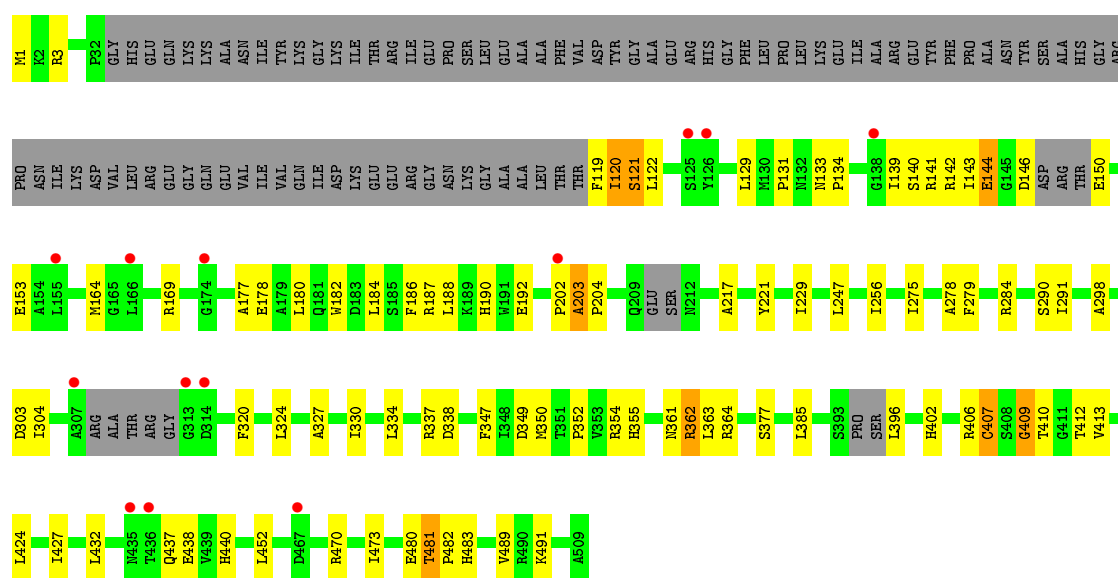


• Molecule 1: RIBONUCLEASE E

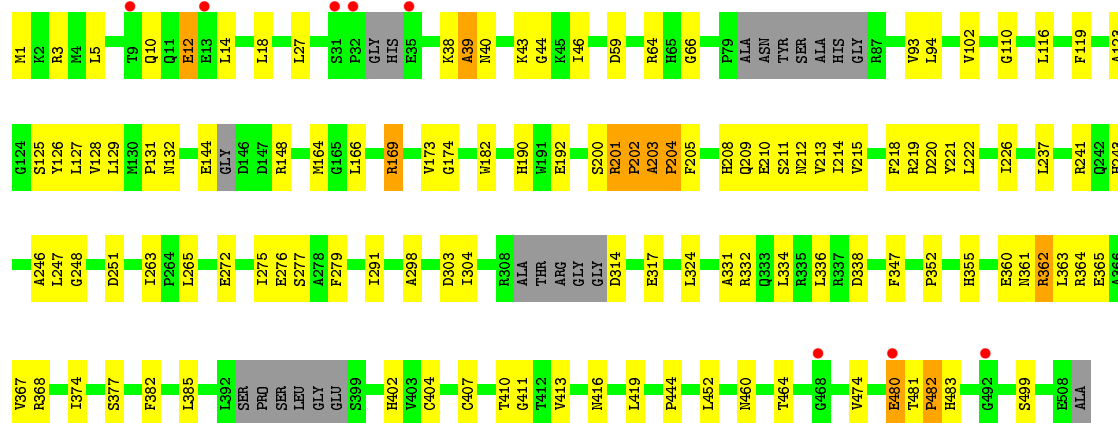




• Molecule 1: RIBONUCLEASE E



• Molecule 1: RIBONUCLEASE E



• Molecule 2: 5'-R(*UP*UP)-3'

Chain E:  100%

U1
U2

- Molecule 2: 5'-R(*UP*UP)-3'

Chain F:  100%

U1
U2

- Molecule 3: 5'-R(*UP*UP*GP)-3'

Chain G:  33% 33% 33%

U1
U2
G3

- Molecule 3: 5'-R(*UP*UP*GP)-3'

Chain H:  33% 100%

U1
U2
G3

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.89Å 121.25Å 242.23Å 90.00° 99.47° 90.00°	Depositor
Resolution (Å)	24.98 – 3.50 24.86 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.98-3.50) 99.9 (24.86-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 3.46Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.317 , 0.351 0.296 , 0.323	Depositor DCC
R_{free} test set	3402 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.077 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	13186	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0546e-03.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	1/3511 (0.0%)	0.54	0/4773
1	B	0.30	0/2951	0.57	3/4007 (0.1%)
1	C	0.30	0/3008	0.60	6/4099 (0.1%)
1	D	0.31	0/3684	0.57	6/5009 (0.1%)
2	E	1.80	1/44 (2.3%)	1.24	0/64
2	F	1.67	1/44 (2.3%)	1.09	0/64
3	G	1.51	1/70 (1.4%)	1.12	0/105
3	H	1.47	1/70 (1.4%)	1.29	0/105
All	All	0.37	5/13382 (0.0%)	0.59	15/18226 (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	A	0	1
1	D	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	U	OP3-P	-10.50	1.48	1.61
2	E	1	U	OP3-P	-10.37	1.48	1.61
3	G	1	U	OP3-P	-10.34	1.48	1.61
2	F	1	U	OP3-P	-10.20	1.49	1.61
1	A	185	SER	CB-OG	7.53	1.52	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	ALA	N-CA-CB	-10.24	95.77	110.10
1	C	203	ALA	N-CA-C	9.79	137.44	111.00
1	D	200	SER	CB-CA-C	8.87	126.96	110.10
1	C	121	SER	N-CA-CB	-7.73	98.91	110.50
1	B	402	HIS	N-CA-C	-6.87	92.44	111.00
1	C	202	PRO	CB-CA-C	6.82	129.04	112.00
1	D	201	ARG	C-N-CD	-6.80	105.65	120.60
1	D	39	ALA	CB-CA-C	-5.79	101.42	110.10
1	C	409	GLY	N-CA-C	5.73	127.42	113.10
1	B	220	ASP	CB-CA-C	-5.55	99.29	110.40
1	D	211	SER	N-CA-C	5.47	125.76	111.00
1	D	482	PRO	CB-CA-C	-5.31	98.73	112.00
1	B	402	HIS	N-CA-CB	5.30	120.14	110.60
1	D	201	ARG	N-CA-CB	-5.25	101.16	110.60
1	C	349	ASP	CB-CG-OD2	5.21	122.99	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	ALA	Peptide
1	D	203	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3465	0	3309	252	0
1	B	2915	0	2767	158	0
1	C	2966	0	2763	118	0
1	D	3628	0	3443	162	0
2	E	41	0	21	1	0
2	F	41	0	21	0	0
3	G	64	0	32	1	0
3	H	64	0	32	5	0
4	A	1	0	0	0	0
4	D	1	0	0	2	0
All	All	13186	0	12388	647	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 25.

All (647) 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:A:7:ASN:CB	1:A:266:PHE:HE2	1.09	1.65
1:A:7:ASN:HB2	1:A:266:PHE:CE2	1.26	1.63
1:C:139:ILE:CD1	1:C:143:ILE:HD13	1.27	1.60
1:A:244:ILE:CD1	1:A:256:ILE:HD11	1.36	1.54
1:C:139:ILE:CD1	1:C:143:ILE:CD1	1.83	1.54
1:D:352:PRO:HG2	1:D:355:HIS:CD2	1.49	1.47
1:B:7:ASN:CB	1:B:266:PHE:HE2	1.28	1.42
1:B:7:ASN:CB	1:B:266:PHE:CE2	2.07	1.37
1:B:146:ASP:HA	1:B:149:THR:CB	1.57	1.34
1:A:244:ILE:HD12	1:A:256:ILE:CD1	1.62	1.29
1:B:7:ASN:HB3	1:B:266:PHE:CE2	1.69	1.27
1:C:407:CYS:SG	1:C:410:THR:O	1.92	1.27
1:C:139:ILE:HD12	1:C:143:ILE:CD1	1.52	1.26
1:D:212:ASN:OD1	1:D:215:VAL:HG23	1.29	1.25
1:A:444:PRO:HG2	1:A:480:GLU:O	1.39	1.23
1:D:352:PRO:CG	1:D:355:HIS:CD2	2.21	1.23
1:A:444:PRO:CG	1:A:480:GLU:O	1.87	1.22
1:A:244:ILE:CD1	1:A:256:ILE:CD1	2.17	1.21
1:A:201:ARG:HD3	1:A:205:PHE:CZ	1.76	1.19
1:C:139:ILE:CG1	1:C:143:ILE:HD13	1.70	1.19
1:B:7:ASN:OD1	1:B:232:ASP:OD1	1.56	1.18
1:B:264:PRO:HG2	1:B:267:SER:CB	1.73	1.18
1:D:352:PRO:CG	1:D:355:HIS:HD2	1.56	1.18
1:D:212:ASN:CG	1:D:215:VAL:HG23	1.66	1.16
1:A:101:ILE:HG22	1:A:120:ILE:HD11	1.20	1.15
1:C:139:ILE:HD11	1:C:143:ILE:CD1	1.56	1.15
1:A:102:VAL:HG11	1:A:116:LEU:HD13	1.25	1.15
1:A:169:ARG:HG2	1:A:169:ARG:HH11	1.00	1.15
1:A:432:LEU:HD22	1:B:263:ILE:HD13	1.15	1.14
1:B:7:ASN:HB2	1:B:266:PHE:CE2	1.74	1.14
1:C:406:ARG:NH2	1:C:481:THR:HG23	1.63	1.13
1:A:237:LEU:HD11	1:A:256:ILE:HG22	1.20	1.12
1:D:40:ASN:OD1	1:D:210:GLU:N	1.82	1.12
1:B:419:LEU:HD21	1:B:481:THR:O	1.49	1.12
1:B:144:GLU:O	1:B:147:ASP:CB	1.96	1.12
1:A:266:PHE:HD1	1:A:271:ILE:HD11	1.14	1.11
1:D:203:ALA:HB1	1:D:204:PRO:HD3	1.23	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:PRO:CB	1:D:355:HIS:HD2	1.65	1.09
1:B:481:THR:HG22	1:B:482:PRO:CD	1.80	1.09
1:D:182:TRP:CH2	1:D:222:LEU:O	2.07	1.07
1:B:444:PRO:HD2	1:B:447:ILE:HD12	1.35	1.06
1:A:244:ILE:HD11	1:A:256:ILE:HD11	1.09	1.06
1:C:377:SER:O	1:C:385:LEU:HD11	1.56	1.06
1:C:139:ILE:CD1	1:C:143:ILE:HD12	1.79	1.04
1:A:237:LEU:HD11	1:A:256:ILE:CG2	1.87	1.03
1:A:218:PHE:HD1	1:A:222:LEU:HD11	1.24	1.03
1:B:216:ARG:O	1:B:220:ASP:HB2	1.59	1.03
1:C:139:ILE:HD12	1:C:143:ILE:HD12	1.31	1.02
1:B:481:THR:HG22	1:B:482:PRO:HD3	1.03	1.02
1:A:203:ALA:HB1	1:A:204:PRO:HD3	1.38	1.01
1:C:377:SER:O	1:C:385:LEU:CD1	2.08	1.01
1:C:362:ARG:HH11	1:C:362:ARG:CG	1.74	1.01
1:B:264:PRO:HG2	1:B:267:SER:HB2	1.03	1.00
1:A:44:GLY:HA2	1:A:204:PRO:CB	1.92	1.00
1:A:44:GLY:HA2	1:A:204:PRO:HB3	1.43	0.99
1:D:59:ASP:O	1:D:204:PRO:HG3	1.62	0.99
1:A:214:ILE:HG23	1:A:218:PHE:CE2	1.98	0.99
1:A:7:ASN:CB	1:A:266:PHE:CE2	2.01	0.98
1:A:266:PHE:CD1	1:A:271:ILE:HD11	1.97	0.98
1:D:201:ARG:CG	1:D:202:PRO:HD2	1.94	0.98
1:A:7:ASN:HB3	1:A:266:PHE:HE2	1.26	0.98
1:B:481:THR:CG2	1:B:482:PRO:HD3	1.93	0.98
1:A:425:ARG:HB3	1:B:272:GLU:HG2	1.41	0.98
1:D:39:ALA:HB3	1:D:210:GLU:CB	1.94	0.98
1:A:244:ILE:HD12	1:A:256:ILE:HD12	1.46	0.97
1:D:128:VAL:O	1:D:166:LEU:HD12	1.63	0.97
1:B:449:SER:OG	1:D:474:VAL:HG23	1.64	0.97
1:C:144:GLU:OE1	1:C:144:GLU:HA	1.65	0.96
1:D:404:CYS:HG	4:D:1509:ZN:ZN	0.64	0.95
1:D:44:GLY:HA2	1:D:204:PRO:HB3	1.46	0.95
1:C:139:ILE:O	3:H:2:U:H4'	1.67	0.95
1:A:432:LEU:HD22	1:B:263:ILE:CD1	1.96	0.95
1:B:7:ASN:HB3	1:B:266:PHE:HE2	0.78	0.94
1:A:291:ILE:CG2	1:A:302:ILE:CG2	2.45	0.94
1:D:201:ARG:HG2	1:D:202:PRO:HD2	1.48	0.93
1:A:59:ASP:O	1:A:204:PRO:HG3	1.67	0.93
1:A:444:PRO:HG3	1:A:480:GLU:O	1.69	0.93
1:D:352:PRO:HB2	1:D:355:HIS:HD2	1.31	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:PRO:HB2	1:D:355:HIS:CD2	2.04	0.93
1:B:266:PHE:HD1	1:B:271:ILE:HD11	1.35	0.92
1:A:237:LEU:CD1	1:A:256:ILE:CG2	2.47	0.92
1:B:352:PRO:HG2	1:B:355:HIS:ND1	1.85	0.91
1:C:140:SER:O	1:C:143:ILE:HG23	1.70	0.91
1:A:444:PRO:HD2	1:A:447:ILE:HD12	1.50	0.91
1:B:264:PRO:CG	1:B:267:SER:HB2	1.98	0.91
1:D:182:TRP:CZ2	1:D:222:LEU:O	2.24	0.90
1:B:419:LEU:CD2	1:B:481:THR:O	2.20	0.90
1:C:139:ILE:HG13	1:C:143:ILE:HD13	1.53	0.90
1:A:214:ILE:HG23	1:A:218:PHE:HE2	1.36	0.89
1:D:212:ASN:OD1	1:D:215:VAL:CG2	2.19	0.89
1:D:129:LEU:HA	1:D:166:LEU:HD13	1.55	0.89
1:D:212:ASN:ND2	1:D:215:VAL:HG23	1.87	0.89
1:A:382:PHE:HE1	1:B:388:SER:HG	1.15	0.89
1:D:352:PRO:HG2	1:D:355:HIS:NE2	1.87	0.89
1:B:146:ASP:CA	1:B:149:THR:CB	2.48	0.88
1:C:406:ARG:NH2	1:C:481:THR:CG2	2.35	0.88
1:A:169:ARG:HG2	1:A:169:ARG:NH1	1.79	0.88
1:A:59:ASP:O	1:A:204:PRO:CG	2.21	0.88
1:C:1:MET:SD	1:C:3:ARG:NH1	2.47	0.88
1:A:432:LEU:CD2	1:B:263:ILE:HD13	2.01	0.88
1:A:291:ILE:CG2	1:A:302:ILE:HG23	2.02	0.88
1:B:481:THR:CG2	1:B:482:PRO:CD	2.50	0.88
1:A:201:ARG:HD3	1:A:205:PHE:CE2	2.09	0.88
1:C:406:ARG:HH21	1:C:481:THR:HG23	1.38	0.88
1:D:59:ASP:O	1:D:204:PRO:CG	2.22	0.87
1:B:481:THR:CG2	1:B:482:PRO:N	2.37	0.87
1:D:119:PHE:HA	1:D:132:ASN:HD22	1.37	0.87
1:D:46:ILE:CD1	1:D:94:LEU:HD13	2.04	0.87
1:C:139:ILE:HB	1:C:143:ILE:HG21	1.54	0.87
1:A:465:ARG:HD3	1:B:262:GLU:HG3	1.57	0.87
1:B:262:GLU:OE1	1:B:262:GLU:HA	1.72	0.87
1:C:362:ARG:HG3	1:C:362:ARG:HH11	1.38	0.86
1:D:203:ALA:CB	1:D:204:PRO:HD3	2.03	0.86
1:D:212:ASN:ND2	1:D:215:VAL:CG2	2.38	0.86
1:B:377:SER:O	1:B:385:LEU:HD11	1.74	0.86
1:B:266:PHE:CD1	1:B:271:ILE:HD11	2.09	0.86
1:A:101:ILE:CG2	1:A:120:ILE:HD11	2.04	0.85
1:A:377:SER:O	1:A:385:LEU:HD11	1.76	0.85
1:B:119:PHE:N	1:B:132:ASN:HD22	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:ARG:HE	1:B:482:PRO:HG3	1.39	0.84
1:B:481:THR:HG23	1:B:482:PRO:N	1.91	0.84
1:B:377:SER:O	1:B:385:LEU:CD1	2.26	0.84
1:D:201:ARG:CG	1:D:202:PRO:CD	2.56	0.84
1:A:377:SER:O	1:A:385:LEU:CD1	2.26	0.83
1:D:44:GLY:HA2	1:D:204:PRO:CB	2.08	0.82
1:B:216:ARG:O	1:B:220:ASP:CB	2.27	0.82
1:C:406:ARG:HH21	1:C:481:THR:CG2	1.93	0.82
1:A:101:ILE:HG22	1:A:120:ILE:CD1	2.08	0.82
1:A:43:LYS:O	1:A:204:PRO:CB	2.27	0.82
1:A:201:ARG:HD3	1:A:205:PHE:CE1	2.15	0.82
1:A:414:ARG:HH22	1:A:422:SER:HB2	1.44	0.82
1:A:73:ILE:HG21	1:A:93:VAL:HG11	1.61	0.81
1:C:139:ILE:HD11	1:C:143:ILE:HD11	1.59	0.81
1:A:131:PRO:HA	1:A:164:MET:HB3	1.61	0.81
1:A:203:ALA:CB	1:A:204:PRO:HD3	2.09	0.81
1:D:212:ASN:CG	1:D:215:VAL:CG2	2.48	0.81
1:D:481:THR:OG1	1:D:482:PRO:HD3	1.79	0.81
1:D:444:PRO:CG	1:D:480:GLU:O	2.29	0.81
1:D:352:PRO:CB	1:D:355:HIS:CD2	2.51	0.81
1:A:291:ILE:HD13	1:A:330:ILE:CG1	2.10	0.80
1:D:128:VAL:C	1:D:166:LEU:HD12	2.00	0.80
1:D:1:MET:HE2	1:D:3:ARG:CZ	2.11	0.80
1:A:169:ARG:CG	1:A:169:ARG:HH11	1.91	0.80
1:C:139:ILE:HD12	1:C:143:ILE:HD13	1.21	0.80
1:D:377:SER:O	1:D:385:LEU:HD11	1.82	0.80
1:A:7:ASN:HB2	1:A:266:PHE:CD2	2.15	0.79
1:A:201:ARG:HB3	1:A:205:PHE:CZ	2.17	0.79
1:A:266:PHE:HD1	1:A:271:ILE:CD1	1.93	0.79
1:A:44:GLY:CA	1:A:204:PRO:HB3	2.12	0.79
1:A:214:ILE:O	1:A:218:PHE:HD2	1.66	0.79
1:C:406:ARG:HH22	1:C:481:THR:HG23	1.47	0.79
1:A:250:PRO:O	1:A:253:SER:HB2	1.83	0.79
1:B:218:PHE:O	1:B:222:LEU:HB2	1.81	0.79
1:A:241:ARG:HH21	1:A:256:ILE:HG22	1.47	0.79
1:A:243:HIS:O	1:A:247:LEU:HG	1.83	0.78
1:A:102:VAL:CG1	1:A:116:LEU:HD13	2.11	0.78
1:A:212:ASN:OD1	1:A:215:VAL:CG2	2.31	0.78
1:D:1:MET:CE	1:D:3:ARG:CZ	2.61	0.78
1:A:291:ILE:CD1	1:A:330:ILE:HG13	2.13	0.78
1:A:218:PHE:CD1	1:A:222:LEU:HD11	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:TYR:HE1	1:A:118:THR:HB	1.49	0.77
1:D:1:MET:HE1	1:D:3:ARG:NH1	1.99	0.77
1:A:402:HIS:O	1:B:412:THR:HA	1.84	0.77
1:A:291:ILE:HG23	1:A:302:ILE:CG2	2.12	0.77
1:A:465:ARG:CD	1:B:262:GLU:HG3	2.14	0.77
1:D:201:ARG:HG2	1:D:202:PRO:CD	2.14	0.77
1:B:25:TYR:HA	1:B:332:ARG:HD2	1.66	0.76
1:D:46:ILE:HD13	1:D:94:LEU:HD13	1.67	0.76
1:D:131:PRO:HA	1:D:164:MET:HB3	1.67	0.76
1:A:291:ILE:HG21	1:A:302:ILE:CG2	2.16	0.75
1:B:266:PHE:HD1	1:B:271:ILE:CD1	1.99	0.75
1:D:1:MET:CE	1:D:3:ARG:NE	2.49	0.75
1:A:7:ASN:HB3	1:A:266:PHE:CE2	2.05	0.75
1:D:377:SER:O	1:D:385:LEU:CD1	2.35	0.75
1:D:1:MET:HE1	1:D:3:ARG:HH11	1.52	0.74
1:B:419:LEU:HD23	1:B:447:ILE:HD11	1.68	0.74
1:A:212:ASN:OD1	1:A:215:VAL:HG23	1.88	0.74
1:B:25:TYR:HA	1:B:332:ARG:CD	2.17	0.74
1:D:38:LYS:O	1:D:210:GLU:CB	2.36	0.74
1:D:212:ASN:HD21	1:D:215:VAL:CG2	2.00	0.74
1:D:46:ILE:HD11	1:D:94:LEU:HD13	1.68	0.73
1:C:143:ILE:HG13	1:C:143:ILE:O	1.89	0.73
1:C:481:THR:OG1	1:C:482:PRO:HD3	1.88	0.73
1:A:363:LEU:HD23	1:A:385:LEU:HD21	1.70	0.73
1:A:127:LEU:HD22	1:A:166:LEU:HD21	1.70	0.73
1:A:161:PRO:HG2	1:A:164:MET:SD	2.28	0.72
1:A:129:LEU:HD21	1:A:188:LEU:HD23	1.69	0.72
1:B:447:ILE:HD11	1:B:481:THR:O	1.89	0.72
1:A:104:ILE:HA	1:A:116:LEU:HD23	1.72	0.72
1:A:291:ILE:HD13	1:A:330:ILE:HG13	1.69	0.72
1:D:201:ARG:HG3	1:D:202:PRO:HD2	1.69	0.72
1:D:407:CYS:HG	4:D:1509:ZN:ZN	1.04	0.72
1:A:237:LEU:HD11	1:A:241:ARG:HH21	1.55	0.71
1:A:7:ASN:OD1	1:A:232:ASP:OD1	2.08	0.71
1:C:131:PRO:HA	1:C:164:MET:HB2	1.72	0.71
1:D:1:MET:CE	1:D:3:ARG:NH1	2.54	0.71
1:D:444:PRO:HG2	1:D:480:GLU:O	1.90	0.71
1:C:144:GLU:CA	1:C:144:GLU:OE1	2.38	0.71
1:C:362:ARG:HH11	1:C:362:ARG:HG2	1.55	0.71
1:B:419:LEU:CD2	1:B:447:ILE:HD11	2.21	0.70
1:C:131:PRO:HA	1:C:164:MET:CB	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ASN:HA	1:D:208:HIS:O	1.91	0.70
1:A:137:GLY:HA2	1:A:166:LEU:O	1.89	0.70
1:D:127:LEU:HD13	1:D:166:LEU:HD21	1.73	0.70
1:B:416:ASN:ND2	1:B:481:THR:OG1	2.25	0.70
1:C:412:THR:O	1:C:412:THR:HG22	1.91	0.70
1:C:1:MET:SD	1:C:3:ARG:CZ	2.80	0.70
1:A:362:ARG:O	1:A:365:GLU:N	2.25	0.70
1:A:77:TYR:CE1	1:A:118:THR:HB	2.27	0.70
1:A:403:VAL:HG12	1:A:404:CYS:H	1.57	0.69
1:D:129:LEU:CA	1:D:166:LEU:HD13	2.21	0.69
1:D:444:PRO:HG3	1:D:480:GLU:O	1.91	0.69
1:A:303:ASP:HB2	1:B:298:ALA:HB2	1.73	0.69
1:D:203:ALA:HB1	1:D:204:PRO:CD	2.14	0.69
1:C:279:PHE:HA	1:C:396:LEU:HD11	1.74	0.69
1:D:363:LEU:O	1:D:367:VAL:HG22	1.92	0.69
1:A:298:ALA:HB2	1:B:303:ASP:HB2	1.75	0.69
1:A:203:ALA:HB1	1:A:204:PRO:CD	2.21	0.68
1:A:363:LEU:O	1:A:367:VAL:HG22	1.94	0.68
1:C:139:ILE:O	3:H:2:U:C5'	2.41	0.68
1:A:170:THR:O	1:A:173:VAL:HG23	1.94	0.68
1:B:444:PRO:HB3	1:B:480:GLU:HA	1.75	0.68
1:D:123:ALA:O	1:D:219:ARG:HD2	1.93	0.68
1:A:108:GLU:HA	1:A:113:GLY:O	1.93	0.68
1:D:272:GLU:O	1:D:276:GLU:HG2	1.92	0.68
1:C:139:ILE:O	3:H:2:U:C4'	2.42	0.68
1:C:337:ARG:O	1:C:338:ASP:HB2	1.93	0.68
1:D:129:LEU:HA	1:D:166:LEU:CD1	2.24	0.67
1:D:201:ARG:HB3	1:D:205:PHE:CZ	2.28	0.67
1:A:43:LYS:O	1:A:204:PRO:HB2	1.93	0.67
1:D:481:THR:HG1	1:D:482:PRO:HD3	1.60	0.67
1:A:214:ILE:HG23	1:A:218:PHE:CD2	2.30	0.67
1:D:314:ASP:HB3	1:D:317:GLU:HB3	1.75	0.67
1:A:44:GLY:HA2	1:A:204:PRO:HB2	1.76	0.67
1:A:137:GLY:CA	1:A:166:LEU:O	2.43	0.67
1:A:18:LEU:HD11	1:A:221:TYR:HD1	1.60	0.66
1:A:201:ARG:HB3	1:A:205:PHE:CE1	2.30	0.66
1:B:352:PRO:HG2	1:B:355:HIS:CE1	2.30	0.66
1:B:216:ARG:CD	1:B:219:ARG:NH2	2.58	0.66
1:B:5:LEU:CD2	1:B:230:LEU:HD12	2.26	0.66
1:A:119:PHE:HA	1:A:132:ASN:HD22	1.58	0.66
1:A:314:ASP:HB3	1:A:317:GLU:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ALA:HB2	1:A:14:LEU:HD13	1.77	0.66
1:A:425:ARG:CB	1:B:272:GLU:HG2	2.23	0.66
1:B:216:ARG:HD2	1:B:219:ARG:NH2	2.10	0.66
1:B:352:PRO:CG	1:B:355:HIS:ND1	2.58	0.66
1:D:209:GLN:HG2	1:D:212:ASN:HD22	1.60	0.65
1:B:352:PRO:HG2	1:B:355:HIS:CG	2.31	0.65
1:B:352:PRO:CG	1:B:355:HIS:CE1	2.79	0.65
1:B:444:PRO:CD	1:B:447:ILE:HD12	2.18	0.65
1:A:419:LEU:HD21	1:A:481:THR:O	1.95	0.65
1:A:291:ILE:HG23	1:A:302:ILE:HG22	1.79	0.65
1:B:262:GLU:CA	1:B:262:GLU:OE1	2.44	0.65
1:D:128:VAL:C	1:D:166:LEU:CD1	2.64	0.65
1:A:23:ARG:NH2	1:A:332:ARG:HE	1.95	0.65
1:B:169:ARG:CG	1:B:169:ARG:HH11	2.09	0.65
1:D:212:ASN:OD1	1:D:215:VAL:N	2.28	0.65
1:D:14:LEU:CD2	1:D:213:VAL:HG11	2.27	0.64
1:A:47:THR:HG21	1:A:65:HIS:CD2	2.31	0.64
1:C:327:ALA:O	1:C:363:LEU:HD12	1.96	0.64
1:A:419:LEU:CD2	1:A:481:THR:O	2.45	0.64
1:B:119:PHE:N	1:B:132:ASN:ND2	2.45	0.64
1:D:5:LEU:HB3	1:D:265:LEU:HD21	1.80	0.64
1:C:129:LEU:HG	1:C:131:PRO:HD3	1.80	0.64
1:A:214:ILE:O	1:A:218:PHE:CD2	2.49	0.64
1:C:119:PHE:O	1:C:120:ILE:HG23	1.97	0.64
1:C:352:PRO:HG2	1:C:355:HIS:ND1	2.12	0.63
1:A:127:LEU:HB3	1:A:166:LEU:HD11	1.79	0.63
1:A:291:ILE:HG12	1:A:304:ILE:HG12	1.79	0.63
1:A:243:HIS:O	1:A:247:LEU:CG	2.47	0.63
1:C:203:ALA:HB3	1:C:204:PRO:HD3	1.81	0.63
1:D:43:LYS:O	1:D:204:PRO:CB	2.47	0.63
1:B:444:PRO:HB3	1:B:480:GLU:CA	2.26	0.63
1:C:362:ARG:NH1	1:C:362:ARG:CG	2.43	0.63
1:A:382:PHE:CE1	1:B:388:SER:HB3	2.33	0.62
1:A:414:ARG:NH1	1:B:276:GLU:OE2	2.28	0.62
1:A:201:ARG:CD	1:A:205:PHE:CE1	2.82	0.62
1:A:201:ARG:CD	1:A:205:PHE:CZ	2.69	0.62
1:A:78:PHE:CE1	1:A:93:VAL:HG22	2.33	0.62
1:C:352:PRO:HG2	1:C:355:HIS:CE1	2.34	0.62
1:A:222:LEU:HD21	1:A:229:ILE:HD11	1.81	0.62
1:A:479:MET:CE	1:A:483:HIS:CD2	2.81	0.62
1:C:362:ARG:NH1	1:C:362:ARG:HG2	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:PRO:CD	1:A:447:ILE:HD12	2.28	0.62
1:D:212:ASN:ND2	1:D:215:VAL:HG21	2.14	0.62
1:D:243:HIS:O	1:D:247:LEU:HB2	2.00	0.61
1:D:44:GLY:CA	1:D:204:PRO:HB3	2.24	0.61
1:B:182:TRP:O	1:B:186:PHE:HD1	1.83	0.61
1:A:212:ASN:OD1	1:A:215:VAL:HG21	2.00	0.61
1:A:46:ILE:HD13	1:A:94:LEU:HB3	1.82	0.61
1:C:330:ILE:O	1:C:334:LEU:HG	1.99	0.61
1:C:291:ILE:HG22	1:C:304:ILE:HG12	1.82	0.61
1:A:361:ASN:O	1:A:364:ARG:HB2	2.00	0.60
1:C:352:PRO:HB2	1:C:355:HIS:ND1	2.16	0.60
1:C:139:ILE:CB	1:C:143:ILE:HG21	2.29	0.60
1:B:145:GLY:C	1:B:147:ASP:N	2.51	0.60
1:C:350:MET:SD	1:C:355:HIS:O	2.60	0.60
1:C:406:ARG:HH21	1:C:481:THR:CB	2.14	0.60
1:D:39:ALA:C	1:D:210:GLU:CB	2.69	0.60
1:A:101:ILE:CG2	1:A:120:ILE:CD1	2.74	0.59
1:D:182:TRP:HH2	1:D:222:LEU:O	1.81	0.59
1:A:444:PRO:CG	1:A:480:GLU:C	2.68	0.59
1:C:438:GLU:HG2	1:C:470:ARG:HB2	1.83	0.59
1:C:437:GLN:HB2	1:C:491:LYS:HA	1.84	0.59
1:B:452:LEU:HD13	1:D:452:LEU:HB3	1.84	0.59
1:A:119:PHE:HA	1:A:132:ASN:ND2	2.17	0.59
1:A:414:ARG:NH2	1:A:422:SER:HB2	2.16	0.59
1:C:327:ALA:O	1:C:363:LEU:CD1	2.49	0.59
1:B:145:GLY:O	1:B:149:THR:N	2.35	0.59
1:C:298:ALA:HB2	1:D:303:ASP:HB2	1.84	0.59
1:A:151:LEU:O	1:A:155:LEU:N	2.27	0.59
1:A:147:ASP:OD2	1:A:173:VAL:CG1	2.51	0.59
1:A:480:GLU:C	1:A:482:PRO:HD2	2.23	0.59
1:A:404:CYS:SG	1:B:406:ARG:HG2	2.43	0.59
1:B:131:PRO:HA	1:B:164:MET:CB	2.33	0.59
1:B:7:ASN:ND2	1:B:266:PHE:CD2	2.71	0.59
1:B:145:GLY:O	1:B:148:ARG:N	2.37	0.58
1:D:39:ALA:CB	1:D:210:GLU:CB	2.77	0.58
1:C:150:GLU:O	1:C:153:GLU:N	2.32	0.58
1:C:407:CYS:HB2	1:C:412:THR:HB	1.84	0.58
1:D:14:LEU:HD23	1:D:213:VAL:HG11	1.85	0.58
1:D:131:PRO:HA	1:D:164:MET:CB	2.33	0.58
1:B:481:THR:N	1:B:482:PRO:HD2	2.19	0.58
1:A:291:ILE:HG21	1:A:302:ILE:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:ILE:HD12	1:C:347:PHE:HA	1.86	0.58
1:A:291:ILE:HD13	1:A:330:ILE:HG12	1.86	0.58
1:C:119:PHE:O	1:C:120:ILE:CG2	2.52	0.58
1:A:131:PRO:HA	1:A:164:MET:CB	2.31	0.57
1:B:216:ARG:O	1:B:220:ASP:N	2.31	0.57
1:D:190:HIS:ND1	1:D:247:LEU:HA	2.19	0.57
1:B:208:HIS:HE1	1:B:215:VAL:HG11	1.69	0.57
1:D:102:VAL:HG11	1:D:116:LEU:HD13	1.85	0.57
1:B:146:ASP:C	1:B:149:THR:H	2.08	0.57
1:B:24:LEU:O	1:B:332:ARG:HD2	2.03	0.57
1:D:222:LEU:HA	1:D:226:ILE:HD12	1.86	0.57
1:C:409:GLY:HA2	1:D:411:GLY:O	2.05	0.57
1:C:413:VAL:CB	1:D:402:HIS:CD2	2.87	0.57
1:A:237:LEU:CD1	1:A:256:ILE:HG21	2.31	0.57
1:A:147:ASP:OD2	1:A:173:VAL:HG11	2.05	0.57
1:C:327:ALA:HA	1:C:363:LEU:HD13	1.87	0.57
1:B:452:LEU:HD13	1:D:452:LEU:CB	2.35	0.57
1:A:43:LYS:O	1:A:204:PRO:CA	2.53	0.56
1:A:237:LEU:HD12	1:A:256:ILE:HG21	1.86	0.56
1:A:432:LEU:CD2	1:B:263:ILE:CD1	2.74	0.56
1:A:218:PHE:CE1	1:A:244:ILE:HD11	2.40	0.56
1:D:481:THR:N	1:D:482:PRO:CD	2.68	0.56
1:D:64:ARG:NH1	1:D:110:GLY:O	2.37	0.56
1:D:125:SER:OG	1:D:220:ASP:HA	2.05	0.56
1:D:460:ASN:O	1:D:464:THR:HG22	2.06	0.56
1:A:201:ARG:CB	1:A:205:PHE:CZ	2.88	0.56
1:A:129:LEU:CD2	1:A:188:LEU:HD23	2.35	0.55
1:A:190:HIS:ND1	1:A:247:LEU:HA	2.21	0.55
1:A:293:ILE:HG12	1:A:302:ILE:HG12	1.89	0.55
1:A:481:THR:N	1:A:482:PRO:HD2	2.22	0.55
1:C:481:THR:OG1	1:C:482:PRO:CD	2.54	0.55
1:B:5:LEU:HD21	1:B:230:LEU:HD12	1.87	0.55
1:A:1:MET:SD	1:A:3:ARG:NH1	2.79	0.55
1:B:7:ASN:ND2	1:B:266:PHE:HD2	2.05	0.55
1:B:218:PHE:HA	1:B:222:LEU:HG	1.87	0.55
1:C:139:ILE:O	3:H:2:U:H5"	2.07	0.55
1:C:482:PRO:HG2	1:C:483:HIS:CD2	2.41	0.55
1:A:23:ARG:NH2	1:A:332:ARG:NE	2.54	0.55
1:A:403:VAL:HG12	1:A:404:CYS:N	2.21	0.55
1:A:479:MET:HE2	1:A:483:HIS:CD2	2.42	0.55
1:D:214:ILE:CG2	1:D:218:PHE:CE1	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:HIS:CE1	1:C:489:VAL:HG21	2.42	0.55
1:D:291:ILE:HG22	1:D:304:ILE:HG12	1.89	0.55
1:B:1:MET:SD	1:B:3:ARG:NH1	2.80	0.55
1:D:444:PRO:HD3	1:D:483:HIS:O	2.06	0.55
1:A:125:SER:OG	1:A:220:ASP:HA	2.07	0.54
1:A:465:ARG:HD3	1:B:262:GLU:CG	2.34	0.54
1:A:5:LEU:HD22	1:A:265:LEU:HD11	1.88	0.54
1:B:262:GLU:O	1:B:263:ILE:C	2.46	0.54
1:C:413:VAL:CB	1:D:402:HIS:O	2.55	0.54
1:A:143:ILE:HD13	1:A:151:LEU:CD1	2.37	0.54
1:B:324:LEU:HD22	1:B:362:ARG:HD2	1.90	0.54
1:D:5:LEU:HB3	1:D:265:LEU:CD2	2.37	0.54
1:A:68:LEU:HD11	1:A:118:THR:HG23	1.90	0.54
1:D:1:MET:HE3	1:D:3:ARG:NE	2.23	0.54
1:B:169:ARG:HG3	1:B:169:ARG:HH11	1.72	0.54
1:D:201:ARG:HG3	1:D:202:PRO:CD	2.32	0.53
1:D:332:ARG:NH1	1:D:336:LEU:HD11	2.23	0.53
1:D:38:LYS:O	1:D:39:ALA:HB3	2.09	0.53
1:B:352:PRO:HG3	1:B:355:HIS:CE1	2.43	0.53
1:D:173:VAL:HG13	1:D:174:GLY:N	2.23	0.53
1:C:144:GLU:C	1:C:146:ASP:H	2.12	0.53
1:C:184:LEU:O	1:C:188:LEU:HG	2.08	0.53
1:A:414:ARG:HD2	1:B:279:PHE:CD2	2.43	0.53
1:A:479:MET:HE1	1:A:483:HIS:CD2	2.44	0.53
1:B:461:ALA:HA	1:B:464:THR:HG22	1.91	0.53
1:A:46:ILE:CD1	1:A:94:LEU:HD13	2.39	0.53
1:D:203:ALA:CB	1:D:204:PRO:CD	2.83	0.53
1:D:363:LEU:HD23	1:D:385:LEU:HD21	1.91	0.53
1:B:169:ARG:HG3	3:G:1:U:OP2	2.08	0.53
1:A:382:PHE:HE1	1:B:388:SER:CB	2.21	0.52
1:B:406:ARG:NE	1:B:482:PRO:HG3	2.16	0.52
1:C:131:PRO:HA	1:C:164:MET:HB3	1.91	0.52
1:A:9:THR:OG1	1:A:10:GLN:NE2	2.43	0.52
1:D:212:ASN:O	1:D:215:VAL:N	2.42	0.52
1:B:264:PRO:HG2	1:B:267:SER:OG	2.08	0.52
1:C:141:ARG:N	3:H:2:U:OP1	2.41	0.52
1:C:324:LEU:HD22	1:C:362:ARG:HD2	1.91	0.52
1:A:128:VAL:HG22	1:A:169:ARG:HD2	1.92	0.52
1:D:66:GLY:HA3	1:D:116:LEU:HD11	1.91	0.52
1:D:331:ALA:O	1:D:334:LEU:HB2	2.09	0.51
1:B:304:ILE:HD12	1:B:347:PHE:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:ARG:HH11	1:C:290:SER:HB3	1.75	0.51
1:D:40:ASN:OD1	1:D:210:GLU:CB	2.59	0.51
1:A:250:PRO:O	1:A:253:SER:CB	2.55	0.51
1:A:414:ARG:HH22	1:A:422:SER:CB	2.20	0.51
1:A:128:VAL:CG2	1:A:169:ARG:HD2	2.41	0.51
1:A:25:TYR:HA	1:A:332:ARG:HD2	1.92	0.51
1:A:452:LEU:HD13	1:C:452:LEU:HB3	1.91	0.51
1:A:327:ALA:CB	1:A:362:ARG:HG2	2.41	0.51
1:A:327:ALA:HB1	1:A:362:ARG:HG2	1.93	0.51
1:B:444:PRO:HG2	1:B:481:THR:CA	2.41	0.51
1:A:332:ARG:NH1	1:A:336:LEU:HD11	2.26	0.51
1:A:338:ASP:OD1	1:A:338:ASP:O	2.28	0.51
1:A:201:ARG:HG2	1:A:202:PRO:HD2	1.92	0.51
1:A:382:PHE:CE1	1:B:388:SER:CB	2.94	0.51
1:A:481:THR:N	1:A:482:PRO:CD	2.74	0.51
1:A:201:ARG:HB3	1:A:205:PHE:HZ	1.75	0.51
1:A:304:ILE:HD12	1:A:347:PHE:HA	1.93	0.51
1:D:361:ASN:O	1:D:364:ARG:HB2	2.10	0.51
1:A:147:ASP:CG	1:A:173:VAL:HG13	2.31	0.50
1:C:402:HIS:HD2	1:D:413:VAL:HB	1.75	0.50
1:D:237:LEU:CD2	1:D:241:ARG:HE	2.24	0.50
1:B:216:ARG:HD3	1:B:219:ARG:CZ	2.42	0.50
1:B:406:ARG:HH21	1:B:482:PRO:HD3	1.76	0.50
1:B:182:TRP:O	1:B:186:PHE:CD1	2.64	0.50
1:D:127:LEU:HB3	1:D:166:LEU:HD11	1.93	0.50
1:D:43:LYS:O	1:D:204:PRO:HB2	2.11	0.50
1:C:182:TRP:O	1:C:186:PHE:HD1	1.95	0.50
1:D:419:LEU:CD2	1:D:481:THR:O	2.60	0.50
1:A:148:ARG:HA	1:A:151:LEU:HD12	1.93	0.50
1:A:415:ASP:HB2	1:A:418:SER:OG	2.12	0.50
1:A:419:LEU:HD23	1:A:447:ILE:HD11	1.93	0.50
1:B:131:PRO:HA	1:B:164:MET:HB2	1.93	0.50
1:D:404:CYS:O	1:D:407:CYS:O	2.29	0.50
1:A:222:LEU:HA	1:A:226:ILE:HD12	1.92	0.50
1:B:480:GLU:C	1:B:482:PRO:HD2	2.31	0.49
1:A:382:PHE:HE1	1:B:388:SER:OG	1.85	0.49
1:D:338:ASP:O	1:D:338:ASP:OD1	2.30	0.49
1:A:166:LEU:HD12	1:A:167:ILE:H	1.78	0.49
1:C:122:LEU:HD13	1:C:190:HIS:HB3	1.95	0.49
1:D:27:LEU:HD22	1:D:275:ILE:HG12	1.95	0.49
1:A:429:GLU:HG2	1:B:267:SER:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:LEU:N	1:D:166:LEU:CD1	2.75	0.49
1:A:102:VAL:HG13	1:A:116:LEU:HB3	1.94	0.49
1:B:293:ILE:HG12	1:B:302:ILE:HG12	1.95	0.49
1:B:353:VAL:O	1:B:356:GLN:HB2	2.13	0.49
1:C:188:LEU:O	1:C:192:GLU:HG2	2.12	0.49
1:A:203:ALA:CB	1:A:204:PRO:CD	2.85	0.48
1:A:221:TYR:O	1:A:226:ILE:CD1	2.61	0.48
1:A:479:MET:CE	1:A:483:HIS:HD2	2.26	0.48
1:D:129:LEU:CA	1:D:166:LEU:CD1	2.87	0.48
1:A:423:ILE:HD11	1:A:484:TYR:CD2	2.48	0.48
1:B:226:ILE:HG22	1:B:226:ILE:O	2.13	0.48
1:B:144:GLU:OE1	1:B:144:GLU:N	2.46	0.48
1:B:131:PRO:HA	1:B:164:MET:HB3	1.95	0.48
1:A:414:ARG:HD2	1:B:279:PHE:CE2	2.48	0.48
1:A:5:LEU:HD23	1:A:230:LEU:HB2	1.96	0.48
1:C:412:THR:HG22	1:C:482:PRO:HB3	1.94	0.48
1:A:6:ILE:HB	1:A:231:ILE:HG12	1.96	0.48
1:C:327:ALA:CA	1:C:363:LEU:HD13	2.43	0.48
1:C:437:GLN:C	1:C:438:GLU:HG3	2.34	0.48
1:B:403:VAL:HG12	1:B:404:CYS:N	2.27	0.48
1:D:214:ILE:HG23	1:D:218:PHE:CE1	2.48	0.48
1:D:362:ARG:O	1:D:365:GLU:N	2.42	0.48
1:D:474:VAL:HG21	1:D:499:SER:O	2.14	0.48
1:A:357:ARG:HH11	1:A:357:ARG:HA	1.79	0.47
1:A:123:ALA:O	1:A:219:ARG:HD2	2.14	0.47
1:A:251:ASP:C	1:A:253:SER:H	2.17	0.47
1:B:209:GLN:CG	1:B:212:ASN:HB3	2.44	0.47
1:A:375:GLN:NE2	1:B:381:ARG:HH12	2.11	0.47
1:C:284:ARG:NH1	1:C:290:SER:HB3	2.29	0.47
1:C:303:ASP:HB2	1:D:298:ALA:HB2	1.94	0.47
1:A:143:ILE:HG22	1:A:144:GLU:N	2.30	0.47
1:B:338:ASP:O	1:B:338:ASP:OD1	2.33	0.47
1:A:330:ILE:O	1:A:334:LEU:HG	2.14	0.47
1:B:216:ARG:CD	1:B:219:ARG:CZ	2.92	0.47
1:B:241:ARG:NH1	1:B:253:SER:O	2.43	0.47
1:C:327:ALA:HB1	1:C:363:LEU:HB2	1.95	0.47
1:D:1:MET:CE	1:D:3:ARG:HE	2.25	0.47
1:B:264:PRO:O	1:B:267:SER:N	2.48	0.47
1:C:278:ALA:O	1:C:396:LEU:HD13	2.15	0.47
1:A:151:LEU:HD21	1:A:172:GLY:O	2.15	0.47
1:B:413:VAL:HG12	1:B:414:ARG:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:LEU:HD21	1:D:241:ARG:HE	1.80	0.47
1:D:416:ASN:HD21	1:D:481:THR:CG2	2.27	0.47
1:A:291:ILE:HD11	1:A:326:ALA:HB1	1.96	0.46
1:C:119:PHE:C	1:C:120:ILE:HG23	2.36	0.46
1:D:481:THR:N	1:D:482:PRO:HD3	2.28	0.46
1:A:190:HIS:CE1	1:A:247:LEU:HD23	2.51	0.46
1:A:46:ILE:HD13	1:A:94:LEU:HD13	1.97	0.46
1:C:432:LEU:HD21	1:D:263:ILE:HG23	1.98	0.46
1:D:352:PRO:CD	1:D:355:HIS:CD2	2.97	0.46
2:E:2:U:H6	2:E:2:U:O5'	1.97	0.46
1:A:222:LEU:CD2	1:A:229:ILE:HD11	2.45	0.46
1:A:73:ILE:HG21	1:A:93:VAL:CG1	2.40	0.46
1:B:145:GLY:O	1:B:146:ASP:C	2.54	0.46
1:A:452:LEU:HD13	1:C:452:LEU:CB	2.46	0.46
1:B:481:THR:N	1:B:482:PRO:CD	2.78	0.46
1:D:119:PHE:HA	1:D:132:ASN:ND2	2.18	0.46
1:A:74:ALA:HB2	1:A:132:ASN:HD21	1.80	0.46
1:A:40:ASN:OD1	1:A:210:GLU:N	2.35	0.46
1:B:169:ARG:NH1	1:B:169:ARG:CG	2.73	0.46
1:B:482:PRO:HG2	1:B:483:HIS:H	1.80	0.46
1:D:192:GLU:OE2	1:D:192:GLU:HA	2.15	0.46
1:D:93:VAL:HG12	1:D:94:LEU:HG	1.97	0.46
1:B:143:ILE:HD11	1:B:170:THR:HA	1.98	0.46
1:B:403:VAL:CG1	1:B:404:CYS:N	2.79	0.46
1:C:119:PHE:HD2	1:C:120:ILE:HG12	1.80	0.46
1:D:360:GLU:O	1:D:364:ARG:HG3	2.15	0.46
1:D:407:CYS:HB2	1:D:410:THR:OG1	2.15	0.46
1:A:353:VAL:O	1:A:356:GLN:HB2	2.16	0.46
1:A:363:LEU:CD2	1:A:385:LEU:CD2	2.94	0.46
1:D:201:ARG:HB3	1:D:205:PHE:CE1	2.50	0.46
1:A:119:PHE:CD1	1:A:133:ASN:HB3	2.51	0.46
1:C:432:LEU:HD21	1:D:263:ILE:CG2	2.45	0.46
1:A:105:ASP:O	1:A:106:LYS:HG3	2.16	0.46
1:A:18:LEU:HD11	1:A:221:TYR:CD1	2.46	0.46
1:A:448:ALA:HB3	1:A:475:PRO:HB3	1.97	0.46
1:B:440:HIS:CD2	1:B:472:VAL:HB	2.51	0.46
1:C:412:THR:CG2	1:C:412:THR:O	2.62	0.46
1:C:480:GLU:O	1:C:481:THR:C	2.54	0.46
1:A:102:VAL:CG1	1:A:116:LEU:HB3	2.47	0.45
1:A:147:ASP:OD2	1:A:173:VAL:HG13	2.15	0.45
1:C:352:PRO:CG	1:C:355:HIS:ND1	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LEU:HD12	1:A:256:ILE:CG2	2.37	0.45
1:A:330:ILE:HD13	1:A:345:ILE:HD13	1.97	0.45
1:C:139:ILE:CG1	1:C:143:ILE:HG21	2.45	0.45
1:A:217:ALA:O	1:A:221:TYR:HB2	2.16	0.45
1:D:18:LEU:HD11	1:D:221:TYR:HD2	1.82	0.45
1:A:160:LEU:HD12	1:A:161:PRO:HD2	1.98	0.45
1:A:38:LYS:O	1:A:39:ALA:HB3	2.17	0.45
1:A:363:LEU:HG	1:A:376:ILE:HD13	1.99	0.45
1:D:365:GLU:O	1:D:368:ARG:HB3	2.15	0.45
1:A:78:PHE:CE1	1:A:93:VAL:CG2	3.00	0.45
1:B:27:LEU:HD22	1:B:275:ILE:HG12	1.98	0.45
1:B:291:ILE:HG22	1:B:304:ILE:HG12	1.97	0.45
1:A:219:ARG:CZ	1:A:220:ASP:OD2	2.65	0.45
1:A:233:ASN:ND2	1:A:236:VAL:HG23	2.30	0.45
1:A:363:LEU:HD23	1:A:385:LEU:CD2	2.42	0.44
1:D:277:SER:C	1:D:279:PHE:H	2.19	0.44
1:B:182:TRP:CZ3	1:B:186:PHE:HE1	2.35	0.44
1:D:10:GLN:HB3	1:D:12:GLU:OE2	2.17	0.44
1:B:407:CYS:SG	1:B:410:THR:OG1	2.66	0.44
1:B:447:ILE:CD1	1:B:481:THR:O	2.62	0.44
1:C:121:SER:HB2	1:C:129:LEU:O	2.17	0.44
1:C:377:SER:HB3	1:D:382:PHE:HE1	1.82	0.44
1:D:404:CYS:HG	1:D:407:CYS:HG	1.66	0.44
1:A:42:TYR:CE2	1:A:206:LEU:HD13	2.53	0.44
1:B:401:HIS:ND1	1:B:401:HIS:N	2.66	0.44
1:C:144:GLU:C	1:C:146:ASP:N	2.70	0.44
1:C:402:HIS:CD2	1:D:413:VAL:HB	2.51	0.44
1:D:246:ALA:C	1:D:248:GLY:H	2.21	0.44
1:A:404:CYS:SG	1:B:406:ARG:HB3	2.58	0.44
1:D:201:ARG:HA	1:D:202:PRO:HD3	1.53	0.44
1:D:202:PRO:O	1:D:205:PHE:HE1	2.00	0.44
1:B:419:LEU:HD21	1:B:447:ILE:HD11	2.00	0.44
1:B:272:GLU:HA	1:B:275:ILE:HD12	1.99	0.44
1:B:406:ARG:HH21	1:B:481:THR:HG22	1.82	0.43
1:D:144:GLU:O	1:D:148:ARG:CB	2.66	0.43
1:A:212:ASN:HD21	1:A:243:HIS:CE1	2.36	0.43
1:A:291:ILE:HG22	1:A:302:ILE:HG23	1.97	0.43
1:A:428:GLU:HG2	1:B:264:PRO:HG3	1.99	0.43
1:C:409:GLY:O	1:D:411:GLY:HA3	2.17	0.43
1:A:476:ASN:ND2	1:A:479:MET:SD	2.91	0.43
1:D:416:ASN:ND2	1:D:481:THR:HG22	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LYS:N	1:A:107:GLU:OE1	2.52	0.43
1:C:337:ARG:HB3	1:C:396:LEU:HB2	1.99	0.43
1:A:429:GLU:CG	1:B:267:SER:HA	2.49	0.43
1:A:77:TYR:HE1	1:A:118:THR:CB	2.26	0.43
1:B:447:ILE:O	1:B:451:LEU:HG	2.19	0.43
1:A:423:ILE:HD13	1:A:443:VAL:CG1	2.48	0.43
1:D:1:MET:HE2	1:D:3:ARG:NH1	2.30	0.43
1:B:182:TRP:CE3	1:B:186:PHE:HE1	2.37	0.43
1:C:177:ALA:O	1:C:178:GLU:C	2.57	0.43
1:C:320:PHE:CG	1:C:355:HIS:HD2	2.35	0.43
1:D:419:LEU:HD21	1:D:481:THR:O	2.19	0.43
1:C:217:ALA:O	1:C:221:TYR:HB2	2.19	0.42
1:C:275:ILE:O	1:C:278:ALA:HB3	2.18	0.42
1:A:69:PRO:HG2	1:A:72:GLU:HG2	2.01	0.42
1:B:222:LEU:HA	1:B:222:LEU:HD23	1.80	0.42
1:B:360:GLU:O	1:B:361:ASN:C	2.58	0.42
1:A:99:GLU:C	1:A:100:VAL:HG23	2.39	0.42
1:A:426:LEU:HD23	1:A:486:VAL:HG21	2.00	0.42
1:A:231:ILE:HB	1:A:237:LEU:HD13	2.00	0.42
1:C:406:ARG:O	1:C:482:PRO:HG3	2.20	0.42
1:D:481:THR:CB	1:D:482:PRO:HD3	2.46	0.42
1:A:143:ILE:HG22	1:A:148:ARG:CB	2.50	0.42
1:A:87:ARG:HA	1:A:88:PRO:HD3	1.88	0.42
1:B:203:ALA:N	1:B:204:PRO:CD	2.82	0.42
1:B:324:LEU:HA	1:B:362:ARG:HD3	2.02	0.42
1:B:334:LEU:CD2	1:B:343:ILE:HD13	2.49	0.42
1:D:324:LEU:HD22	1:D:362:ARG:CD	2.48	0.42
1:B:437:GLN:HB2	1:B:491:LYS:HA	2.02	0.42
1:C:337:ARG:HG2	1:C:396:LEU:HD22	2.02	0.42
1:C:452:LEU:HD11	1:C:473:ILE:O	2.20	0.42
1:D:1:MET:HE3	1:D:3:ARG:HE	1.84	0.42
1:A:237:LEU:CD2	1:A:258:LEU:HB2	2.50	0.42
1:A:1:MET:SD	1:A:3:ARG:CZ	3.08	0.42
1:A:403:VAL:CG1	1:A:404:CYS:H	2.31	0.42
1:A:481:THR:OG1	1:A:482:PRO:HD3	2.19	0.42
1:A:59:ASP:O	1:A:204:PRO:HG2	2.14	0.42
1:D:304:ILE:HD12	1:D:347:PHE:HA	2.00	0.42
1:A:240:ALA:O	1:A:244:ILE:HG13	2.20	0.42
1:B:217:ALA:O	1:B:221:TYR:N	2.31	0.42
1:B:1:MET:SD	1:B:3:ARG:CZ	3.08	0.42
1:D:174:GLY:O	1:D:368:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:LEU:HD13	1:B:500:TYR:OH	2.20	0.41
1:C:178:GLU:O	1:C:182:TRP:HB2	2.20	0.41
1:C:361:ASN:O	1:C:364:ARG:HB2	2.19	0.41
1:D:251:ASP:N	1:D:251:ASP:OD2	2.51	0.41
1:A:75:ARG:HA	1:A:78:PHE:CD2	2.55	0.41
1:C:133:ASN:HA	1:C:134:PRO:HD3	1.87	0.41
1:C:352:PRO:CB	1:C:355:HIS:ND1	2.83	0.41
1:B:12:GLU:OE2	1:B:12:GLU:N	2.50	0.41
1:C:122:LEU:CD1	1:C:187:ARG:O	2.68	0.41
1:D:201:ARG:HG2	1:D:202:PRO:N	2.35	0.41
1:C:177:ALA:O	1:C:180:LEU:N	2.50	0.41
1:A:342:LEU:HD22	1:B:382:PHE:HB3	2.01	0.41
1:D:367:VAL:HB	1:D:374:ILE:HD13	2.01	0.41
1:D:38:LYS:O	1:D:39:ALA:CB	2.68	0.41
1:A:148:ARG:O	1:A:151:LEU:HB2	2.21	0.41
1:A:303:ASP:CB	1:B:298:ALA:HB2	2.48	0.41
1:C:424:LEU:HA	1:C:427:ILE:HD12	2.03	0.41
1:D:277:SER:C	1:D:279:PHE:N	2.74	0.41
1:A:221:TYR:O	1:A:226:ILE:HD11	2.20	0.41
1:B:120:ILE:CG2	1:B:121:SER:N	2.83	0.41
1:B:359:VAL:O	1:B:362:ARG:HB3	2.21	0.41
1:A:251:ASP:C	1:A:253:SER:N	2.74	0.41
1:A:77:TYR:CZ	1:A:100:VAL:HG13	2.56	0.41
1:C:229:ILE:HB	1:C:256:ILE:HG12	2.02	0.41
1:C:190:HIS:ND1	1:C:247:LEU:HA	2.36	0.41
1:C:1:MET:SD	1:C:3:ARG:NE	2.94	0.41
1:A:104:ILE:HA	1:A:116:LEU:CD2	2.48	0.40
1:A:362:ARG:O	1:A:363:LEU:C	2.59	0.40
1:B:7:ASN:ND2	1:B:266:PHE:CE2	2.89	0.40
1:B:330:ILE:O	1:B:334:LEU:HG	2.22	0.40
1:C:377:SER:O	1:C:385:LEU:HD12	2.11	0.40
1:D:46:ILE:HD13	1:D:94:LEU:HB3	2.03	0.40
1:B:126:TYR:O	1:B:169:ARG:HB2	2.21	0.40
1:A:59:ASP:HB2	1:A:65:HIS:HD2	1.86	0.40
1:A:46:ILE:HD11	1:A:94:LEU:HD13	2.03	0.40
1:D:126:TYR:O	1:D:169:ARG:HB2	2.21	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	451/509 (89%)	424 (94%)	25 (6%)	2 (0%)	34	72
1	B	380/509 (75%)	354 (93%)	25 (7%)	1 (0%)	41	75
1	C	399/509 (78%)	380 (95%)	17 (4%)	2 (0%)	29	68
1	D	475/509 (93%)	441 (93%)	32 (7%)	2 (0%)	34	72
All	All	1705/2036 (84%)	1599 (94%)	99 (6%)	7 (0%)	34	72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	LEU
1	D	202	PRO
1	B	482	PRO
1	D	204	PRO
1	C	120	ILE
1	A	110	GLY
1	C	481	THR

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	345/433 (80%)	342 (99%)	3 (1%)	78	90
1	B	288/433 (66%)	284 (99%)	4 (1%)	67	85
1	C	287/433 (66%)	281 (98%)	6 (2%)	53	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	361/433 (83%)	357 (99%)	4 (1%)	73	88
All	All	1281/1732 (74%)	1264 (99%)	17 (1%)	69	86

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	ARG
1	A	306	SER
1	A	404	CYS
1	B	144	GLU
1	B	169	ARG
1	B	262	GLU
1	B	479	MET
1	C	142	ARG
1	C	144	GLU
1	C	169	ARG
1	C	354	ARG
1	C	362	ARG
1	C	407	CYS
1	D	12	GLU
1	D	169	ARG
1	D	362	ARG
1	D	480	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	65	HIS
1	A	132	ASN
1	A	280	GLN
1	A	375	GLN
1	A	416	ASN
1	A	483	HIS
1	A	485	HIS
1	B	10	GLN
1	B	208	HIS
1	B	355	HIS
1	B	416	ASN
1	C	375	GLN
1	C	402	HIS

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Mol	Chain	Res	Type
1	C	416	ASN
1	C	440	HIS
1	D	10	GLN
1	D	65	HIS
1	D	132	ASN
1	D	208	HIS
1	D	355	HIS
1	D	416	ASN
1	D	506	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	1/2 (50%)	0	0
2	F	1/2 (50%)	1 (100%)	0
3	G	2/3 (66%)	1 (50%)	0
3	H	2/3 (66%)	1 (50%)	0
All	All	6/10 (60%)	3 (50%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	F	2	U
3	G	3	G
3	H	3	G

There are no RNA pucker outliers to report.

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 [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	468/509 (91%)	-0.17	11 (2%) 59 53	68, 107, 151, 261	0
1	B	398/509 (78%)	0.03	10 (2%) 57 51	71, 129, 161, 289	0
1	C	411/509 (80%)	0.00	13 (3%) 47 42	80, 125, 164, 304	0
1	D	487/509 (95%)	-0.16	8 (1%) 72 66	71, 106, 149, 251	0
2	E	2/2 (100%)	0.04	0 100 100	109, 109, 109, 124	0
2	F	2/2 (100%)	0.41	0 100 100	128, 128, 128, 140	0
3	G	3/3 (100%)	0.43	0 100 100	122, 122, 140, 149	0
3	H	3/3 (100%)	1.06	1 (33%) 0 0	133, 133, 135, 153	0
All	All	1774/2046 (86%)	-0.08	43 (2%) 59 53	68, 117, 158, 304	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	PRO	4.8
1	C	138	GLY	4.3
1	C	125	SER	4.0
1	B	137	GLY	3.8
1	A	87	ARG	3.6
1	D	32	PRO	3.6
1	D	468	GLY	3.6
1	B	468	GLY	3.5
1	D	31	SER	3.5
1	C	202	PRO	3.4
1	A	227	GLY	3.3
1	B	467	ASP	3.3
1	D	35	GLU	3.0
1	C	166	LEU	2.9
1	D	480	GLU	2.9
1	B	480	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	467	ASP	2.8
1	A	496	PRO	2.8
1	A	22	GLN	2.7
1	A	13	GLU	2.7
1	C	314	ASP	2.7
1	A	12	GLU	2.6
1	B	11	GLN	2.6
1	D	492	GLY	2.6
1	B	405	PRO	2.6
1	B	487	LEU	2.6
1	B	12	GLU	2.4
1	C	174	GLY	2.4
1	B	432	LEU	2.3
1	A	436	THR	2.3
1	C	313	GLY	2.2
1	C	435	ASN	2.2
1	C	126	TYR	2.2
1	A	467	ASP	2.2
1	A	31	SER	2.2
1	C	307	ALA	2.1
1	D	9	THR	2.1
1	C	436	THR	2.1
1	B	138	GLY	2.1
3	H	3	G	2.1
1	A	147	ASP	2.0
1	D	13	GLU	2.0
1	C	155	LEU	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. 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	B-factors(\AA^2)	Q<0.9
4	ZN	D	1509	1/1	0.90	0.05	112,112,112,112	0
4	ZN	A	1506	1/1	0.92	0.11	97,97,97,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.