



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:22 PM UTC

PDB ID : 2VRT / pdb_00002vrt
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

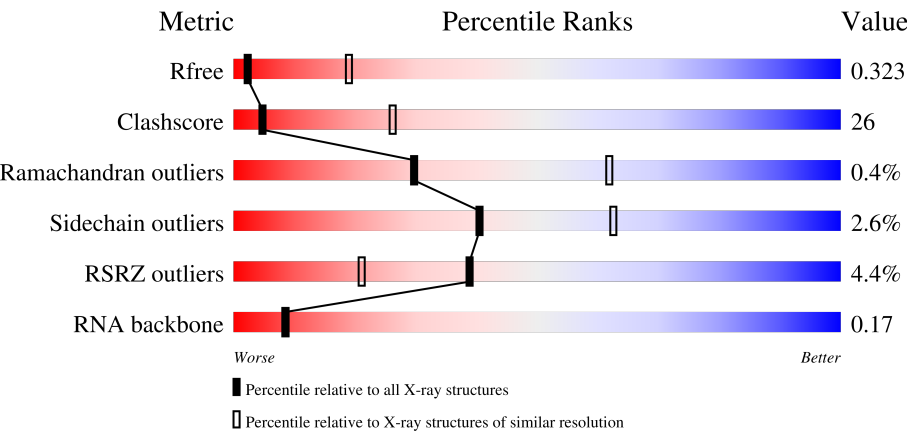
1 Overall quality at a glance i

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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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 of 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>4%</div><div>57%</div><div>33%</div><div>8%</div></div>
1	B	509	<div><div>4%</div><div>56%</div><div>21%</div><div>22%</div></div>
1	C	509	<div><div>3%</div><div>63%</div><div>16%</div><div>19%</div></div>
1	D	509	<div><div>5%</div><div>71%</div><div>22%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
2	E	2	<div><div></div><div>50%</div><div>50%</div></div>
2	F	2	<div><div></div><div>50%</div><div>50%</div></div>
3	G	3	<div><div></div><div>33%</div><div>67%</div></div>
3	H	3	<div><div></div><div>33%</div><div>67%</div></div>

2 Entry composition

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			

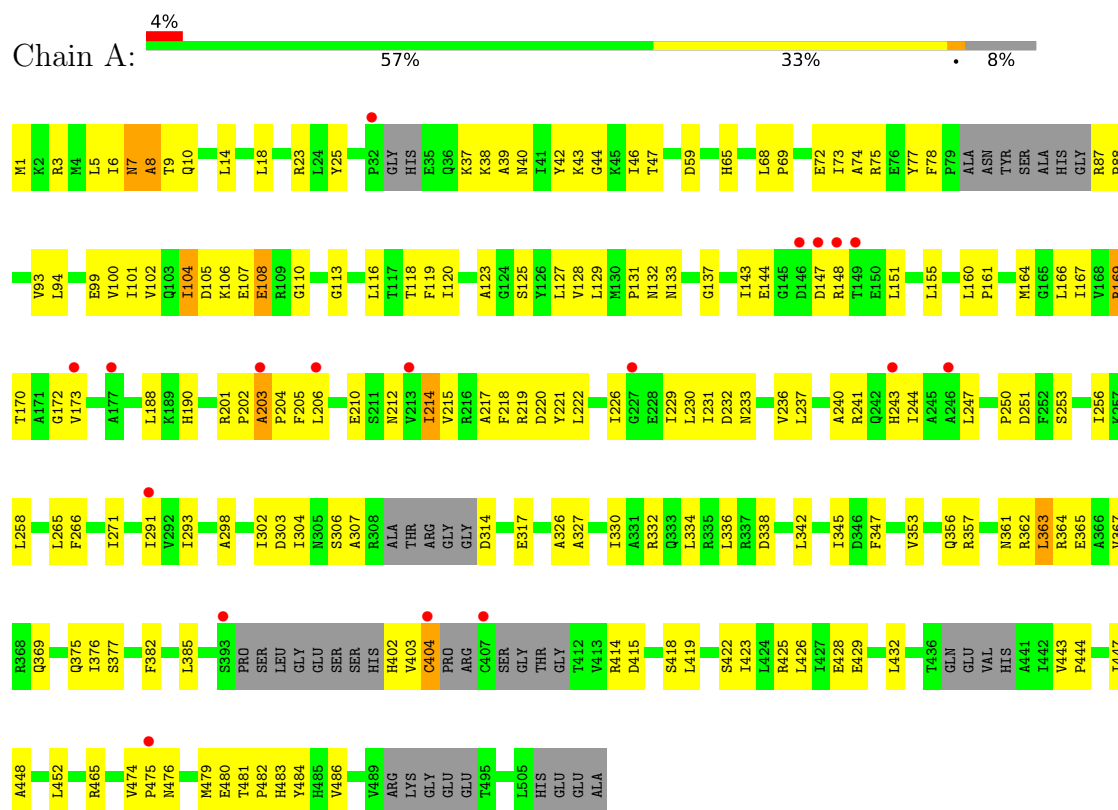
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

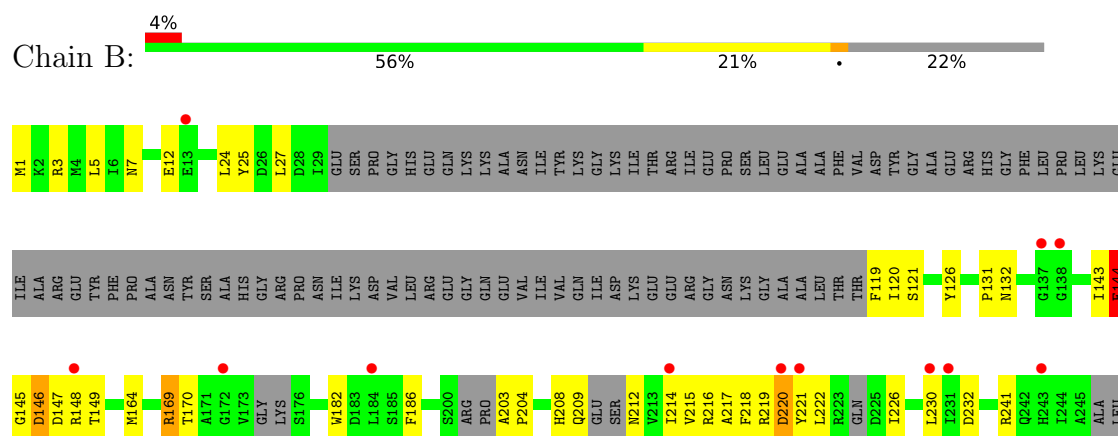
3 Residue-property plots

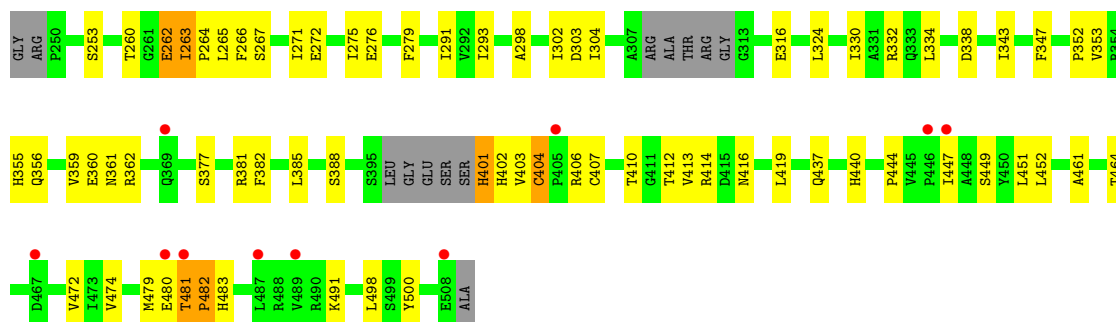
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

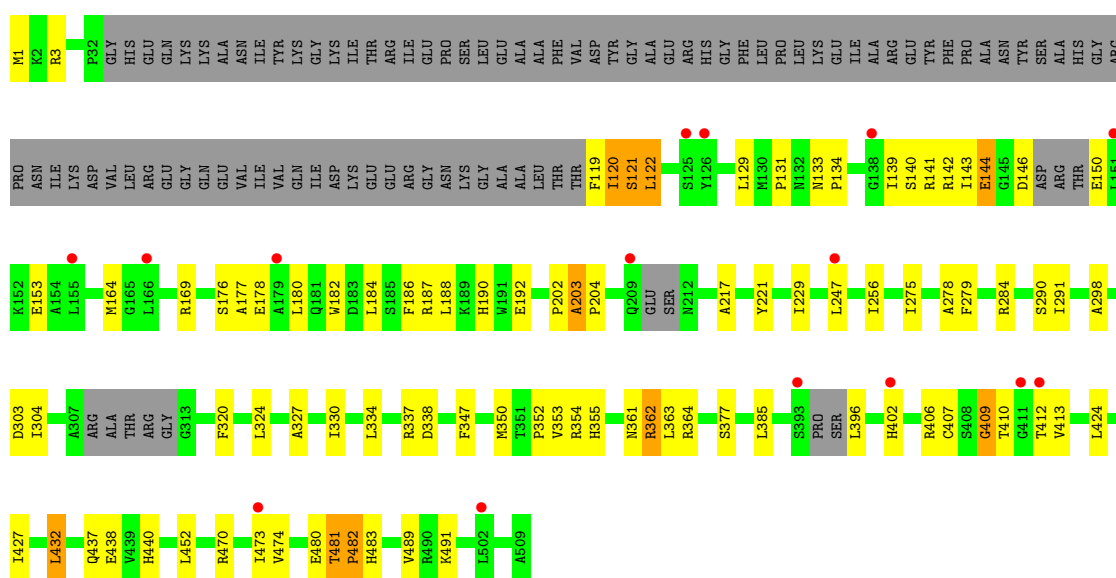


• Molecule 1: RIBONUCLEASE E

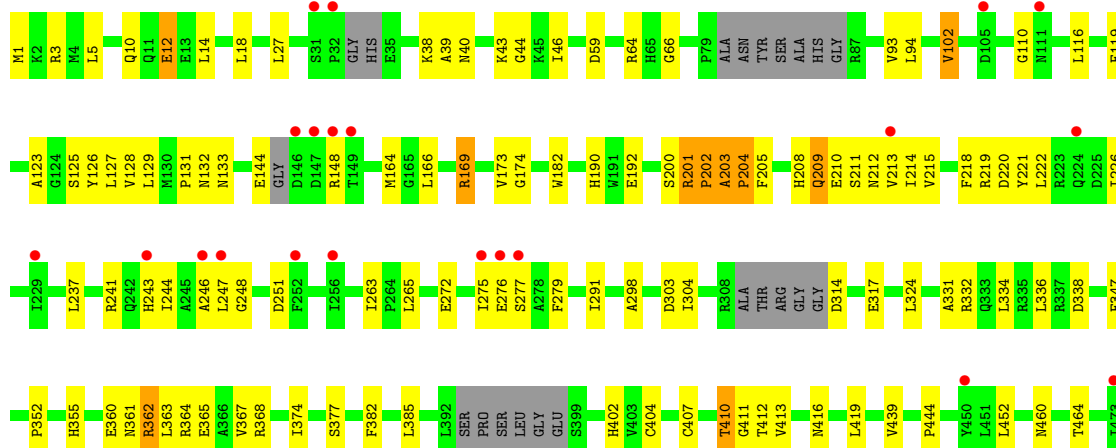


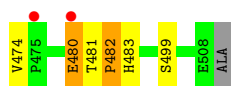


• Molecule 1: RIBONUCLEASE E



• Molecule 1: RIBONUCLEASE E





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

Chain E: 50% 50%



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

Chain F: 50% 50%



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

Chain G: 33% 67%



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

Chain H: 33% 67%



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 24.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.98-3.50) 99.6 (24.98-3.50)	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 (10.06%)	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)	0.27 , 94.7	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	0.85	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	0.40	0/3511	0.85	3/4773 (0.1%)
1	B	0.40	0/2951	0.89	8/4007 (0.2%)
1	C	0.40	0/3008	0.94	9/4099 (0.2%)
1	D	0.41	0/3684	0.86	8/5009 (0.2%)
2	E	0.84	0/44	1.02	0/64
2	F	0.56	0/44	0.75	0/64
3	G	0.82	0/70	0.83	0/105
3	H	0.67	0/70	0.98	0/105
All	All	0.41	0/13382	0.88	28/18226 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	ALA	N-CA-C	18.43	137.44	112.55
1	C	202	PRO	CB-CA-C	11.80	129.04	111.22
1	C	203	ALA	N-CA-CB	-9.96	95.77	110.11
1	B	220	ASP	N-CA-C	9.29	123.11	111.69
1	C	409	GLY	N-CA-C	9.11	127.42	115.40
1	D	200	SER	CB-CA-C	8.89	126.96	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	THR	N-CA-C	8.68	120.82	111.36
1	D	211	SER	N-CA-C	8.64	125.76	107.70
1	B	402	HIS	N-CA-C	-8.62	92.44	110.80
1	B	146	ASP	N-CA-C	-8.04	101.89	112.34
1	C	121	SER	N-CA-CB	-8.01	98.91	111.56
1	D	482	PRO	CB-CA-C	-7.77	98.73	111.56
1	D	209	GLN	N-CA-C	-7.49	98.94	110.10
1	C	122	LEU	N-CA-C	7.03	119.57	108.67
1	B	220	ASP	CB-CA-C	-6.24	99.29	110.70
1	A	8	ALA	N-CA-C	6.21	120.48	112.41
1	D	133	ASN	CA-C-N	6.20	126.32	119.87
1	D	133	ASN	C-N-CA	6.20	126.32	119.87
1	C	202	PRO	CA-C-N	-6.14	112.46	120.44
1	C	202	PRO	C-N-CA	-6.14	112.46	120.44
1	A	7	ASN	N-CA-C	6.06	118.71	107.99
1	D	410	THR	N-CA-C	5.75	119.48	112.23
1	C	482	PRO	CB-CA-C	-5.73	103.25	111.62
1	B	402	HIS	N-CA-CB	5.71	120.14	110.49
1	B	144	GLU	CB-CA-C	5.29	119.74	109.33
1	D	201	ARG	N-CA-CB	-5.18	101.16	110.37
1	A	307	ALA	N-CA-C	5.13	116.57	110.97
1	B	404	CYS	CB-CA-C	5.10	116.68	109.08

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	253	0
1	B	2915	0	2767	164	0
1	C	2966	0	2763	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3628	0	3443	158	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	1	0
All	All	13186	0	12388	653	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 26.

All (653) 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:D:212:ASN:CG	1:D:215:VAL:HG23	1.66	1.20
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:479:MET:HE2	1:A:483:HIS:CD2	1.85	1.10
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:B:481:THR:HG22	1:B:482:PRO:HD3	1.03	1.02
1:C:139:ILE:HD12	1:C:143:ILE:HD12	1.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:SER:OG	1:D:474:VAL:HG23	1.64	0.97
1:D:404:CYS:HG	4:D:1509:ZN:ZN	0.64	0.97
1:C:144:GLU:OE1	1:C:144:GLU:HA	1.65	0.96
1:C:139:ILE:O	3:H:2:U:H4'	1.67	0.95
1:D:44:GLY:HA2	1:D:204:PRO:HB3	1.46	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
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:D:1:MET:HE2	1:D:3:ARG:NH1	1.85	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:C:362:ARG:HG3	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:D:1:MET:HE2	1:D:3:ARG:CZ	2.05	0.86
1:A:101:ILE:CG2	1:A:120:ILE:HD11	2.04	0.85
1:D:212:ASN:CG	1:D:215:VAL:CG2	2.48	0.85
1:D:128:VAL:C	1:D:166:LEU:HD12	2.00	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
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:A:479:MET:HE2	1:A:483:HIS:HD2	1.39	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:43:LYS:O	1:A:204:PRO:CB	2.27	0.82
1:A:101:ILE:HG22	1:A:120:ILE:CD1	2.08	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: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:A:169:ARG:HH11	1:A:169:ARG:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:77:TYR:HE1	1:A:118:THR:HB	1.49	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: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:O	1:C:143:ILE:HG13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:ARG:HG3	1:D:202:PRO:HD2	1.69	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:OE1	1:C:144:GLU:CA	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
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:D:128:VAL:C	1:D:166:LEU:CD1	2.64	0.70
1:C:1:MET:SD	1:C:3:ARG:CZ	2.80	0.70
1:A:77:TYR:CE1	1:A:118:THR:HB	2.27	0.70
1:A:362:ARG:O	1:A:365:GLU:N	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:5:LEU:CD2	1:B:230:LEU:HD12	2.26	0.66
1:B:216:ARG:CD	1:B:219:ARG:NH2	2.58	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
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:479:MET:HE2	1:A:483:HIS:NE2	2.12	0.65
1:A:291:ILE:HG23	1:A:302:ILE:HG22	1.79	0.65
1:B:145:GLY:C	1:B:147:ASP:N	2.51	0.65
1:B:262:GLU:OE1	1:B:262:GLU:CA	2.44	0.65
1:A:23:ARG:NH2	1:A:332:ARG:HE	1.95	0.65
1:B:169:ARG:HH11	1:B:169:ARG:CG	2.09	0.65
1:D:39:ALA:C	1:D:210:GLU:CB	2.69	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:A:444:PRO:CG	1:A:480:GLU:C	2.68	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:A:480:GLU:C	1:A:482:PRO:HD2	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:362:ARG:CG	1:C:362:ARG:NH1	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:78:PHE:CE1	1:A:93:VAL:HG22	2.33	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: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:C:362:ARG:HG2	1:C:362:ARG:NH1	2.11	0.62
1:A:444:PRO:CD	1:A:447:ILE:HD12	2.28	0.62
1:B:146:ASP:C	1:B:149:THR:H	2.08	0.62
1:B:444:PRO:HB3	1:B:480:GLU:CA	2.26	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:D:1:MET:HE3	1:D:3:ARG:NE	2.15	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:C:350:MET:SD	1:C:355:HIS:O	2.60	0.60
1:A:382:PHE:HE1	1:B:388:SER:OG	1.85	0.60
1:C:406:ARG:HH21	1:C:481:THR:CB	2.14	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:B:452:LEU:HD13	1:D:452:LEU:HB3	1.84	0.59
1:C:437:GLN:HB2	1:C:491:LYS:HA	1.84	0.59
1:C:438:GLU:HG2	1:C:470:ARG:HB2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:262:GLU:O	1:B:263:ILE:C	2.46	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
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:24:LEU:O	1:B:332:ARG:HD2	2.03	0.57
1:C:409:GLY:HA2	1:D:411:GLY:O	2.05	0.57
1:D:222:LEU:HA	1:D:226:ILE:HD12	1.86	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: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:481:THR:N	1:D:482:PRO:CD	2.68	0.56
1:C:144:GLU:C	1:C:146:ASP:H	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:147:ASP:CG	1:A:173:VAL:HG13	2.31	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:D:214:ILE:CG2	1:D:218:PHE:CE1	2.90	0.55
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:B:480:GLU:C	1:B:482:PRO:HD2	2.31	0.54
1:A:5:LEU:HD22	1:A:265:LEU:HD11	1.88	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:B:169:ARG:HH11	1:B:169:ARG:HG3	1.72	0.54
1:D:201:ARG:HG3	1:D:202:PRO:CD	2.32	0.53
1:A:382:PHE:HE1	1:B:388:SER:CB	2.21	0.53
1:D:38:LYS:O	1:D:39:ALA:HB3	2.09	0.53
1:D:332:ARG:NH1	1:D:336:LEU:HD11	2.23	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:GLN:C	1:C:438:GLU:HG3	2.34	0.52
1:B:406:ARG:NE	1:B:482:PRO:HG3	2.16	0.52
1:A:251:ASP:C	1:A:253:SER:H	2.17	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:7:ASN:CG	1:B:232:ASP:OD1	2.47	0.51
1:B:304:ILE:HD12	1:B:347:PHE:HA	1.92	0.51
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:C:119:PHE:C	1:C:120:ILE:HG23	2.36	0.51
1:A:25:TYR:HA	1:A:332:ARG:HD2	1.92	0.51
1:A:128:VAL:CG2	1:A:169:ARG:HD2	2.41	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:145:GLY:O	1:B:146:ASP:C	2.54	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: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:C:480:GLU:O	1:C:481:THR:C	2.54	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:43:LYS:O	1:D:204:PRO:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:LEU:HB3	1:D:166:LEU:HD11	1.93	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:A:444:PRO:HG2	1:A:480:GLU:C	2.29	0.49
1:D:338:ASP:OD1	1:D:338:ASP:O	2.30	0.49
1:A:166:LEU:HD12	1:A:167:ILE:H	1.78	0.49
1:D:277:SER:C	1:D:279:PHE:H	2.19	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
1:D:129:LEU:N	1:D:166:LEU:CD1	2.75	0.49
1:C:144:GLU:C	1:C:146:ASP:N	2.70	0.49
1:D:246:ALA:C	1:D:248:GLY:H	2.21	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: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:O	1:B:226:ILE:HG22	2.13	0.48
1:B:144:GLU:N	1:B:144:GLU:OE1	2.46	0.48
1:A:414:ARG:HD2	1:B:279:PHE:CE2	2.48	0.48
1:B:131:PRO:HA	1:B:164:MET:HB3	1.95	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:A:99:GLU:C	1:A:100:VAL:HG23	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ALA:O	1:A:219:ARG:HD2	2.14	0.47
1:A:375:GLN:NE2	1:B:381:ARG:HH12	2.11	0.47
1:B:209:GLN:CG	1:B:212:ASN:HB3	2.44	0.47
1:C:284:ARG:NH1	1:C:290:SER:HB3	2.29	0.47
1:C:177:ALA:O	1:C:178:GLU:C	2.57	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:OD1	1:B:338:ASP:O	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:360:GLU:O	1:B:361:ASN:C	2.58	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
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:D:481:THR:N	1:D:482:PRO:HD3	2.28	0.46
1:A:46:ILE:HD13	1:A:94:LEU:HD13	1.97	0.46
1:A:190:HIS:CE1	1:A:247:LEU:HD23	2.51	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:O5'	2:E:2:U:H6	1.97	0.46
1:A:73:ILE:HG21	1:A:93:VAL:CG1	2.40	0.46
1:A:222:LEU:CD2	1:A:229:ILE:HD11	2.45	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:40:ASN:OD1	1:A:210:GLU:N	2.35	0.46
1:A:74:ALA:HB2	1:A:132:ASN:HD21	1.80	0.46
1:B:169:ARG:CG	1:B:169:ARG:NH1	2.73	0.46
1:B:482:PRO:HG2	1:B:483:HIS:H	1.80	0.46
1:D:93:VAL:HG12	1:D:94:LEU:HG	1.97	0.46
1:D:192:GLU:OE2	1:D:192:GLU:HA	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:18:LEU:HD11	1:A:221:TYR:CD1	2.46	0.46
1:A:105:ASP:O	1:A:106:LYS:HG3	2.16	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:O	1:C:412:THR:CG2	2.62	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:A:251:ASP:C	1:A:253:SER:N	2.74	0.45
1:C:352:PRO:CG	1:C:355:HIS:ND1	2.79	0.45
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:38:LYS:O	1:A:39:ALA:HB3	2.17	0.45
1:A:160:LEU:HD12	1:A:161:PRO:HD2	1.98	0.45
1:A:362:ARG:O	1:A:363:LEU:C	2.59	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:B:316:GLU:CD	1:B:355:HIS:HE1	2.25	0.45
1:A:363:LEU:HD23	1:A:385:LEU:CD2	2.42	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:A:42:TYR:CE2	1:A:206:LEU:HD13	2.53	0.44
1:B:7:ASN:CG	1:B:266:PHE:CE2	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:HIS:ND1	1:B:401:HIS:N	2.66	0.44
1:C:402:HIS:CD2	1:D:413:VAL:HB	2.51	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:B:126:TYR:C	1:B:169:ARG:HB2	2.42	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
1:C:176:SER:O	1:C:177:ALA:C	2.60	0.43
1:A:37:LYS:N	1:A:107:GLU:OE1	2.52	0.43
1:C:480:GLU:C	1:C:482:PRO:HD2	2.43	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:B:182:TRP:CE3	1:B:186:PHE:HE1	2.37	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:HD23	1:B:222:LEU:HA	1.80	0.42
1:A:426:LEU:HD23	1:A:486:VAL:HG21	2.00	0.42
1:A:484:TYR:CD1	1:A:484:TYR:C	2.98	0.42
1:A:231:ILE:HB	1:A:237:LEU:HD13	2.00	0.42
1:D:277:SER:C	1:D:279:PHE:N	2.74	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:87:ARG:HA	1:A:88:PRO:HD3	1.88	0.42
1:A:143:ILE:HG22	1:A:148:ARG:CB	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1:MET:SD	1:A:3:ARG:CZ	3.08	0.42
1:A:59:ASP:O	1:A:204:PRO:HG2	2.14	0.42
1:A:237:LEU:CD2	1:A:258:LEU:HB2	2.50	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: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:1:MET:SD	1:B:3:ARG:CZ	3.08	0.42
1:B:217:ALA:O	1:B:221:TYR:N	2.31	0.42
1:D:174:GLY:O	1:D:368:ARG:HG3	2.20	0.42
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:OD2	1:D:251:ASP:N	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:D:1:MET:CE	1:D:3:ARG:HH11	2.32	0.41
1:A:342:LEU:HD22	1:B:382:PHE:HB3	2.01	0.41
1:B:7:ASN:OD1	1:B:232:ASP:CG	2.52	0.41
1:D:38:LYS:O	1:D:39:ALA:CB	2.68	0.41
1:D:367:VAL:HB	1:D:374:ILE:HD13	2.01	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: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:145:GLY:C	1:B:147:ASP:H	2.26	0.41
1:B:359:VAL:O	1:B:362:ARG:HB3	2.21	0.41
1:A:77:TYR:CZ	1:A:100:VAL:HG13	2.56	0.41
1:C:190:HIS:ND1	1:C:247:LEU:HA	2.36	0.41
1:C:229:ILE:HB	1:C:256:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:SD	1:C:3:ARG:NE	2.94	0.41
1:A:362:ARG:C	1:A:364:ARG:N	2.78	0.40
1:B:264:PRO:O	1:B:265:LEU:C	2.63	0.40
1:A:104:ILE:HA	1:A:116:LEU:CD2	2.48	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:46:ILE:HD11	1:A:94:LEU:HD13	2.03	0.40
1:A:59:ASP:HB2	1:A:65:HIS:HD2	1.86	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	451/509 (89%)	424 (94%)	25 (6%)	2 (0%)	30	62
1	B	380/509 (75%)	354 (93%)	25 (7%)	1 (0%)	36	67
1	C	399/509 (78%)	380 (95%)	17 (4%)	2 (0%)	24	57
1	D	475/509 (93%)	441 (93%)	32 (7%)	2 (0%)	30	62
All	All	1705/2036 (84%)	1599 (94%)	99 (6%)	7 (0%)	30	62

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	LEU
1	D	202	PRO
1	B	482	PRO

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Mol	Chain	Res	Type
1	D	204	PRO
1	C	120	ILE
1	A	110	GLY
1	C	481	THR

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	345/433 (80%)	337 (98%)	8 (2%)	44	64
1	B	288/433 (66%)	279 (97%)	9 (3%)	35	59
1	C	287/433 (66%)	279 (97%)	8 (3%)	38	61
1	D	361/433 (83%)	353 (98%)	8 (2%)	45	65
All	All	1281/1732 (74%)	1248 (97%)	33 (3%)	40	62

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ILE
1	A	108	GLU
1	A	169	ARG
1	A	214	ILE
1	A	306	SER
1	A	369	GLN
1	A	404	CYS
1	A	474	VAL
1	B	144	GLU
1	B	169	ARG
1	B	214	ILE
1	B	262	GLU
1	B	263	ILE
1	B	401	HIS
1	B	474	VAL
1	B	479	MET
1	B	481	THR

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Mol	Chain	Res	Type
1	C	142	ARG
1	C	144	GLU
1	C	169	ARG
1	C	353	VAL
1	C	354	ARG
1	C	362	ARG
1	C	432	LEU
1	C	474	VAL
1	D	12	GLU
1	D	102	VAL
1	D	169	ARG
1	D	244	ILE
1	D	362	ARG
1	D	412	THR
1	D	439	VAL
1	D	480	GLU

Sometimes 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	305	ASN
1	A	375	GLN
1	A	416	ASN
1	A	466	GLN
1	B	208	HIS
1	B	305	ASN
1	B	355	HIS
1	B	416	ASN
1	B	466	GLN
1	C	133	ASN
1	C	305	ASN
1	C	402	HIS
1	C	416	ASN
1	C	440	HIS
1	C	466	GLN
1	D	132	ASN
1	D	208	HIS
1	D	305	ASN
1	D	355	HIS

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Mol	Chain	Res	Type
1	D	416	ASN

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 oligosaccharides 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%)	0.58	18 (3%)	44 24	68, 107, 151, 261	0
1	B	398/509 (78%)	0.63	22 (5%)	30 18	71, 129, 161, 289	0
1	C	411/509 (80%)	0.57	15 (3%)	46 25	80, 125, 164, 304	0
1	D	487/509 (95%)	0.60	23 (4%)	36 20	71, 106, 149, 251	0
2	E	2/2 (100%)	0.59	0	100 100	109, 109, 109, 124	0
2	F	2/2 (100%)	0.95	0	100 100	128, 128, 128, 140	0
3	G	3/3 (100%)	0.47	0	100 100	122, 122, 140, 149	0
3	H	3/3 (100%)	0.91	0	100 100	133, 133, 135, 153	0
All	All	1774/2046 (86%)	0.59	78 (4%)	39 21	68, 117, 158, 304	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	CYS	5.3
1	B	138	GLY	4.9
1	D	146	ASP	4.4
1	D	213	VAL	3.9
1	A	147	ASP	3.7
1	A	146	ASP	3.6
1	B	480	GLU	3.5
1	D	147	ASP	3.5
1	A	227	GLY	3.4
1	B	405	PRO	3.4
1	A	213	VAL	3.3
1	C	138	GLY	3.1
1	B	137	GLY	3.1
1	B	481	THR	3.1
1	C	126	TYR	3.0
1	B	230	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	475	PRO	2.9
1	C	411	GLY	2.9
1	D	148	ARG	2.9
1	B	369	GLN	2.8
1	D	105	ASP	2.7
1	C	155	LEU	2.7
1	A	32	PRO	2.7
1	B	221	TYR	2.7
1	C	179	ALA	2.6
1	A	149	THR	2.6
1	A	173	VAL	2.6
1	B	148	ARG	2.6
1	A	404	CYS	2.5
1	D	31	SER	2.5
1	D	276	GLU	2.5
1	D	252	PHE	2.5
1	B	489	VAL	2.5
1	D	149	THR	2.4
1	D	243	HIS	2.4
1	C	502	LEU	2.4
1	D	224	GLN	2.4
1	B	214	ILE	2.4
1	B	243	HIS	2.4
1	C	209	GLN	2.4
1	C	247	LEU	2.4
1	B	508	GLU	2.3
1	B	220	ASP	2.3
1	A	206	LEU	2.3
1	C	166	LEU	2.3
1	B	13	GLU	2.3
1	C	125	SER	2.3
1	A	148	ARG	2.3
1	C	412	THR	2.3
1	D	275	ILE	2.3
1	A	203	ALA	2.3
1	A	243	HIS	2.2
1	C	151	LEU	2.2
1	A	475	PRO	2.2
1	A	291	ILE	2.2
1	A	177	ALA	2.2
1	C	473	ILE	2.1
1	C	393	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	467	ASP	2.1
1	D	229	ILE	2.1
1	D	450	TYR	2.1
1	B	446	PRO	2.1
1	D	246	ALA	2.1
1	B	447	ILE	2.1
1	D	256	ILE	2.1
1	D	247	LEU	2.1
1	D	111	ASN	2.1
1	D	32	PRO	2.1
1	B	231	ILE	2.1
1	D	277	SER	2.1
1	C	402	HIS	2.0
1	D	473	ILE	2.0
1	B	172	GLY	2.0
1	A	393	SER	2.0
1	B	184	LEU	2.0
1	B	487	LEU	2.0
1	D	480	GLU	2.0
1	A	246	ALA	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 oligosaccharides 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(Å ²)	Q<0.9
4	ZN	D	1509	1/1	0.96	0.06	112,112,112,112	0
4	ZN	A	1506	1/1	0.97	0.13	97,97,97,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.