



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:53 AM UTC

PDB ID : 4IRY / pdb_00004iry
Title : Influenza A virus tail-loop free nucleoprotein at 2.8 Å resolution
Authors : Ye, Q.; Mata, D.A.; Tao, Y.J.
Deposited on : 2013-01-15
Resolution : 2.80 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

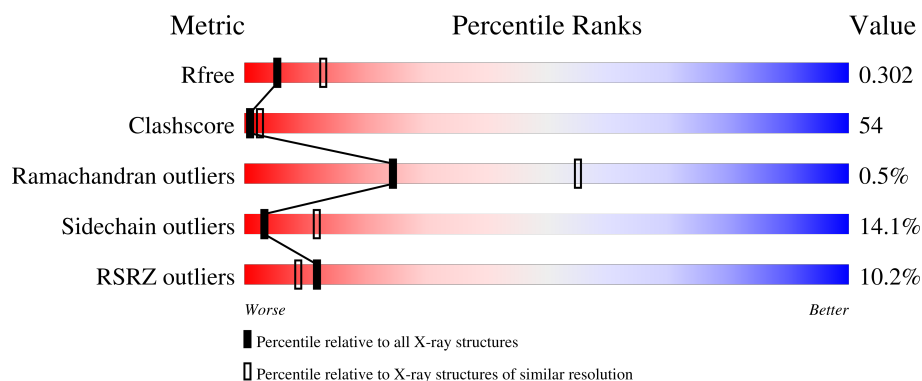
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	483	10% 28% 45% 10% 16%
1	B	483	7% 33% 43% 12% 12%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 6586 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 Nucleocapsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	424	Total	C	N	O	S	8	0	0
			3373	2089	630	629	25			
1	A	404	Total	C	N	O	S	0	0	0
			3213	1992	597	599	25			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	425	GLY	-	linker	UNP Q1K9H2
B	426	GLY	-	linker	UNP Q1K9H2
B	427	GLY	-	linker	UNP Q1K9H2
B	428	GLY	-	linker	UNP Q1K9H2
B	429	SER	-	linker	UNP Q1K9H2
B	499	LEU	-	expression tag	UNP Q1K9H2
B	500	GLU	-	expression tag	UNP Q1K9H2
B	501	HIS	-	expression tag	UNP Q1K9H2
B	502	HIS	-	expression tag	UNP Q1K9H2
B	503	HIS	-	expression tag	UNP Q1K9H2
B	504	HIS	-	expression tag	UNP Q1K9H2
B	505	HIS	-	expression tag	UNP Q1K9H2
B	506	HIS	-	expression tag	UNP Q1K9H2
A	425	GLY	-	linker	UNP Q1K9H2
A	426	GLY	-	linker	UNP Q1K9H2
A	427	GLY	-	linker	UNP Q1K9H2
A	428	GLY	-	linker	UNP Q1K9H2
A	429	SER	-	linker	UNP Q1K9H2
A	499	LEU	-	expression tag	UNP Q1K9H2
A	500	GLU	-	expression tag	UNP Q1K9H2
A	501	HIS	-	expression tag	UNP Q1K9H2
A	502	HIS	-	expression tag	UNP Q1K9H2
A	503	HIS	-	expression tag	UNP Q1K9H2
A	504	HIS	-	expression tag	UNP Q1K9H2
A	505	HIS	-	expression tag	UNP Q1K9H2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	506	HIS	-	expression tag	UNP Q1K9H2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	60.18Å 155.62Å 97.77Å 90.00° 90.94° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	96.1 (50.00-2.80) 97.1 (50.00-2.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.298 0.260 , 0.302	Depositor DCC
R_{free} test set	2109 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6586	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.80	3/3261 (0.1%)	1.36	50/4375 (1.1%)
1	B	0.80	7/3430 (0.2%)	1.28	41/4608 (0.9%)
All	All	0.80	10/6691 (0.1%)	1.32	91/8983 (1.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	SER	C-N	-6.96	1.25	1.33
1	B	117	ARG	C-N	-6.76	1.24	1.33
1	B	128	ASP	C-N	-5.95	1.25	1.33
1	B	79	LEU	C-N	-5.41	1.26	1.33
1	B	477	PRO	N-CA	-5.36	1.40	1.47
1	A	50	SER	CA-C	-5.22	1.46	1.53
1	B	201	ILE	CA-CB	5.14	1.60	1.54
1	A	231	GLN	CA-CB	-5.13	1.47	1.54
1	B	475	ILE	C-N	-5.13	1.27	1.33
1	B	476	VAL	CA-C	-5.06	1.47	1.52

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	ASN	CA-CB-CG	-11.18	101.42	112.60
1	A	149	GLN	OE1-CD-NE2	-10.27	112.33	122.60
1	A	168	GLN	OE1-CD-NE2	-10.05	112.55	122.60
1	B	364	GLN	OE1-CD-NE2	-9.93	112.67	122.60
1	B	311	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	B	308	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	A	235	GLN	OE1-CD-NE2	-9.78	112.83	122.60
1	A	42	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	B	231	GLN	OE1-CD-NE2	-9.70	112.90	122.60
1	A	311	GLN	OE1-CD-NE2	-9.70	112.91	122.60
1	A	122	GLN	OE1-CD-NE2	-9.54	113.06	122.60
1	A	231	GLN	OE1-CD-NE2	-9.51	113.09	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	GLN	OE1-CD-NE2	-9.41	113.19	122.60
1	A	58	GLN	OE1-CD-NE2	-9.32	113.28	122.60
1	A	488	PHE	N-CA-C	9.20	124.69	113.38
1	A	482	SER	N-CA-C	-7.71	102.20	111.69
1	A	42	GLN	CG-CD-NE2	7.50	127.65	116.40
1	A	168	GLN	CG-CD-NE2	7.42	127.53	116.40
1	A	373	THR	N-CA-C	-7.41	101.98	113.02
1	A	336	ALA	N-CA-C	7.32	121.53	112.59
1	A	235	GLN	CG-CD-NE2	7.06	126.99	116.40
1	B	299	VAL	CB-CA-C	-7.00	103.13	111.94
1	A	197	ILE	N-CA-C	-6.95	104.08	110.82
1	B	149	GLN	CG-CD-NE2	6.94	126.81	116.40
1	A	231	GLN	CG-CD-NE2	6.88	126.71	116.40
1	B	364	GLN	CG-CD-NE2	6.86	126.69	116.40
1	B	308	GLN	CG-CD-NE2	6.81	126.62	116.40
1	B	311	GLN	CG-CD-NE2	6.67	126.40	116.40
1	A	199	ARG	CA-C-N	-6.61	110.94	122.83
1	A	199	ARG	C-N-CA	-6.61	110.94	122.83
1	A	353	VAL	CA-C-N	6.56	126.48	119.85
1	A	353	VAL	C-N-CA	6.56	126.48	119.85
1	B	231	GLN	CG-CD-NE2	6.52	126.18	116.40
1	A	247	ASN	CB-CA-C	6.49	118.93	109.20
1	B	386	TRP	N-CA-C	-6.44	99.54	109.52
1	A	311	GLN	CG-CD-NE2	6.42	126.03	116.40
1	B	315	LEU	N-CA-C	-6.41	100.56	110.10
1	A	149	GLN	CG-CD-NE2	6.40	126.00	116.40
1	A	215	THR	N-CA-C	-6.36	104.44	111.82
1	A	245	SER	CA-C-N	6.31	129.03	120.38
1	A	245	SER	C-N-CA	6.31	129.03	120.38
1	A	58	GLN	CG-CD-NE2	6.31	125.86	116.40
1	A	122	GLN	CG-CD-NE2	6.30	125.86	116.40
1	B	166	LEU	N-CA-C	-6.29	104.23	112.41
1	B	124	ASN	O-C-N	-6.21	114.71	122.35
1	B	439	ASP	N-CA-C	-6.20	104.52	111.28
1	B	201	ILE	CA-CB-CG1	6.15	120.86	110.40
1	A	220	GLU	N-CA-C	-6.14	104.14	111.69
1	A	73	GLU	CA-C-N	6.12	131.28	122.40
1	A	73	GLU	C-N-CA	6.12	131.28	122.40
1	B	291	PHE	N-CA-C	6.10	117.80	111.03
1	A	265	ILE	N-CA-C	-6.01	106.39	111.56
1	A	387	ALA	N-CA-C	5.95	118.46	109.41
1	A	349	GLY	N-CA-C	-5.91	107.66	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ASN	CA-CB-CG	-5.89	106.71	112.60
1	B	36	ILE	N-CA-C	-5.77	104.73	110.62
1	A	477	PRO	CA-C-N	-5.69	115.44	122.84
1	A	477	PRO	C-N-CA	-5.69	115.44	122.84
1	B	298	LEU	N-CA-C	-5.68	105.68	113.30
1	B	381	LEU	N-CA-C	5.63	119.69	112.26
1	B	388	ILE	CB-CA-C	-5.62	103.05	110.98
1	A	315	LEU	N-CA-C	-5.62	102.17	110.48
1	B	302	ASP	CA-C-N	5.56	125.26	119.64
1	B	302	ASP	C-N-CA	5.56	125.26	119.64
1	A	288	GLY	N-CA-C	-5.52	107.41	114.37
1	B	167	MET	N-CA-C	5.49	119.98	113.28
1	B	299	VAL	N-CA-C	5.48	117.39	111.58
1	B	148	TYR	N-CA-C	5.47	118.41	109.59
1	B	349	GLY	N-CA-C	-5.45	107.49	114.85
1	B	26	ARG	CA-C-N	5.37	127.75	120.44
1	B	26	ARG	C-N-CA	5.37	127.75	120.44
1	B	170	SER	N-CA-C	5.32	118.56	111.75
1	A	385	TYR	CB-CA-C	-5.30	98.93	109.79
1	A	247	ASN	CA-C-N	5.22	125.52	119.93
1	A	247	ASN	C-N-CA	5.22	125.52	119.93
1	B	307	LEU	CA-C-N	5.19	127.18	120.44
1	B	307	LEU	C-N-CA	5.19	127.18	120.44
1	A	182	ALA	N-CA-C	-5.18	105.71	111.36
1	A	79	LEU	N-CA-C	5.17	117.23	108.02
1	B	173	PRO	N-CA-CB	5.15	108.14	103.15
1	A	176	SER	N-CA-C	5.13	117.60	109.96
1	B	374	MET	N-CA-C	5.12	117.65	110.23
1	A	73	GLU	CB-CA-C	-5.12	105.00	111.86
1	B	330	TRP	N-CA-C	-5.11	105.40	110.97
1	A	253	PHE	N-CA-C	-5.09	102.97	111.37
1	B	125	ASN	N-CA-C	5.08	118.59	111.74
1	B	198	LYS	CA-C-N	-5.08	112.59	120.31
1	B	198	LYS	C-N-CA	-5.08	112.59	120.31
1	A	175	ARG	N-CA-C	5.06	118.49	112.72
1	B	176	SER	CA-C-N	5.04	131.29	121.41
1	B	176	SER	C-N-CA	5.04	131.29	121.41

There are no chirality outliers.

There are no planarity outliers.

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	3213	0	3208	347	0
1	B	3373	0	3346	366	0
All	All	6586	0	6554	704	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 54.

All (704) 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:B:26:ARG:HH11	1:B:26:ARG:CG	1.34	1.39
1:B:199:ARG:HG3	1:B:206:PHE:CE2	1.63	1.33
1:A:65:ARG:HD3	1:A:79:LEU:CD1	1.56	1.32
1:A:196:MET:HG3	1:A:219:TYR:CE1	1.69	1.26
1:B:120:TRP:CZ2	1:B:129:ALA:HB3	1.77	1.20
1:A:365:ILE:HD13	1:A:365:ILE:O	1.41	1.20
1:A:115:GLU:O	1:A:119:ILE:HG13	1.46	1.15
1:A:75:ARG:O	1:A:175:ARG:HG3	1.47	1.14
1:B:82:HIS:CD2	1:B:84:SER:H	1.66	1.12
1:B:262:SER:HA	1:B:448:MET:HE3	1.25	1.11
1:B:339:GLU:CD	1:B:389:ARG:HH12	1.59	1.09
1:B:199:ARG:HG3	1:B:206:PHE:CZ	1.88	1.08
1:B:26:ARG:HH11	1:B:26:ARG:HG2	0.97	1.08
1:B:82:HIS:CD2	1:B:83:PRO:HD2	1.88	1.08
1:B:364:GLN:O	1:B:365:ILE:HD13	1.54	1.08
1:A:25:ILE:HD13	1:A:25:ILE:H	1.18	1.08
1:B:66:MET:HE3	1:B:93:GLY:HA2	1.37	1.05
1:B:316:ILE:HG23	1:B:375:GLU:HB3	1.38	1.04
1:B:149:GLN:CG	1:B:151:THR:HG23	1.88	1.03
1:A:196:MET:HG3	1:A:219:TYR:HE1	0.95	1.02
1:A:198:LYS:HE3	1:A:253:PHE:CE2	1.94	1.02
1:A:65:ARG:HH11	1:A:79:LEU:HD11	1.23	1.02
1:A:440:MET:HE2	1:A:440:MET:HA	1.36	1.01
1:B:77:LYS:HA	1:B:175:ARG:HB2	1.05	1.00
1:A:189:MET:CE	1:A:189:MET:HA	1.91	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:HIS:HB3	1:B:85:ALA:HB2	1.39	0.99
1:A:65:ARG:HD3	1:A:79:LEU:HD13	1.44	0.98
1:B:199:ARG:CG	1:B:206:PHE:CE2	2.46	0.98
1:B:77:LYS:HA	1:B:175:ARG:CB	1.93	0.98
1:B:26:ARG:HG2	1:B:26:ARG:NH1	1.70	0.98
1:B:26:ARG:CG	1:B:26:ARG:NH1	2.09	0.98
1:B:66:MET:CE	1:B:93:GLY:HA2	1.94	0.97
1:A:31:LYS:HA	1:A:292:GLU:HG2	1.47	0.97
1:A:324:HIS:CD2	1:A:359:SER:H	1.81	0.97
1:A:197:ILE:HG23	1:A:248:PRO:HB2	1.47	0.97
1:B:26:ARG:HH11	1:B:26:ARG:HG3	1.25	0.97
1:B:120:TRP:HZ2	1:B:129:ALA:HB3	1.21	0.97
1:B:213:ARG:O	1:B:217:ILE:HD13	1.62	0.96
1:B:180:GLY:O	1:B:184:LYS:HG3	1.66	0.96
1:A:463:VAL:CG2	1:A:475:ILE:HB	1.96	0.96
1:B:152:ARG:HA	1:B:152:ARG:HH11	1.31	0.95
1:A:198:LYS:HE3	1:A:253:PHE:HE2	1.26	0.95
1:A:365:ILE:HD13	1:A:365:ILE:C	1.93	0.94
1:A:266:LEU:HD13	1:A:447:LEU:HD23	1.51	0.93
1:A:120:TRP:HZ2	1:A:129:ALA:HB3	1.32	0.92
1:B:98:ARG:HD2	1:B:107:GLU:OE1	1.69	0.92
1:B:77:LYS:CA	1:B:175:ARG:HB2	1.98	0.91
1:B:80:GLU:HG3	1:B:173:PRO:HD3	1.51	0.91
1:B:82:HIS:CD2	1:B:83:PRO:CD	2.54	0.91
1:A:65:ARG:CD	1:A:79:LEU:CD1	2.47	0.90
1:A:324:HIS:HD2	1:A:359:SER:H	1.14	0.90
1:B:262:SER:HA	1:B:448:MET:CE	2.02	0.90
1:B:82:HIS:HD2	1:B:84:SER:H	1.06	0.89
1:B:82:HIS:HD2	1:B:84:SER:N	1.69	0.89
1:A:318:PRO:HG2	1:A:373:THR:HG22	1.56	0.88
1:B:484:GLU:CD	1:B:484:GLU:H	1.83	0.87
1:B:325:LYS:HB2	1:B:360:THR:HG21	1.57	0.86
1:A:389:ARG:HE	1:A:391:ARG:CB	1.87	0.86
1:A:189:MET:HA	1:A:189:MET:HE3	1.56	0.86
1:A:25:ILE:O	1:A:29:VAL:HG22	1.76	0.86
1:A:200:GLY:C	1:A:201:ILE:HG13	1.99	0.86
1:B:26:ARG:NH1	1:B:26:ARG:HG3	1.86	0.86
1:A:180:GLY:O	1:A:183:VAL:HG22	1.75	0.85
1:A:65:ARG:HD3	1:A:79:LEU:HD11	1.58	0.85
1:B:212:GLY:O	1:B:216:ARG:HB3	1.76	0.85
1:B:82:HIS:CG	1:B:83:PRO:HD2	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:MET:CG	1:A:219:TYR:CE1	2.59	0.84
1:B:205:ASN:O	1:B:205:ASN:ND2	2.10	0.84
1:B:82:HIS:CG	1:B:83:PRO:CD	2.61	0.84
1:A:65:ARG:HD3	1:A:79:LEU:HD12	1.59	0.83
1:A:464:PHE:HD2	1:A:473:SER:O	1.60	0.83
1:A:120:TRP:CZ2	1:A:129:ALA:HB3	2.13	0.83
1:B:179:ALA:O	1:B:183:VAL:HG23	1.79	0.83
1:B:194:ILE:HG23	1:B:253:PHE:CE2	2.13	0.82
1:B:212:GLY:O	1:B:216:ARG:CB	2.27	0.82
1:A:112:ASP:OD1	1:A:112:ASP:N	2.13	0.82
1:A:266:LEU:CD1	1:A:447:LEU:HD23	2.10	0.82
1:B:159:MET:HE1	1:B:191:MET:CB	2.10	0.81
1:A:91:LYS:HA	1:A:113:LYS:HD3	1.62	0.81
1:A:299:VAL:HG12	1:A:299:VAL:O	1.80	0.81
1:A:65:ARG:HH11	1:A:79:LEU:CD1	1.92	0.81
1:A:68:LEU:HD22	1:A:78:TYR:HB3	1.62	0.81
1:B:343:VAL:HA	1:B:479:PHE:HE1	1.45	0.81
1:A:76:ASN:O	1:A:175:ARG:HB2	1.81	0.81
1:B:314:SER:HB3	1:B:379:LEU:HD21	1.63	0.80
1:A:232:THR:O	1:A:236:ARG:HG3	1.81	0.80
1:B:324:HIS:HD2	1:B:359:SER:OG	1.63	0.80
1:A:189:MET:HA	1:A:189:MET:HE2	1.63	0.80
1:B:199:ARG:NE	1:B:206:PHE:HZ	1.80	0.79
1:B:200:GLY:HA2	1:B:206:PHE:CB	2.13	0.79
1:B:79:LEU:CD2	1:B:81:GLU:OE1	2.30	0.79
1:B:120:TRP:HZ2	1:B:129:ALA:CB	1.96	0.79
1:B:314:SER:CB	1:B:379:LEU:HD21	2.13	0.79
1:B:465:GLU:HG2	1:B:475:ILE:HD11	1.65	0.79
1:B:316:ILE:CG2	1:B:375:GLU:HB3	2.13	0.78
1:B:67:VAL:HG12	1:B:68:LEU:HD23	1.65	0.78
1:B:312:VAL:O	1:B:379:LEU:HG	1.83	0.78
1:B:174:ARG:O	1:B:174:ARG:HG2	1.84	0.78
1:B:167:MET:CE	1:B:187:GLY:HA3	2.14	0.78
1:B:343:VAL:HA	1:B:479:PHE:CE1	2.19	0.78
1:B:189:MET:HE3	1:B:225:ILE:CG2	2.14	0.77
1:B:149:GLN:OE1	1:B:491:ASP:HB3	1.84	0.77
1:B:159:MET:HE1	1:B:191:MET:HB2	1.66	0.77
1:B:77:LYS:HD3	1:B:78:TYR:CE1	2.19	0.77
1:B:482:SER:O	1:A:261:ARG:HD3	1.85	0.76
1:A:167:MET:HE1	1:A:187:GLY:C	2.09	0.76
1:B:82:HIS:NE2	1:B:83:PRO:HD2	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ARG:HD3	1:A:369:GLU:OE1	1.85	0.76
1:B:193:LEU:HD23	1:B:222:MET:HE3	1.67	0.76
1:A:168:GLN:HG3	1:A:270:VAL:HG11	1.67	0.76
1:B:189:MET:HE3	1:B:225:ILE:HG21	1.67	0.76
1:A:150:ARG:HD3	1:A:170:SER:OG	1.85	0.75
1:A:151:THR:HA	1:A:154:LEU:HD12	1.68	0.75
1:A:180:GLY:O	1:A:183:VAL:CG2	2.35	0.75
1:A:77:LYS:HA	1:A:175:ARG:HB2	1.69	0.74
1:A:152:ARG:HB2	1:A:495:GLU:OE1	1.87	0.74
1:B:79:LEU:HD23	1:B:81:GLU:OE1	1.88	0.74
1:B:149:GLN:HG3	1:B:151:THR:HG23	1.69	0.74
1:A:440:MET:HA	1:A:440:MET:CE	2.13	0.73
1:A:70:ALA:HB1	1:A:117:ARG:HD3	1.70	0.73
1:B:82:HIS:CD2	1:B:83:PRO:N	2.57	0.73
1:B:167:MET:HE2	1:B:187:GLY:HA3	1.70	0.73
1:B:115:GLU:O	1:B:119:ILE:HD12	1.89	0.73
1:B:339:GLU:CD	1:B:389:ARG:NH1	2.41	0.73
1:B:74:ARG:HG2	1:B:74:ARG:O	1.88	0.73
1:A:91:LYS:HB3	1:A:111:TYR:O	1.88	0.73
1:B:149:GLN:CG	1:B:151:THR:CG2	2.67	0.73
1:A:62:THR:O	1:A:66:MET:SD	2.47	0.73
1:B:59:ASN:O	1:B:62:THR:HG22	1.89	0.72
1:A:290:ASP:HB3	1:A:293:ARG:HE	1.52	0.72
1:B:120:TRP:CE2	1:B:129:ALA:HB3	2.25	0.72
1:B:149:GLN:HG2	1:B:151:THR:HG23	1.70	0.72
1:B:296:TYR:CE1	1:B:302:ASP:HB3	2.25	0.71
1:A:189:MET:HE1	1:A:192:GLU:OE1	1.89	0.71
1:B:156:ARG:HG3	1:B:156:ARG:HH11	1.55	0.71
1:B:78:TYR:HE2	1:B:133:LEU:HB2	1.56	0.71
1:A:76:ASN:O	1:A:175:ARG:CB	2.37	0.71
1:A:59:ASN:O	1:A:63:ILE:HG12	1.90	0.70
1:B:78:TYR:CE2	1:B:133:LEU:HB2	2.26	0.70
1:A:275:CYS:C	1:A:276:LEU:HD23	2.17	0.69
1:B:470:LYS:HG3	1:B:471:ALA:N	2.07	0.69
1:A:180:GLY:HA2	1:A:183:VAL:HG22	1.75	0.69
1:A:113:LYS:O	1:A:117:ARG:HG2	1.92	0.69
1:A:233:ALA:O	1:A:237:THR:HG23	1.92	0.69
1:A:463:VAL:HG23	1:A:475:ILE:HB	1.74	0.69
1:B:205:ASN:ND2	1:B:208:ARG:O	2.25	0.69
1:A:375:GLU:CD	1:A:376:SER:H	2.01	0.69
1:A:389:ARG:HE	1:A:391:ARG:HB2	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PHE:CZ	1:A:67:VAL:HG13	2.26	0.68
1:B:120:TRP:CZ2	1:B:129:ALA:CB	2.66	0.68
1:B:197:ILE:O	1:B:201:ILE:HB	1.94	0.68
1:B:149:GLN:HG3	1:B:151:THR:CG2	2.23	0.68
1:B:152:ARG:HD3	1:B:156:ARG:NH1	2.07	0.68
1:B:189:MET:CE	1:B:225:ILE:HG21	2.23	0.68
1:B:82:HIS:CE1	1:B:83:PRO:HD2	2.28	0.68
1:B:199:ARG:NE	1:B:206:PHE:CZ	2.62	0.68
1:A:318:PRO:HG3	1:A:373:THR:O	1.93	0.68
1:B:316:ILE:CD1	1:B:322:PRO:HG3	2.24	0.67
1:A:168:GLN:HG2	1:A:185:GLY:HA3	1.77	0.67
1:B:477:PRO:HB2	1:B:479:PHE:CE2	2.30	0.67
1:A:246:ARG:O	1:A:247:ASN:OD1	2.13	0.67
1:A:63:ILE:HA	1:A:66:MET:SD	2.34	0.67
1:B:470:LYS:CD	1:B:471:ALA:H	2.07	0.67
1:B:347:ILE:HD12	1:B:461:ARG:HE	1.60	0.67
1:B:307:LEU:O	1:B:310:SER:HB3	1.94	0.67
1:B:324:HIS:CD2	1:B:359:SER:OG	2.47	0.66
1:A:59:ASN:O	1:A:63:ILE:CG1	2.43	0.66
1:A:181:ALA:HB1	1:A:225:ILE:HD13	1.76	0.66
1:A:463:VAL:HG22	1:A:475:ILE:HB	1.77	0.66
1:B:79:LEU:HD21	1:B:81:GLU:OE1	1.94	0.66
1:B:26:ARG:CG	1:B:295:GLY:HA3	2.26	0.66
1:A:225:ILE:HG22	1:A:229:LYS:HE2	1.77	0.66
1:B:150:ARG:HH12	1:B:171:THR:HG22	1.61	0.66
1:A:117:ARG:O	1:A:121:ARG:HG2	1.96	0.66
1:A:371:MET:HE2	1:A:371:MET:HA	1.77	0.66
1:A:440:MET:HE2	1:A:440:MET:CA	2.18	0.66
1:B:305:ARG:O	1:B:308:GLN:HB2	1.95	0.66
1:A:200:GLY:O	1:A:201:ILE:HG13	1.96	0.65
1:B:162:ARG:HA	1:A:489:PHE:CE2	2.31	0.65
1:A:219:TYR:CE1	1:A:222:MET:HE1	2.32	0.65
1:A:345:SER:HA	1:A:352:VAL:HG23	1.79	0.65
1:A:317:ARG:HG2	1:A:374:MET:HE1	1.78	0.65
1:A:306:LEU:O	1:A:310:SER:HB2	1.95	0.65
1:B:57:ILE:HG21	1:B:363:VAL:CG2	2.26	0.65
1:B:157:THR:HG22	1:B:194:ILE:HG21	1.77	0.65
1:B:347:ILE:CD1	1:B:461:ARG:HE	2.08	0.65
1:B:152:ARG:HD3	1:B:156:ARG:HH12	1.61	0.65
1:B:308:GLN:NE2	1:B:382:ARG:HB3	2.12	0.65
1:A:138:ILE:HD13	1:A:183:VAL:HG11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:O	1:A:48:LYS:HG2	1.97	0.65
1:A:215:THR:O	1:A:219:TYR:HD2	1.79	0.65
1:B:62:THR:HG21	1:B:96:ILE:HD13	1.77	0.65
1:B:149:GLN:CD	1:B:151:THR:HG23	2.22	0.65
1:B:104:TRP:HE1	1:B:376:SER:HB2	1.61	0.64
1:B:307:LEU:O	1:B:310:SER:CB	2.46	0.64
1:B:498:ASN:HD22	1:B:498:ASN:C	2.05	0.64
1:A:40:TYR:CE2	1:A:279:CYS:HA	2.32	0.64
1:A:324:HIS:HD2	1:A:359:SER:N	1.93	0.64
1:B:150:ARG:NH1	1:B:171:THR:HG22	2.13	0.64
1:B:325:LYS:CB	1:B:360:THR:HG21	2.27	0.64
1:A:217:ILE:O	1:A:221:ARG:HG3	1.98	0.64
1:A:92:THR:CG2	1:A:116:ILE:CD1	2.76	0.64
1:B:470:LYS:CG	1:B:471:ALA:N	2.60	0.64
1:A:120:TRP:HZ2	1:A:129:ALA:CB	2.07	0.64
1:B:24:GLU:HG3	1:B:25:ILE:HD13	1.80	0.63
1:A:167:MET:O	1:A:170:SER:HB3	1.98	0.63
1:B:199:ARG:CG	1:B:206:PHE:CZ	2.73	0.63
1:A:167:MET:CE	1:A:187:GLY:C	2.71	0.63
1:B:470:LYS:HD2	1:B:471:ALA:H	1.63	0.63
1:A:45:THR:O	1:A:48:LYS:CG	2.46	0.63
1:A:58:GLN:HG3	1:A:315:LEU:HD12	1.79	0.63
1:B:47:LEU:O	1:B:48:LYS:HG3	1.97	0.63
1:B:26:ARG:HG2	1:B:295:GLY:HA3	1.81	0.63
1:A:343:VAL:HG12	1:A:479:PHE:CZ	2.34	0.63
1:B:181:ALA:O	1:B:229:LYS:NZ	2.26	0.63
1:B:98:ARG:HH11	1:B:107:GLU:CD	2.06	0.62
1:A:167:MET:HE2	1:A:167:MET:HA	1.81	0.62
1:B:497:ASP:O	1:B:498:ASN:HB2	1.99	0.62
1:A:343:VAL:HA	1:A:479:PHE:HE1	1.64	0.62
1:B:47:LEU:O	1:B:98:ARG:NH2	2.32	0.62
1:B:240:ASP:O	1:B:244:GLU:HG2	1.98	0.62
1:B:484:GLU:OE2	1:A:261:ARG:NH2	2.33	0.62
1:A:343:VAL:HA	1:A:479:PHE:CE1	2.35	0.62
1:B:41:ILE:CD1	1:B:286:ALA:HB2	2.30	0.62
1:B:193:LEU:HD21	1:B:222:MET:HB2	1.82	0.62
1:B:301:ILE:HG12	1:B:386:TRP:CE2	2.35	0.61
1:B:26:ARG:HB3	1:B:295:GLY:HA3	1.82	0.61
1:A:180:GLY:C	1:A:183:VAL:HG22	2.26	0.61
1:A:192:GLU:O	1:A:196:MET:HE2	1.99	0.61
1:A:363:VAL:HG12	1:A:363:VAL:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:GLN:OE1	1:B:185:GLY:HA3	2.00	0.61
1:A:354:PRO:HD2	1:A:357:LYS:HD2	1.82	0.61
1:A:238:MET:HB2	1:A:259:LEU:HD11	1.80	0.61
1:B:200:GLY:HA2	1:B:206:PHE:CG	2.35	0.61
1:A:237:THR:OG1	1:A:440:MET:HG3	2.01	0.61
1:A:327:GLN:HE21	1:A:331:MET:HE1	1.65	0.61
1:B:40:TYR:CE2	1:B:279:CYS:HA	2.35	0.61
1:B:196:MET:SD	1:B:222:MET:HE2	2.40	0.61
1:A:276:LEU:HD23	1:A:276:LEU:N	2.16	0.61
1:A:492:ASN:HD22	1:A:492:ASN:C	2.07	0.61
1:B:162:ARG:HA	1:A:489:PHE:CD2	2.36	0.61
1:A:31:LYS:CA	1:A:292:GLU:HG2	2.26	0.61
1:B:281:TYR:O	1:B:285:VAL:HG13	2.01	0.61
1:B:162:ARG:HH22	1:A:486:SER:H	1.49	0.60
1:B:301:ILE:HG12	1:B:386:TRP:CD2	2.36	0.60
1:A:382:ARG:CG	1:A:382:ARG:HH11	2.14	0.60
1:B:177:GLY:O	1:B:181:ALA:CB	2.49	0.60
1:A:160:ASP:O	1:A:163:MET:HB2	2.01	0.60
1:A:92:THR:HG22	1:A:116:ILE:CD1	2.32	0.60
1:A:217:ILE:HG13	1:A:218:ALA:N	2.17	0.60
1:A:21:ASN:N	1:A:24:GLU:OE2	2.35	0.60
1:B:341:LEU:HD22	1:B:352:VAL:O	2.02	0.60
1:B:182:ALA:O	1:B:271:ALA:HB3	2.02	0.59
1:B:120:TRP:HE1	1:B:129:ALA:H	1.50	0.59
1:B:384:ARG:HG2	1:B:384:ARG:HH11	1.67	0.59
1:A:115:GLU:O	1:A:119:ILE:CG1	2.37	0.59
1:A:340:ASP:HB3	1:A:343:VAL:HG22	1.82	0.59
1:B:212:GLY:O	1:B:216:ARG:N	2.33	0.59
1:B:106:ARG:HB2	1:B:371:MET:SD	2.43	0.59
1:A:179:ALA:O	1:A:182:ALA:HB3	2.03	0.59
1:A:317:ARG:HA	1:A:374:MET:CE	2.33	0.59
1:A:382:ARG:HH11	1:A:382:ARG:HG3	1.68	0.59
1:A:477:PRO:HB2	1:A:479:PHE:CE2	2.38	0.59
1:A:302:ASP:HB2	1:A:303:PRO:HD3	1.85	0.59
1:B:27:ALA:O	1:B:31:LYS:CB	2.51	0.59
1:B:82:HIS:CD2	1:B:84:SER:N	2.46	0.58
1:B:200:GLY:HA2	1:B:206:PHE:HB3	1.85	0.58
1:B:314:SER:HB2	1:B:379:LEU:HD21	1.86	0.58
1:A:284:ALA:HB2	1:A:306:LEU:HD11	1.85	0.58
1:B:66:MET:HE3	1:B:93:GLY:CA	2.22	0.58
1:A:215:THR:O	1:A:219:TYR:CD2	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASN:O	1:A:227:LYS:HB3	2.03	0.58
1:A:47:LEU:O	1:A:98:ARG:NH1	2.36	0.58
1:B:470:LYS:CG	1:B:471:ALA:H	2.16	0.58
1:A:59:ASN:OD1	1:A:97:TYR:HD1	1.86	0.58
1:A:384:ARG:HD3	1:A:385:TYR:CE1	2.39	0.58
1:B:34:ASP:OD1	1:B:291:PHE:HB2	2.03	0.58
1:B:71:PHE:CE2	1:B:117:ARG:HG2	2.38	0.58
1:A:31:LYS:HG2	1:A:292:GLU:CG	2.34	0.58
1:B:82:HIS:HD2	1:B:85:ALA:H	1.52	0.57
1:A:77:LYS:CA	1:A:175:ARG:HB2	2.34	0.57
1:A:180:GLY:CA	1:A:183:VAL:HG22	2.34	0.57
1:B:199:ARG:HE	1:B:206:PHE:HZ	1.50	0.57
1:B:347:ILE:HD12	1:B:461:ARG:HH21	1.69	0.57
1:B:27:ALA:O	1:B:31:LYS:HB2	2.05	0.57
1:B:72:ASP:O	1:B:75:ARG:HG2	2.04	0.57
1:A:31:LYS:HG2	1:A:292:GLU:HG2	1.85	0.57
1:A:299:VAL:O	1:A:299:VAL:CG1	2.53	0.57
1:B:152:ARG:HD2	1:B:156:ARG:NH2	2.20	0.57
1:A:238:MET:CE	1:A:255:ASP:OD1	2.53	0.57
1:B:25:ILE:HD13	1:B:25:ILE:N	2.19	0.57
1:B:139:TRP:CZ2	1:B:277:PRO:HG3	2.39	0.57
1:B:59:ASN:O	1:B:63:ILE:HG12	2.05	0.57
1:A:63:ILE:O	1:A:67:VAL:HG22	2.05	0.57
1:A:65:ARG:CD	1:A:79:LEU:HD13	2.25	0.57
1:A:167:MET:CE	1:A:187:GLY:HA3	2.34	0.57
1:B:57:ILE:HG21	1:B:363:VAL:HG21	1.87	0.57
1:A:76:ASN:O	1:A:175:ARG:CG	2.53	0.56
1:A:348:ARG:HG2	1:A:348:ARG:HH11	1.70	0.56
1:B:156:ARG:HG3	1:B:156:ARG:NH1	2.15	0.56
1:B:65:ARG:HH11	1:B:79:LEU:HD11	1.69	0.56
1:B:77:LYS:HG2	1:B:176:SER:HB2	1.86	0.56
1:A:307:LEU:HA	1:A:310:SER:HB2	1.86	0.56
1:B:82:HIS:HB3	1:B:85:ALA:CB	2.25	0.56
1:B:117:ARG:O	1:B:121:ARG:HG3	2.05	0.56
1:A:58:GLN:HB2	1:A:97:TYR:CE1	2.41	0.56
1:A:76:ASN:C	1:A:175:ARG:HB2	2.31	0.56
1:B:104:TRP:NE1	1:B:376:SER:HB2	2.21	0.56
1:A:65:ARG:CD	1:A:79:LEU:HD11	2.24	0.56
1:A:276:LEU:HD13	1:A:307:LEU:HG	1.88	0.56
1:B:26:ARG:O	1:B:30:GLY:N	2.35	0.56
1:B:484:GLU:HG3	1:A:160:ASP:OD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ILE:HD12	1:B:448:MET:HE2	1.86	0.55
1:A:92:THR:HG21	1:A:116:ILE:CD1	2.36	0.55
1:B:307:LEU:HD11	1:B:333:CYS:HB3	1.87	0.55
1:A:380:GLU:OE2	1:A:382:ARG:HG3	2.07	0.55
1:A:97:TYR:OH	1:A:365:ILE:HD12	2.07	0.55
1:A:318:PRO:CG	1:A:373:THR:O	2.54	0.55
1:B:152:ARG:HD2	1:B:156:ARG:HH22	1.71	0.55
1:B:317:ARG:NH1	1:B:369:GLU:OE2	2.39	0.55
1:B:149:GLN:CD	1:B:151:THR:CG2	2.80	0.55
1:A:168:GLN:HG2	1:A:185:GLY:CA	2.36	0.55
1:B:159:MET:HE1	1:B:191:MET:CA	2.37	0.55
1:B:308:GLN:CG	1:B:466:LEU:HD11	2.38	0.55
1:A:305:ARG:HG3	1:A:306:LEU:N	2.22	0.55
1:A:50:SER:O	1:A:51:ASP:C	2.49	0.54
1:B:70:ALA:HB1	1:B:117:ARG:HG3	1.88	0.54
1:B:317:ARG:HB2	1:B:320:GLU:CD	2.33	0.54
1:A:22:ALA:HA	1:A:25:ILE:HD11	1.90	0.54
1:B:255:ASP:O	1:B:258:PHE:HB3	2.07	0.54
1:B:115:GLU:O	1:B:119:ILE:CD1	2.56	0.54
1:B:159:MET:CE	1:B:191:MET:HA	2.38	0.54
1:B:199:ARG:CG	1:B:206:PHE:HE2	2.17	0.54
1:B:301:ILE:CD1	1:B:469:GLU:HA	2.37	0.54
1:B:305:ARG:HA	1:B:308:GLN:HB2	1.89	0.54
1:B:308:GLN:HG3	1:B:466:LEU:CD1	2.37	0.54
1:B:382:ARG:HG3	1:B:382:ARG:HH11	1.72	0.54
1:A:192:GLU:O	1:A:196:MET:HG2	2.08	0.54
1:A:317:ARG:CG	1:A:374:MET:HE1	2.37	0.54
1:A:64:GLU:O	1:A:67:VAL:HG23	2.08	0.54
1:A:382:ARG:HG3	1:A:382:ARG:NH1	2.23	0.54
1:B:43:MET:CE	1:B:119:ILE:HD13	2.38	0.53
1:A:159:MET:HE1	1:A:191:MET:HA	1.89	0.53
1:A:75:ARG:O	1:A:175:ARG:CG	2.39	0.53
1:A:345:SER:CA	1:A:352:VAL:HG23	2.39	0.53
1:B:115:GLU:OE1	1:B:118:ARG:NH1	2.38	0.53
1:B:64:GLU:O	1:B:68:LEU:HG	2.09	0.53
1:B:363:VAL:HG22	1:B:363:VAL:O	2.08	0.53
1:B:82:HIS:CD2	1:B:85:ALA:H	2.26	0.53
1:B:308:GLN:CD	1:B:466:LEU:HD11	2.33	0.53
1:B:463:VAL:CG2	1:B:475:ILE:HB	2.38	0.53
1:B:163:MET:HE2	1:B:261:ARG:HG2	1.89	0.53
1:A:391:ARG:O	1:A:391:ARG:HG3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:VAL:HG23	1:B:475:ILE:HB	1.90	0.53
1:A:39:PHE:CE2	1:A:67:VAL:HG13	2.44	0.53
1:B:157:THR:HG22	1:B:194:ILE:CG2	2.39	0.53
1:B:56:LEU:HD23	1:B:59:ASN:ND2	2.24	0.53
1:A:189:MET:CE	1:A:189:MET:CA	2.72	0.53
1:A:252:GLU:HA	1:A:255:ASP:HB2	1.90	0.53
1:A:314:SER:HB2	1:A:379:LEU:HD11	1.90	0.53
1:A:24:GLU:H	1:A:24:GLU:CD	2.16	0.52
1:A:167:MET:HE1	1:A:187:GLY:O	2.08	0.52
1:A:240:ASP:OD1	1:A:243:ARG:NH1	2.42	0.52
1:A:468:ASP:OD1	1:A:472:THR:HB	2.09	0.52
1:B:364:GLN:C	1:B:365:ILE:HD13	2.32	0.52
1:B:67:VAL:HA	1:B:116:ILE:CG2	2.39	0.52
1:B:124:ASN:CG	1:B:129:ALA:HB2	2.35	0.52
1:A:25:ILE:HG12	1:A:26:ARG:H	1.75	0.52
1:B:207:TRP:HH2	1:B:219:TYR:HB2	1.72	0.52
1:A:69:SER:HA	1:A:79:LEU:HD23	1.92	0.52
1:B:194:ILE:HG23	1:B:253:PHE:CZ	2.44	0.52
1:B:159:MET:HE1	1:B:191:MET:HA	1.92	0.52
1:B:355:ARG:HD3	1:B:487:TYR:CZ	2.45	0.52
1:B:316:ILE:HD13	1:B:322:PRO:HG3	1.90	0.52
1:A:159:MET:HE1	1:A:191:MET:CB	2.39	0.52
1:A:492:ASN:C	1:A:492:ASN:ND2	2.67	0.52
1:B:41:ILE:HD11	1:B:285:VAL:HG22	1.91	0.52
1:B:91:LYS:HG2	1:B:110:LEU:HD22	1.92	0.52
1:A:22:ALA:CA	1:A:25:ILE:HD11	2.40	0.52
1:A:39:PHE:CE2	1:A:67:VAL:CG1	2.93	0.52
1:A:56:LEU:HG	1:A:58:GLN:HG2	1.92	0.52
1:B:26:ARG:CB	1:B:295:GLY:HA3	2.40	0.51
1:B:163:MET:HG2	1:B:166:LEU:HD12	1.92	0.51
1:A:25:ILE:H	1:A:25:ILE:CD1	1.95	0.51
1:A:106:ARG:NH2	1:A:369:GLU:O	2.43	0.51
1:A:98:ARG:HH21	1:A:107:GLU:CD	2.18	0.51
1:B:66:MET:HE2	1:B:93:GLY:HA2	1.87	0.51
1:A:92:THR:HG22	1:A:92:THR:O	2.10	0.51
1:B:203:ASP:OD2	1:B:206:PHE:N	2.43	0.51
1:A:124:ASN:O	1:A:125:ASN:HB2	2.10	0.51
1:B:252:GLU:N	1:B:252:GLU:CD	2.69	0.51
1:A:37:GLY:HA3	1:A:285:VAL:HG21	1.92	0.51
1:A:365:ILE:C	1:A:365:ILE:CD1	2.62	0.51
1:A:492:ASN:HD22	1:A:493:ALA:N	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LYS:O	1:A:91:LYS:HG3	2.11	0.51
1:A:189:MET:CE	1:A:192:GLU:OE1	2.58	0.51
1:A:317:ARG:HB2	1:A:320:GLU:CD	2.36	0.51
1:A:389:ARG:HE	1:A:391:ARG:HB3	1.70	0.51
1:A:22:ALA:C	1:A:25:ILE:HD11	2.36	0.51
1:A:185:GLY:HA2	1:A:270:VAL:HG21	1.93	0.51
1:A:214:ARG:HD2	1:A:217:ILE:HD11	1.93	0.51
1:B:143:LEU:HD11	1:B:363:VAL:HG11	1.92	0.51
1:B:325:LYS:CA	1:B:360:THR:HG21	2.41	0.51
1:A:249:GLY:N	1:A:252:GLU:OE1	2.30	0.51
1:B:91:LYS:HG3	1:B:112:ASP:HA	1.92	0.50
1:B:167:MET:HE1	1:B:187:GLY:C	2.36	0.50
1:B:184:LYS:O	1:B:229:LYS:HE3	2.11	0.50
1:A:34:ASP:OD2	1:A:38:ARG:NH2	2.44	0.50
1:B:382:ARG:HG3	1:B:382:ARG:NH1	2.26	0.50
1:A:72:ASP:O	1:A:75:ARG:HG3	2.11	0.50
1:A:167:MET:HE3	1:A:187:GLY:HA3	1.92	0.50
1:A:300:GLY:O	1:A:303:PRO:HD2	2.12	0.50
1:A:62:THR:CG2	1:A:95:PRO:HD2	2.42	0.50
1:B:318:PRO:O	1:B:319:ASN:HB2	2.12	0.50
1:A:69:SER:HA	1:A:79:LEU:CD2	2.41	0.50
1:B:75:ARG:HH21	1:B:78:TYR:HE1	1.57	0.50
1:A:43:MET:O	1:A:47:LEU:HG	2.11	0.50
1:A:168:GLN:NE2	1:A:338:PHE:CG	2.79	0.50
1:B:92:THR:O	1:B:110:LEU:HD23	2.12	0.50
1:B:340:ASP:OD1	1:B:342:ARG:HB2	2.10	0.50
1:B:76:ASN:O	1:B:173:PRO:HB2	2.12	0.50
1:A:188:THR:O	1:A:192:GLU:HG3	2.12	0.50
1:A:317:ARG:HA	1:A:374:MET:HE1	1.94	0.49
1:B:129:ALA:O	1:B:133:LEU:HG	2.12	0.49
1:B:384:ARG:HD3	1:B:385:TYR:CZ	2.48	0.49
1:A:45:THR:O	1:A:48:LYS:HG3	2.12	0.49
1:A:64:GLU:OE1	1:A:140:HIS:HE1	1.95	0.49
1:A:184:LYS:O	1:A:229:LYS:HE3	2.12	0.49
1:B:41:ILE:O	1:B:45:THR:HG23	2.12	0.49
1:B:115:GLU:O	1:B:119:ILE:CG1	2.60	0.49
1:B:301:ILE:HD11	1:B:469:GLU:HA	1.93	0.49
1:A:182:ALA:O	1:A:271:ALA:HB3	2.12	0.49
1:A:318:PRO:HG2	1:A:373:THR:CG2	2.37	0.49
1:B:43:MET:HE3	1:B:119:ILE:HG21	1.94	0.49
1:B:82:HIS:CG	1:B:83:PRO:N	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ALA:H	1:B:369:GLU:HG3	1.77	0.49
1:A:91:LYS:HD3	1:A:112:ASP:HA	1.95	0.49
1:B:365:ILE:HD12	1:B:374:MET:HE3	1.95	0.48
1:A:139:TRP:CZ2	1:A:277:PRO:HG3	2.48	0.48
1:A:290:ASP:HB3	1:A:293:ARG:NE	2.25	0.48
1:A:65:ARG:NH1	1:A:79:LEU:CD1	2.69	0.48
1:B:47:LEU:C	1:B:48:LYS:CG	2.87	0.48
1:B:177:GLY:O	1:B:181:ALA:HB2	2.12	0.48
1:A:37:GLY:HA2	1:A:282:GLY:HA2	1.95	0.48
1:B:200:GLY:O	1:B:203:ASP:O	2.31	0.48
1:B:339:GLU:CG	1:B:389:ARG:HH12	2.22	0.48
1:B:62:THR:O	1:B:66:MET:HG3	2.14	0.48
1:B:380:GLU:OE1	1:B:382:ARG:HG3	2.13	0.48
1:A:114:GLU:O	1:A:118:ARG:HB2	2.14	0.48
1:B:308:GLN:NE2	1:B:382:ARG:CB	2.76	0.48
1:B:366:ALA:N	1:B:369:GLU:HG3	2.29	0.48
1:B:479:PHE:HB3	1:B:481:MET:HE3	1.96	0.48
1:A:79:LEU:O	1:A:79:LEU:HG	2.03	0.48
1:B:484:GLU:OE2	1:A:261:ARG:CZ	2.62	0.48
1:B:41:ILE:HD11	1:B:286:ALA:HB2	1.95	0.48
1:B:190:VAL:O	1:B:194:ILE:HG12	2.14	0.48
1:B:199:ARG:CB	1:B:206:PHE:CE2	2.96	0.48
1:B:303:PRO:O	1:B:307:LEU:HB2	2.14	0.48
1:A:189:MET:HE2	1:A:189:MET:CA	2.37	0.48
1:A:363:VAL:O	1:A:363:VAL:CG1	2.62	0.48
1:B:41:ILE:HD13	1:B:286:ALA:HB2	1.95	0.47
1:B:177:GLY:O	1:B:181:ALA:N	2.39	0.47
1:B:238:MET:O	1:B:242:VAL:HG23	2.14	0.47
1:A:32:MET:HE2	1:A:33:ILE:HD13	1.95	0.47
1:A:160:ASP:H	1:A:163:MET:HE3	1.79	0.47
1:A:345:SER:HA	1:A:352:VAL:CG2	2.44	0.47
1:B:379:LEU:N	1:B:379:LEU:HD23	2.29	0.47
1:A:62:THR:HG23	1:A:95:PRO:HD2	1.95	0.47
1:B:356:GLY:HA2	1:B:492:ASN:HB2	1.96	0.47
1:B:353:VAL:HB	1:B:354:PRO:CD	2.45	0.47
1:A:130:THR:O	1:A:134:THR:HG23	2.14	0.47
1:A:163:MET:SD	1:A:260:ALA:HB1	2.53	0.47
1:A:238:MET:HE3	1:A:255:ASP:OD1	2.15	0.47
1:B:216:ARG:NE	1:B:220:GLU:OE2	2.46	0.47
1:A:62:THR:HG21	1:A:95:PRO:N	2.30	0.47
1:A:64:GLU:OE1	1:A:140:HIS:CE1	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ARG:HG3	1:A:162:ARG:O	2.12	0.47
1:A:252:GLU:O	1:A:253:PHE:C	2.56	0.47
1:A:288:GLY:O	1:A:289:TYR:C	2.55	0.47
1:B:167:MET:HE1	1:B:187:GLY:HA3	1.95	0.47
1:B:477:PRO:HB2	1:B:479:PHE:CD2	2.50	0.47
1:B:498:ASN:C	1:B:498:ASN:ND2	2.73	0.47
1:A:115:GLU:OE1	1:A:118:ARG:NH1	2.48	0.47
1:B:167:MET:O	1:B:168:GLN:C	2.57	0.47
1:B:171:THR:HB	1:B:496:TYR:CZ	2.49	0.47
1:B:313:TYR:CE1	1:B:378:THR:HG22	2.50	0.47
1:A:184:LYS:O	1:A:270:VAL:HG13	2.15	0.47
1:A:214:ARG:O	1:A:217:ILE:HG12	2.15	0.47
1:A:348:ARG:HG2	1:A:348:ARG:NH1	2.30	0.47
1:B:308:GLN:HE21	1:B:382:ARG:HB3	1.79	0.47
1:A:66:MET:HG2	1:A:92:THR:HG23	1.96	0.47
1:A:266:LEU:HD11	1:A:447:LEU:HD23	1.96	0.47
1:A:390:THR:CG2	1:A:461:ARG:HG2	2.45	0.47
1:B:26:ARG:HB3	1:B:295:GLY:CA	2.44	0.46
1:B:41:ILE:HD11	1:B:285:VAL:CG2	2.45	0.46
1:B:151:THR:HA	1:B:154:LEU:HD12	1.95	0.46
1:B:484:GLU:CD	1:B:484:GLU:N	2.62	0.46
1:B:98:ARG:NH1	1:B:107:GLU:OE2	2.48	0.46
1:A:38:ARG:O	1:A:39:PHE:C	2.58	0.46
1:A:217:ILE:CG1	1:A:218:ALA:N	2.78	0.46
1:A:232:THR:HG21	1:A:447:LEU:HD21	1.97	0.46
1:B:167:MET:HE1	1:B:187:GLY:CA	2.46	0.46
1:A:445:ILE:HA	1:A:448:MET:SD	2.55	0.46
1:B:68:LEU:O	1:B:72:ASP:HB2	2.15	0.46
1:B:106:ARG:NH2	1:B:367:SER:O	2.48	0.46
1:A:100:VAL:HG23	1:A:100:VAL:O	2.15	0.46
1:B:212:GLY:O	1:B:216:ARG:HB2	2.15	0.46
1:B:226:LEU:O	1:B:229:LYS:HB2	2.15	0.46
1:B:380:GLU:OE2	1:B:382:ARG:NH1	2.49	0.46
1:B:56:LEU:HG	1:B:58:GLN:HG2	1.97	0.46
1:B:252:GLU:CD	1:B:252:GLU:H	2.23	0.46
1:B:321:ASN:OD1	1:B:323:ALA:HB3	2.15	0.46
1:A:244:GLU:OE1	1:A:244:GLU:HA	2.15	0.46
1:B:74:ARG:O	1:B:74:ARG:CG	2.54	0.46
1:A:39:PHE:CZ	1:A:43:MET:HG3	2.51	0.46
1:A:217:ILE:O	1:A:220:GLU:HB2	2.16	0.46
1:B:39:PHE:CZ	1:B:43:MET:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ARG:HD3	1:A:482:SER:O	2.15	0.46
1:A:60:SER:O	1:A:64:GLU:CG	2.64	0.46
1:B:384:ARG:HG2	1:B:384:ARG:NH1	2.30	0.45
1:B:61:LEU:CD2	1:B:139:TRP:HE1	2.29	0.45
1:B:384:ARG:HG2	1:B:384:ARG:O	2.16	0.45
1:B:445:ILE:O	1:B:448:MET:HB2	2.17	0.45
1:A:111:TYR:HB3	1:A:116:ILE:HD11	1.98	0.45
1:A:340:ASP:O	1:A:343:VAL:HG22	2.15	0.45
1:B:355:ARG:HD3	1:B:487:TYR:CE2	2.51	0.45
1:A:365:ILE:HA	1:A:369:GLU:OE2	2.16	0.45
1:B:70:ALA:CB	1:B:117:ARG:HG3	2.46	0.45
1:B:116:ILE:N	1:B:116:ILE:HD13	2.30	0.45
1:B:480:ASP:OD2	1:B:483:ASN:CG	2.60	0.45
1:A:99:ARG:O	1:A:99:ARG:HG2	2.15	0.45
1:B:29:VAL:HG12	1:B:296:TYR:HB3	1.99	0.45
1:B:168:GLN:HB3	1:B:338:PHE:CE1	2.52	0.45
1:A:152:ARG:HB2	1:A:495:GLU:CD	2.41	0.45
1:B:181:ALA:HB2	1:B:225:ILE:HD13	1.99	0.45
1:B:325:LYS:NZ	1:B:362:GLY:O	2.47	0.45
1:A:92:THR:CG2	1:A:116:ILE:HD12	2.47	0.45
1:A:253:PHE:O	1:A:257:ILE:HG12	2.16	0.45
1:A:464:PHE:CD2	1:A:473:SER:O	2.52	0.45
1:B:58:GLN:HG3	1:B:315:LEU:HG	1.98	0.45
1:B:185:GLY:O	1:B:186:VAL:C	2.60	0.45
1:B:205:ASN:ND2	1:B:205:ASN:C	2.73	0.45
1:B:475:ILE:HG22	1:B:476:VAL:N	2.32	0.45
1:A:25:ILE:HG12	1:A:26:ARG:N	2.31	0.45
1:A:43:MET:HE2	1:A:46:GLU:HB2	1.99	0.45
1:A:90:LYS:C	1:A:91:LYS:HG3	2.42	0.45
1:A:238:MET:HE2	1:A:238:MET:HB3	1.89	0.45
1:B:40:TYR:CD2	1:B:279:CYS:HA	2.52	0.45
1:B:152:ARG:NH2	1:A:492:ASN:OD1	2.50	0.45
1:A:167:MET:CE	1:A:187:GLY:CA	2.95	0.45
1:A:277:PRO:HB2	1:A:279:CYS:SG	2.56	0.45
1:A:477:PRO:HB2	1:A:479:PHE:CZ	2.50	0.45
1:B:167:MET:CE	1:B:187:GLY:CA	2.91	0.45
1:B:180:GLY:O	1:B:184:LYS:CG	2.50	0.45
1:B:312:VAL:HG12	1:B:379:LEU:HD12	1.98	0.45
1:A:113:LYS:H	1:A:113:LYS:HG2	1.46	0.45
1:A:120:TRP:CZ2	1:A:129:ALA:CB	2.90	0.45
1:B:139:TRP:CH2	1:B:277:PRO:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LYS:HA	1:A:292:GLU:CG	2.33	0.45
1:A:225:ILE:CG2	1:A:229:LYS:HE2	2.46	0.45
1:A:317:ARG:HA	1:A:374:MET:HE2	1.99	0.45
1:B:43:MET:HA	1:B:43:MET:HE2	1.99	0.44
1:B:207:TRP:CH2	1:B:219:TYR:HB2	2.52	0.44
1:B:477:PRO:CB	1:B:479:PHE:CE2	2.99	0.44
1:A:25:ILE:HD13	1:A:25:ILE:N	2.04	0.44
1:A:161:PRO:C	1:A:163:MET:H	2.25	0.44
1:A:180:GLY:O	1:A:183:VAL:N	2.51	0.44
1:A:325:LYS:NZ	1:A:362:GLY:O	2.48	0.44
1:A:472:THR:O	1:A:472:THR:CG2	2.62	0.44
1:B:174:ARG:O	1:B:174:ARG:CG	2.61	0.44
1:B:190:VAL:HG13	1:B:256:LEU:HB3	1.98	0.44
1:A:380:GLU:OE2	1:A:382:ARG:NH1	2.50	0.44
1:B:76:ASN:O	1:B:173:PRO:CB	2.66	0.44
1:A:43:MET:HE2	1:A:43:MET:HA	2.00	0.44
1:A:161:PRO:C	1:A:163:MET:N	2.74	0.44
1:B:78:TYR:CE2	1:B:133:LEU:CB	2.99	0.44
1:B:77:LYS:CA	1:B:175:ARG:CB	2.77	0.44
1:B:159:MET:HE1	1:B:191:MET:CG	2.48	0.44
1:B:160:ASP:O	1:B:163:MET:HB2	2.17	0.44
1:B:207:TRP:O	1:B:208:ARG:HD3	2.18	0.44
1:A:65:ARG:NH1	1:A:79:LEU:HD11	2.08	0.44
1:A:473:SER:HA	1:A:474:PRO:HD3	1.63	0.44
1:B:82:HIS:ND1	1:B:83:PRO:HD2	2.33	0.44
1:A:214:ARG:HD2	1:A:217:ILE:CD1	2.47	0.44
1:B:27:ALA:O	1:B:31:LYS:N	2.41	0.43
1:B:56:LEU:HD11	1:B:315:LEU:HG	2.00	0.43
1:B:386:TRP:CD1	1:B:466:LEU:HA	2.53	0.43
1:A:388:ILE:HG12	1:A:464:PHE:HE1	1.83	0.43
1:B:152:ARG:HB2	1:B:495:GLU:HG3	1.99	0.43
1:B:371:MET:HE3	1:B:374:MET:HG2	2.01	0.43
1:A:296:TYR:HE1	1:A:298:LEU:HD23	1.82	0.43
1:A:389:ARG:HG3	1:A:391:ARG:N	2.33	0.43
1:B:302:ASP:HB2	1:B:303:PRO:HD3	2.00	0.43
1:A:240:ASP:OD1	1:A:243:ARG:CZ	2.66	0.43
1:A:259:LEU:HD23	1:A:259:LEU:HA	1.87	0.43
1:B:60:SER:O	1:B:64:GLU:HG3	2.18	0.43
1:B:67:VAL:HA	1:B:116:ILE:HG21	2.01	0.43
1:B:279:CYS:O	1:B:283:SER:HB2	2.19	0.43
1:B:480:ASP:OD2	1:B:483:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:HD11	1:A:183:VAL:CG2	2.49	0.43
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.88	0.43
1:B:198:LYS:HE2	1:B:253:PHE:CE2	2.54	0.43
1:B:199:ARG:HB2	1:B:206:PHE:HE2	1.84	0.43
1:A:62:THR:HG23	1:A:94:GLY:HA3	1.99	0.43
1:A:160:ASP:HB2	1:A:163:MET:HG3	2.01	0.43
1:A:170:SER:HA	1:A:188:THR:HG23	2.00	0.43
1:A:340:ASP:OD2	1:A:342:ARG:NH2	2.45	0.43
1:A:355:ARG:HB2	1:A:487:TYR:CZ	2.54	0.43
1:A:157:THR:HG22	1:A:157:THR:O	2.18	0.43
1:A:196:MET:HG3	1:A:219:TYR:CZ	2.38	0.43
1:A:284:ALA:O	1:A:287:SER:HB2	2.19	0.43
1:B:172:LEU:HD12	1:B:173:PRO:HD2	2.01	0.43
1:B:312:VAL:CG1	1:B:379:LEU:HD12	2.48	0.43
1:B:317:ARG:HD3	1:B:369:GLU:OE1	2.19	0.43
1:A:58:GLN:CD	1:A:58:GLN:H	2.26	0.43
1:A:484:GLU:H	1:A:484:GLU:HG3	1.44	0.43
1:B:257:ILE:O	1:B:261:ARG:HG3	2.20	0.42
1:A:29:VAL:O	1:A:32:MET:HB3	2.19	0.42
1:A:321:ASN:OD1	1:A:323:ALA:HB3	2.18	0.42
1:A:386:TRP:NE1	1:A:464:PHE:HB2	2.34	0.42
1:B:58:GLN:HE21	1:B:58:GLN:HB3	1.62	0.42
1:B:77:LYS:HD3	1:B:78:TYR:CD1	2.53	0.42
1:A:120:TRP:CE2	1:A:124:ASN:ND2	2.87	0.42
1:A:107:GLU:HG2	1:A:109:ILE:HG23	2.01	0.42
1:B:204:ARG:HA	1:B:204:ARG:HD2	1.72	0.42
1:B:347:ILE:HD12	1:B:461:ARG:NE	2.29	0.42
1:B:355:ARG:O	1:B:358:LEU:HB2	2.19	0.42
1:A:98:ARG:NH2	1:A:107:GLU:OE1	2.41	0.42
1:A:441:ARG:O	1:A:445:ILE:HG13	2.19	0.42
1:B:211:ASN:O	1:B:215:THR:HG23	2.20	0.42
1:B:386:TRP:HD1	1:B:466:LEU:HA	1.83	0.42
1:A:92:THR:HG21	1:A:116:ILE:HD13	2.00	0.42
1:A:498:ASN:HD22	1:A:498:ASN:HA	1.64	0.42
1:A:26:ARG:NH1	1:A:295:GLY:HA3	2.34	0.42
1:A:78:TYR:O	1:A:173:PRO:HG3	2.20	0.42
1:A:112:ASP:OD2	1:A:115:GLU:HB2	2.20	0.42
1:A:152:ARG:O	1:A:156:ARG:HG3	2.19	0.42
1:A:299:VAL:HG13	1:A:389:ARG:HG2	2.00	0.42
1:A:32:MET:HE2	1:A:33:ILE:CD1	2.50	0.42
1:A:107:GLU:OE2	1:A:109:ILE:CG2	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ARG:HG2	1:A:374:MET:CE	2.46	0.42
1:B:151:THR:O	1:B:155:VAL:HG23	2.19	0.42
1:B:217:ILE:O	1:B:221:ARG:HG3	2.19	0.42
1:A:340:ASP:O	1:A:343:VAL:CG2	2.67	0.42
1:B:313:TYR:CE1	1:B:378:THR:CG2	3.03	0.42
1:B:325:LYS:HB2	1:B:360:THR:CG2	2.40	0.42
1:B:346:PHE:HE2	1:B:463:VAL:HG21	1.85	0.42
1:B:444:ILE:O	1:B:448:MET:HG3	2.20	0.42
1:B:29:VAL:O	1:B:33:ILE:HG12	2.20	0.42
1:B:452:ARG:HA	1:B:453:PRO:HD3	1.83	0.42
1:A:26:ARG:HG3	1:A:296:TYR:O	2.20	0.42
1:A:49:LEU:HB3	1:A:53:GLU:HB2	2.02	0.42
1:B:61:LEU:HD23	1:B:61:LEU:HA	1.78	0.41
1:A:92:THR:HG22	1:A:116:ILE:HD11	2.00	0.41
1:B:170:SER:HA	1:B:188:THR:HG23	2.02	0.41
1:A:317:ARG:CG	1:A:317:ARG:HH11	2.32	0.41
1:A:382:ARG:HH11	1:A:382:ARG:CB	2.34	0.41
1:B:61:LEU:HD22	1:B:140:HIS:CD2	2.55	0.41
1:B:475:ILE:CG2	1:B:476:VAL:N	2.83	0.41
1:A:290:ASP:O	1:A:293:ARG:HG3	2.20	0.41
1:B:247:ASN:HD22	1:B:247:ASN:HA	1.69	0.41
1:A:317:ARG:NH1	1:A:317:ARG:HG3	2.34	0.41
1:B:150:ARG:C	1:B:495:GLU:OE1	2.63	0.41
1:A:376:SER:OG	1:A:377:SER:N	2.54	0.41
1:A:382:ARG:HH11	1:A:382:ARG:HB2	1.84	0.41
1:B:75:ARG:O	1:B:175:ARG:HG3	2.20	0.41
1:B:341:LEU:HA	1:B:341:LEU:HD23	1.77	0.41
1:A:225:ILE:O	1:A:226:LEU:C	2.63	0.41
1:B:61:LEU:HD23	1:B:64:GLU:OE1	2.20	0.41
1:A:129:ALA:O	1:A:130:THR:C	2.64	0.41
1:A:172:LEU:HD23	1:A:173:PRO:HD2	2.02	0.41
1:A:324:HIS:HD2	1:A:359:SER:HB2	1.86	0.41
1:A:341:LEU:HD13	1:A:352:VAL:O	2.20	0.41
1:B:301:ILE:HG12	1:B:386:TRP:CE3	2.56	0.41
1:B:354:PRO:O	1:B:355:ARG:C	2.62	0.41
1:A:149:GLN:HB2	1:A:491:ASP:OD2	2.20	0.41
1:A:226:LEU:HD11	1:A:230:PHE:CE2	2.56	0.41
1:A:290:ASP:CB	1:A:293:ARG:HE	2.25	0.41
1:B:307:LEU:O	1:B:310:SER:HB2	2.19	0.41
1:A:24:GLU:HG2	1:A:25:ILE:HD13	2.03	0.41
1:A:66:MET:HB3	1:A:116:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:VAL:O	1:A:477:PRO:C	2.64	0.41
1:B:218:ALA:O	1:B:219:TYR:C	2.64	0.40
1:B:308:GLN:C	1:B:310:SER:H	2.29	0.40
1:A:25:ILE:CD1	1:A:25:ILE:N	2.73	0.40
1:A:127:ASP:OD1	1:A:127:ASP:C	2.65	0.40
1:A:324:HIS:HD2	1:A:359:SER:CB	2.34	0.40
1:A:340:ASP:CG	1:A:342:ARG:HH21	2.26	0.40
1:B:199:ARG:C	1:B:206:PHE:CD2	2.99	0.40
1:B:220:GLU:O	1:B:221:ARG:C	2.63	0.40
1:A:31:LYS:HE2	1:A:292:GLU:OE1	2.21	0.40
1:A:161:PRO:O	1:A:164:CYS:HB3	2.20	0.40
1:A:327:GLN:HG3	1:A:352:VAL:HG13	2.04	0.40
1:B:33:ILE:O	1:B:34:ASP:C	2.65	0.40
1:B:41:ILE:CD1	1:B:285:VAL:CG2	2.98	0.40
1:B:225:ILE:O	1:B:229:LYS:HG3	2.21	0.40
1:B:276:LEU:HB2	1:B:281:TYR:CZ	2.55	0.40
1:B:290:ASP:OD1	1:B:293:ARG:HG2	2.22	0.40
1:A:43:MET:HE3	1:A:119:ILE:CD1	2.51	0.40
1:A:68:LEU:HB3	1:A:79:LEU:HB3	2.02	0.40
1:A:237:THR:OG1	1:A:238:MET:N	2.55	0.40
1:B:257:ILE:O	1:B:260:ALA:HB3	2.21	0.40
1:A:114:GLU:HA	1:A:117:ARG:CG	2.51	0.40
1:B:36:ILE:HD11	1:B:132:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	394/483 (82%)	377 (96%)	14 (4%)	3 (1%)	16	44
1	B	418/483 (86%)	401 (96%)	16 (4%)	1 (0%)	43	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	812/966 (84%)	778 (96%)	30 (4%)	4 (0%)	24 55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	474	PRO
1	A	177	GLY
1	B	83	PRO
1	A	102	GLY

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	344/406 (85%)	291 (85%)	53 (15%)	2 10
1	B	359/406 (88%)	313 (87%)	46 (13%)	4 15
All	All	703/812 (87%)	604 (86%)	99 (14%)	3 12

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	24	GLU
1	B	25	ILE
1	B	26	ARG
1	B	57	ILE
1	B	58	GLN
1	B	62	THR
1	B	65	ARG
1	B	67	VAL
1	B	68	LEU
1	B	81	GLU
1	B	98	ARG
1	B	110	LEU
1	B	112	ASP
1	B	115	GLU

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Mol	Chain	Res	Type
1	B	116	ILE
1	B	122	GLN
1	B	130	THR
1	B	151	THR
1	B	152	ARG
1	B	160	ASP
1	B	168	GLN
1	B	183	VAL
1	B	201	ILE
1	B	231	GLN
1	B	247	ASN
1	B	259	LEU
1	B	270	VAL
1	B	285	VAL
1	B	294	GLU
1	B	309	ASN
1	B	328	LEU
1	B	339	GLU
1	B	358	LEU
1	B	359	SER
1	B	374	MET
1	B	375	GLU
1	B	378	THR
1	B	382	ARG
1	B	445	ILE
1	B	463	VAL
1	B	466	LEU
1	B	472	THR
1	B	482	SER
1	B	484	GLU
1	B	492	ASN
1	B	498	ASN
1	A	24	GLU
1	A	25	ILE
1	A	34	ASP
1	A	43	MET
1	A	44	CYS
1	A	45	THR
1	A	49	LEU
1	A	50	SER
1	A	57	ILE
1	A	58	GLN

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Mol	Chain	Res	Type
1	A	63	ILE
1	A	65	ARG
1	A	66	MET
1	A	67	VAL
1	A	75	ARG
1	A	79	LEU
1	A	92	THR
1	A	101	ASP
1	A	103	LYS
1	A	110	LEU
1	A	111	TYR
1	A	112	ASP
1	A	113	LYS
1	A	127	ASP
1	A	152	ARG
1	A	168	GLN
1	A	170	SER
1	A	189	MET
1	A	247	ASN
1	A	253	PHE
1	A	272	HIS
1	A	276	LEU
1	A	285	VAL
1	A	298	LEU
1	A	305	ARG
1	A	310	SER
1	A	312	VAL
1	A	350	THR
1	A	352	VAL
1	A	358	LEU
1	A	365	ILE
1	A	373	THR
1	A	375	GLU
1	A	382	ARG
1	A	390	THR
1	A	392	SER
1	A	469	GLU
1	A	472	THR
1	A	473	SER
1	A	481	MET
1	A	484	GLU
1	A	492	ASN

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Mol	Chain	Res	Type
1	A	498	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	82	HIS
1	B	142	ASN
1	B	205	ASN
1	B	231	GLN
1	B	235	GLN
1	B	247	ASN
1	B	272	HIS
1	B	308	GLN
1	B	324	HIS
1	B	368	ASN
1	B	483	ASN
1	B	492	ASN
1	B	498	ASN
1	A	42	GLN
1	A	76	ASN
1	A	140	HIS
1	A	142	ASN
1	A	149	GLN
1	A	168	GLN
1	A	241	GLN
1	A	247	ASN
1	A	324	HIS
1	A	327	GLN
1	A	364	GLN
1	A	368	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	404/483 (83%)	0.87	49 (12%) 8 6	31, 63, 97, 120	0
1	B	423/483 (87%)	0.52	35 (8%) 17 12	26, 49, 97, 123	0
All	All	827/966 (85%)	0.69	84 (10%) 12 9	26, 55, 98, 123	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	LEU	6.8
1	B	177	GLY	4.0
1	B	129	ALA	4.0
1	B	207	TRP	3.9
1	A	215	THR	3.8
1	A	310	SER	3.7
1	A	71	PHE	3.6
1	A	201	ILE	3.6
1	A	196	MET	3.6
1	B	23	THR	3.5
1	A	219	TYR	3.4
1	A	90	LYS	3.4
1	B	201	ILE	3.3
1	A	178	ALA	3.3
1	B	79	LEU	3.3
1	B	492	ASN	3.2
1	A	388	ILE	3.2
1	B	78	TYR	3.1
1	B	495	GLU	3.1
1	B	176	SER	3.1
1	A	80	GLU	3.1
1	A	176	SER	3.1
1	A	447	LEU	3.1
1	A	179	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	197	ILE	3.0
1	A	73	GLU	2.9
1	A	180	GLY	2.9
1	A	248	PRO	2.8
1	B	461	ARG	2.8
1	A	234	ALA	2.8
1	A	290	ASP	2.8
1	A	472	THR	2.8
1	B	450	SER	2.7
1	A	439	ASP	2.7
1	A	462	GLY	2.7
1	A	70	ALA	2.6
1	B	83	PRO	2.6
1	B	74	ARG	2.6
1	A	129	ALA	2.6
1	A	112	ASP	2.6
1	B	26	ARG	2.5
1	A	473	SER	2.5
1	A	460	GLY	2.5
1	A	250	ASN	2.5
1	A	475	ILE	2.5
1	A	245	SER	2.5
1	B	80	GLU	2.5
1	B	174	ARG	2.5
1	B	206	PHE	2.5
1	A	498	ASN	2.5
1	A	371	MET	2.4
1	A	114	GLU	2.4
1	A	440	MET	2.4
1	A	177	GLY	2.3
1	B	497	ASP	2.3
1	B	484	GLU	2.3
1	A	109	ILE	2.3
1	B	368	ASN	2.3
1	B	22	ALA	2.3
1	A	363	VAL	2.3
1	B	77	LYS	2.3
1	A	98	ARG	2.3
1	B	89	PRO	2.2
1	B	462	GLY	2.2
1	A	444	ILE	2.2
1	A	68	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	108	LEU	2.2
1	B	247	ASN	2.2
1	A	231	GLN	2.2
1	B	460	GLY	2.2
1	B	310	SER	2.2
1	B	25	ILE	2.1
1	B	86	GLY	2.1
1	B	200	GLY	2.1
1	A	107	GLU	2.1
1	B	199	ARG	2.1
1	B	210	GLU	2.1
1	A	362	GLY	2.1
1	A	479	PHE	2.1
1	A	78	TYR	2.0
1	A	448	MET	2.0
1	B	463	VAL	2.0
1	A	474	PRO	2.0
1	B	363	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.