



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:41 PM UTC

PDB ID : 1MAS / pdb_00001mas
Title : PURINE NUCLEOSIDE HYDROLASE
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Deposited on : 1995-12-18
Resolution : 2.50 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

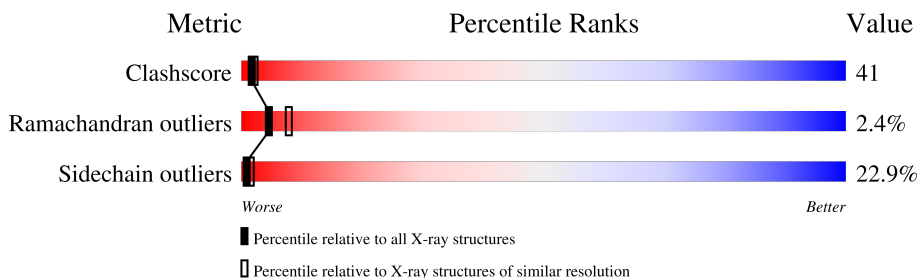
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	
1	B	314	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4693 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 INOSINE-URIDINE NUCLEOSIDE N-RIBOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2356	1497	401	443	15			
1	B	295	Total	C	N	O	S	0	0	0
			2262	1437	388	423	14			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	34	Total	O	0	0
			34	34		

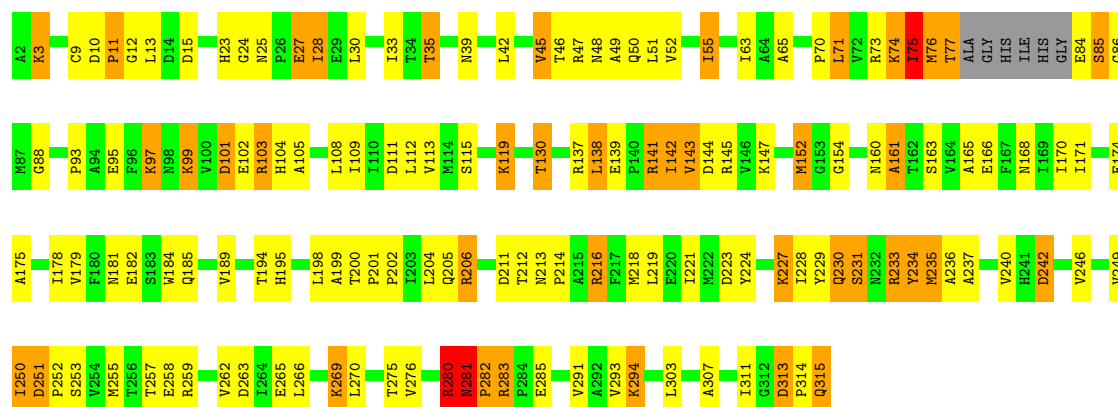
3 Residue-property plots

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. 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. 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.

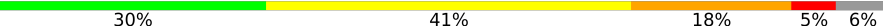
Note EDS was not executed.

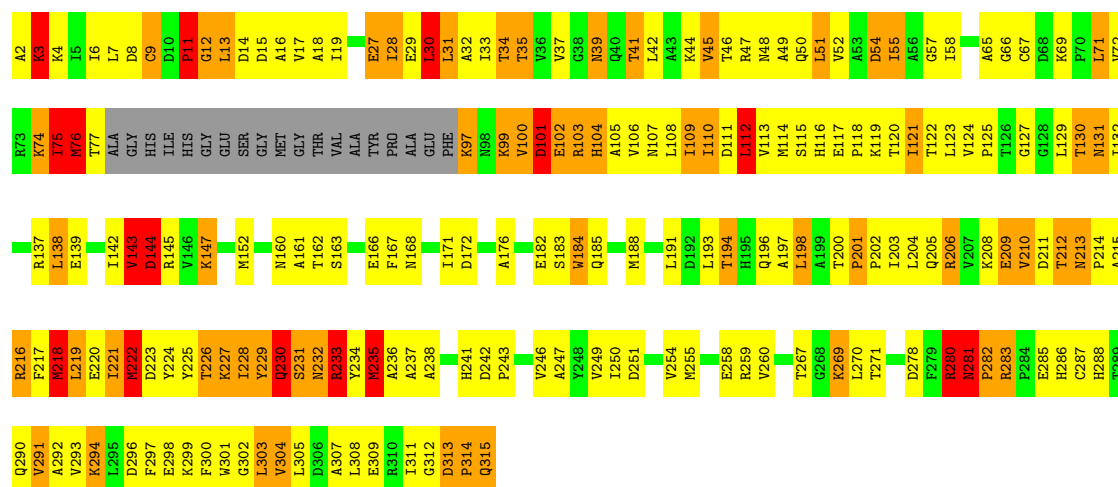
• Molecule 1: INOSINE-URIDINE NUCLEOSIDE N-RIBOHYDROLASE

Chain A: 



• Molecule 1: INOSINE-URIDINE NUCLEOSIDE N-RIBOHYDROLASE

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	63.84Å 131.53Å 90.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 2.50	Depositor
% Data completeness (in resolution range)	89.1 (99.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4693	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.13	1/2399 (0.0%)	1.39	25/3268 (0.8%)
1	B	1.28	16/2302 (0.7%)	1.68	55/3136 (1.8%)
All	All	1.21	17/4701 (0.4%)	1.54	80/6404 (1.2%)

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	B	0	3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	315	GLN	C-OXT	30.27	1.84	1.23
1	B	282	PRO	CA-C	23.24	1.75	1.52
1	B	219	LEU	N-CA	17.83	1.68	1.46
1	B	281	ASN	C-N	-16.01	1.17	1.33
1	B	283	ARG	N-CA	14.19	1.68	1.46
1	B	234	TYR	N-CA	12.66	1.62	1.46
1	B	281	ASN	CA-C	-9.85	1.40	1.52
1	B	101	ASP	N-CA	9.18	1.58	1.46
1	B	222	MET	N-CA	8.29	1.56	1.46
1	B	282	PRO	CA-CB	-6.25	1.45	1.53
1	B	100	VAL	CA-C	6.01	1.60	1.52
1	B	100	VAL	N-CA	5.44	1.54	1.46
1	B	100	VAL	C-N	5.43	1.41	1.33
1	B	144	ASP	CA-CB	-5.41	1.44	1.53
1	B	281	ASN	N-CA	-5.23	1.38	1.46
1	B	131	ASN	N-CA	5.13	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	99	LYS	CA-C	5.03	1.60	1.53

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	ASP	CA-CB-CG	24.35	136.95	112.60
1	B	281	ASN	O-C-N	-23.72	94.04	121.32
1	B	281	ASN	CA-C-N	-18.04	98.04	120.23
1	B	281	ASN	C-N-CA	-18.04	98.04	120.23
1	A	281	ASN	O-C-N	-14.38	104.79	121.32
1	B	222	MET	N-CA-C	-12.14	98.03	111.14
1	A	282	PRO	CB-CA-C	-11.32	102.36	111.87
1	A	85	SER	N-CA-C	10.74	125.10	111.24
1	B	282	PRO	O-C-N	-10.63	111.76	123.03
1	B	219	LEU	N-CA-C	-10.35	98.97	111.69
1	B	234	TYR	N-CA-CB	10.34	127.97	110.49
1	B	75	ILE	N-CA-C	-9.63	100.24	110.36
1	A	280	ARG	N-CA-C	9.61	122.23	110.41
1	B	3	LYS	N-CA-C	9.21	130.43	110.80
1	A	236	ALA	N-CA-C	-9.14	101.40	111.36
1	A	97	LYS	N-CA-C	-8.70	99.51	112.04
1	B	218	MET	N-CA-C	-8.47	102.01	111.07
1	B	102	GLU	N-CA-C	-8.46	102.97	113.20
1	A	12	GLY	N-CA-C	-8.33	93.44	113.18
1	B	282	PRO	CA-N-CD	8.10	123.34	112.00
1	B	218	MET	CA-C-N	-7.79	107.25	120.58
1	B	218	MET	C-N-CA	-7.79	107.25	120.58
1	B	233	ARG	CA-C-N	-7.58	107.06	121.54
1	B	233	ARG	C-N-CA	-7.58	107.06	121.54
1	B	231	SER	N-CA-C	-7.50	104.10	113.55
1	B	76	MET	N-CA-C	7.49	126.76	110.80
1	A	293	VAL	N-CA-C	7.30	117.39	111.62
1	B	112	LEU	N-CA-C	-7.05	102.64	111.11
1	B	230	GLN	CB-CA-C	-6.96	96.57	110.42
1	B	230	GLN	CA-C-N	-6.91	110.50	122.79
1	B	230	GLN	C-N-CA	-6.91	110.50	122.79
1	B	219	LEU	N-CA-CB	-6.90	99.92	110.20
1	B	11	PRO	O-C-N	6.87	131.91	122.64
1	B	271	THR	N-CA-C	6.85	121.34	112.92
1	B	12	GLY	N-CA-C	-6.82	101.30	111.19
1	B	212	THR	N-CA-C	-6.53	99.28	109.72
1	A	86	GLY	N-CA-C	-6.43	97.95	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	VAL	N-CA-C	6.42	119.07	111.05
1	A	175	ALA	N-CA-C	-6.33	104.39	111.28
1	A	161	ALA	N-CA-C	-6.29	103.72	111.33
1	B	127	GLY	N-CA-C	-6.24	102.53	111.20
1	A	93	PRO	N-CA-C	-6.20	102.54	111.22
1	A	130	THR	N-CA-C	6.18	123.97	110.80
1	B	280	ARG	O-C-N	-6.17	115.53	122.75
1	B	67	CYS	N-CA-C	6.16	119.19	110.50
1	A	250	ILE	CB-CA-C	-5.98	104.31	111.97
1	A	179	VAL	N-CA-C	5.98	116.16	110.42
1	B	304	VAL	CB-CA-C	-5.97	104.06	111.70
1	A	102	GLU	N-CA-CB	5.89	119.31	110.53
1	B	143	VAL	CA-C-N	-5.88	112.09	122.26
1	B	143	VAL	C-N-CA	-5.88	112.09	122.26
1	B	115	SER	N-CA-C	5.83	120.12	113.19
1	B	30	LEU	N-CA-C	5.76	118.26	109.62
1	B	291	VAL	N-CA-C	5.74	116.74	108.48
1	B	72	VAL	N-CA-C	5.70	116.12	111.62
1	A	75	ILE	O-C-N	5.68	127.68	121.83
1	B	9	CYS	N-CA-C	5.66	116.86	108.60
1	B	32	ALA	N-CA-C	5.55	116.71	108.60
1	B	198	LEU	N-CA-C	5.53	118.93	110.20
1	A	251	ASP	C-N-CD	-5.47	102.57	125.00
1	B	222	MET	O-C-N	5.42	127.94	122.09
1	B	11	PRO	CA-C-N	5.39	129.29	120.51
1	B	11	PRO	C-N-CA	5.39	129.29	120.51
1	A	165	ALA	N-CA-C	5.35	118.29	109.72
1	B	233	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	B	280	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	B	75	ILE	CB-CA-C	-5.29	105.11	111.88
1	B	282	PRO	N-CD-CG	-5.28	95.28	103.20
1	B	283	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	138	LEU	CA-C-N	-5.27	117.47	122.37
1	A	138	LEU	C-N-CA	-5.27	117.47	122.37
1	A	234	TYR	N-CA-C	5.24	116.93	108.34
1	B	104	HIS	N-CA-C	-5.21	101.47	109.76
1	B	235	MET	N-CA-C	-5.16	99.55	108.52
1	A	39	ASN	N-CA-C	-5.12	106.99	113.18
1	B	54	ASP	N-CA-C	-5.11	104.79	111.02
1	B	286	HIS	N-CA-C	5.11	117.48	108.24
1	B	281	ASN	CA-CB-CG	5.10	117.70	112.60
1	B	267	THR	N-CA-C	5.07	121.16	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	GLN	N-CA-C	-5.01	105.51	110.97

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	218	MET	Peptide
1	B	281	ASN	Mainchain,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	2356	0	2395	136	0
1	B	2262	0	2312	255	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	39	0	0	3	0
3	B	34	0	0	1	0
All	All	4693	0	4707	384	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 41.

All (384) 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:283:ARG:N	1:B:283:ARG:CA	1.68	1.56
1:B:282:PRO:C	1:B:282:PRO:CA	1.75	1.56
1:B:219:LEU:CA	1:B:219:LEU:N	1.68	1.54
1:B:226:THR:CG2	1:B:230:GLN:HE22	1.29	1.44
1:B:226:THR:HG23	1:B:230:GLN:NE2	1.23	1.42
1:A:315:GLN:C	1:A:315:GLN:OXT	1.84	1.21
1:A:11:PRO:HD2	1:A:45:VAL:HG13	1.28	1.16
1:B:11:PRO:HD2	1:B:45:VAL:HG13	1.24	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:MET:HE3	1:B:238:ALA:HA	1.29	1.13
1:A:315:GLN:OXT	1:A:315:GLN:HB3	1.47	1.13
1:A:269:LYS:HE2	1:A:270:LEU:HD21	1.24	1.10
1:B:185:GLN:NE2	1:B:259:ARG:HH22	1.52	1.07
1:B:185:GLN:HE22	1:B:259:ARG:NH2	1.51	1.06
1:B:13:LEU:HD12	1:B:225:TYR:HB2	1.05	1.03
1:B:188:MET:HE2	1:B:291:VAL:HG12	1.40	1.03
1:A:35:THR:HG22	1:A:65:ALA:HA	1.38	1.02
1:B:223:ASP:HA	1:B:226:THR:HB	1.41	1.00
1:A:315:GLN:OXT	1:A:315:GLN:CB	2.09	1.00
1:B:212:THR:HB	1:B:214:PRO:HD2	1.44	0.99
1:A:28:ILE:HD11	1:A:250:ILE:HG12	1.41	0.96
1:B:75:ILE:HD13	1:B:75:ILE:H	1.31	0.95
1:B:269:LYS:HE3	1:B:270:LEU:HG	1.49	0.93
1:B:13:LEU:CD1	1:B:225:TYR:HB2	1.98	0.93
1:A:315:GLN:OXT	1:A:315:GLN:CA	2.20	0.90
1:B:218:MET:C	1:B:219:LEU:CA	2.43	0.90
1:A:28:ILE:CD1	1:A:250:ILE:HG12	2.01	0.90
1:B:13:LEU:HD12	1:B:225:TYR:CB	1.99	0.88
1:B:75:ILE:HG12	1:B:76:MET:H	1.38	0.87
1:A:269:LYS:HE2	1:A:270:LEU:CD2	2.04	0.86
1:B:11:PRO:HD2	1:B:45:VAL:CG1	2.07	0.84
1:B:201:PRO:HG2	1:B:202:PRO:HD3	1.62	0.81
1:A:75:ILE:HD13	1:A:76:MET:H	1.45	0.81
1:B:223:ASP:CA	1:B:226:THR:HB	2.10	0.81
1:B:294:LYS:HB2	1:B:294:LYS:NZ	1.93	0.80
1:A:11:PRO:CD	1:A:45:VAL:HG13	2.11	0.80
1:B:219:LEU:N	1:B:219:LEU:CB	2.46	0.78
1:A:224:TYR:O	1:A:228:ILE:HD13	1.83	0.78
1:A:230:GLN:HG2	1:A:235:MET:CB	2.14	0.78
1:B:11:PRO:HA	1:B:15:ASP:HB2	1.65	0.78
1:A:35:THR:HG21	1:A:46:THR:OG1	1.82	0.78
1:A:101:ASP:OD2	1:A:103:ARG:HG3	1.86	0.76
1:B:194:THR:HB	1:B:241:HIS:HD2	1.49	0.76
1:B:219:LEU:N	1:B:219:LEU:C	2.44	0.76
1:A:139:GLU:OE2	1:A:141:ARG:HB2	1.86	0.75
1:B:282:PRO:C	1:B:282:PRO:CB	2.59	0.74
1:B:307:ALA:O	1:B:311:ILE:HG23	1.89	0.73
1:B:212:THR:CB	1:B:214:PRO:HD2	2.18	0.72
1:B:200:THR:HB	1:B:201:PRO:HD2	1.71	0.72
1:B:212:THR:O	1:B:216:ARG:HG2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ASP:OD2	1:B:299:LYS:HB2	1.89	0.71
1:B:35:THR:HG22	1:B:65:ALA:HA	1.71	0.71
1:A:202:PRO:O	1:A:206:ARG:HG2	1.91	0.71
1:A:227:LYS:O	1:A:231:SER:HB2	1.91	0.71
1:A:230:GLN:HG2	1:A:235:MET:HB3	1.73	0.70
1:B:13:LEU:HG	1:B:221:ILE:HG23	1.72	0.70
1:B:48:ASN:O	1:B:52:VAL:HG23	1.91	0.70
1:A:11:PRO:HA	1:A:15:ASP:HB2	1.73	0.70
1:B:110:ILE:HD13	1:B:139:GLU:HB3	1.73	0.70
1:B:105:ALA:O	1:B:109:ILE:HG13	1.93	0.69
1:B:55:ILE:HD13	1:B:55:ILE:N	2.09	0.68
1:B:219:LEU:O	1:B:222:MET:HB2	1.94	0.68
1:B:75:ILE:HG12	1:B:76:MET:N	2.08	0.68
1:A:115:SER:OG	3:A:918:HOH:O	2.12	0.68
1:A:74:LYS:HD3	1:A:76:MET:CE	2.24	0.67
1:B:9:CYS:HB2	1:B:15:ASP:OD2	1.94	0.67
1:A:75:ILE:H	1:A:75:ILE:CD1	2.08	0.67
1:B:216:ARG:O	1:B:219:LEU:N	2.26	0.67
1:A:48:ASN:O	1:A:52:VAL:HG23	1.95	0.67
1:B:74:LYS:HG2	1:B:76:MET:SD	2.34	0.67
1:B:226:THR:HG22	1:B:227:LYS:N	2.09	0.67
1:B:35:THR:HG21	1:B:46:THR:OG1	1.95	0.67
1:A:281:ASN:HB3	1:A:282:PRO:HD3	1.75	0.67
1:A:235:MET:HG2	1:A:237:ALA:O	1.94	0.66
1:A:35:THR:HG23	1:A:42:LEU:CD1	2.25	0.66
1:B:229:TYR:C	1:B:231:SER:H	2.03	0.66
1:A:307:ALA:O	1:A:311:ILE:HG12	1.94	0.66
1:B:118:PRO:O	1:B:120:THR:HG23	1.95	0.66
1:B:235:MET:HE3	1:B:238:ALA:CA	2.15	0.66
1:A:103:ARG:HE	1:A:108:LEU:HD13	1.61	0.66
1:B:160:ASN:OD1	1:B:161:ALA:N	2.28	0.66
1:B:216:ARG:HG3	1:B:216:ARG:HH11	1.61	0.66
1:B:121:ILE:O	1:B:147:LYS:HB3	1.96	0.65
1:B:281:ASN:ND2	1:B:281:ASN:O	2.29	0.65
1:A:251:ASP:OD1	1:A:252:PRO:HD2	1.96	0.65
1:A:269:LYS:HG2	1:A:270:LEU:HD23	1.79	0.65
1:B:228:ILE:O	1:B:231:SER:HB2	1.97	0.65
1:B:101:ASP:OD1	1:B:103:ARG:HD2	1.96	0.65
1:B:201:PRO:CG	1:B:202:PRO:HD3	2.25	0.65
1:B:219:LEU:HA	1:B:222:MET:HB2	1.79	0.65
1:B:11:PRO:CD	1:B:45:VAL:HG13	2.16	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:HD13	1:A:75:ILE:N	2.12	0.64
1:A:75:ILE:HD13	1:A:75:ILE:H	1.63	0.64
1:A:230:GLN:HG2	1:A:235:MET:HB2	1.80	0.64
1:A:119:LYS:N	1:A:145:ARG:O	2.28	0.64
1:B:214:PRO:HG2	1:B:311:ILE:CD1	2.28	0.63
1:B:51:LEU:CD1	1:B:55:ILE:HD11	2.29	0.63
1:B:188:MET:HE2	1:B:291:VAL:CG1	2.25	0.63
1:A:283:ARG:NH1	1:A:283:ARG:HG3	2.13	0.62
1:A:74:LYS:HD3	1:A:76:MET:SD	2.40	0.62
1:B:235:MET:O	1:B:236:ALA:C	2.43	0.61
1:B:227:LYS:HA	1:B:230:GLN:OE1	2.00	0.61
1:B:111:ASP:O	1:B:112:LEU:C	2.41	0.61
1:B:224:TYR:CE1	1:B:228:ILE:HD11	2.36	0.61
1:A:185:GLN:HE22	1:A:259:ARG:HH22	1.47	0.61
1:B:31:LEU:N	1:B:31:LEU:HD23	2.16	0.60
1:B:34:THR:CG2	1:B:105:ALA:HB1	2.31	0.60
1:B:259:ARG:HG2	1:B:290:GLN:HB3	1.83	0.60
1:B:106:VAL:O	1:B:110:ILE:HG13	2.02	0.60
1:B:219:LEU:N	1:B:220:GLU:N	2.49	0.60
1:B:223:ASP:O	1:B:224:TYR:C	2.44	0.60
1:B:223:ASP:HA	1:B:226:THR:CB	2.23	0.60
1:B:213:ASN:HA	1:B:216:ARG:HG3	1.84	0.59
1:B:226:THR:C	1:B:230:GLN:NE2	2.61	0.59
1:A:152:MET:HE3	1:A:194:THR:HG21	1.84	0.59
1:A:281:ASN:HB3	1:A:282:PRO:CD	2.32	0.59
1:A:11:PRO:HG2	1:A:49:ALA:HB2	1.83	0.59
1:B:129:LEU:HD12	1:B:176:ALA:HA	1.84	0.59
1:B:219:LEU:O	1:B:222:MET:N	2.36	0.59
1:B:11:PRO:HA	1:B:15:ASP:CB	2.33	0.58
1:A:265:GLU:OE1	1:B:270:LEU:HB2	2.03	0.58
1:B:102:GLU:HG3	1:B:102:GLU:O	2.02	0.58
1:B:214:PRO:HG2	1:B:311:ILE:HD12	1.86	0.58
1:B:227:LYS:O	1:B:230:GLN:N	2.36	0.58
1:A:47:ARG:HA	1:A:50:GLN:HE21	1.67	0.58
1:B:121:ILE:HG22	1:B:122:THR:N	2.18	0.58
1:B:259:ARG:NH2	1:B:287:CYS:O	2.31	0.58
1:A:24:GLY:CA	1:A:311:ILE:HD11	2.34	0.58
1:B:51:LEU:O	1:B:55:ILE:HG12	2.04	0.58
1:B:223:ASP:O	1:B:226:THR:HB	2.04	0.58
1:A:218:MET:O	1:A:221:ILE:HG12	2.04	0.57
1:B:194:THR:HB	1:B:241:HIS:CD2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:TYR:C	1:B:231:SER:N	2.62	0.57
1:B:308:LEU:O	1:B:311:ILE:HG12	2.05	0.57
1:B:51:LEU:HD12	1:B:55:ILE:HD11	1.86	0.57
1:A:229:TYR:C	1:A:231:SER:H	2.12	0.57
1:B:193:LEU:HD13	1:B:193:LEU:C	2.30	0.57
1:B:302:GLY:O	1:B:303:LEU:C	2.48	0.57
1:B:303:LEU:HD23	1:B:303:LEU:N	2.19	0.57
1:B:110:ILE:HD13	1:B:139:GLU:CB	2.33	0.56
1:B:246:VAL:O	1:B:249:VAL:HB	2.05	0.56
1:A:280:ARG:NH1	1:B:162:THR:HA	2.20	0.56
1:B:74:LYS:HB3	1:B:76:MET:HB2	1.87	0.56
1:B:296:ASP:O	1:B:297:PHE:C	2.48	0.56
1:B:4:LYS:HE3	1:B:29:GLU:OE1	2.06	0.56
1:B:213:ASN:HA	1:B:216:ARG:NH1	2.20	0.56
1:B:4:LYS:HD3	1:B:31:LEU:HD21	1.88	0.56
1:A:73:ARG:NE	1:A:174:GLU:OE2	2.37	0.56
1:B:34:THR:HG22	1:B:105:ALA:CB	2.36	0.56
1:B:214:PRO:O	1:B:215:ALA:C	2.49	0.56
1:B:12:GLY:O	1:B:13:LEU:C	2.48	0.55
1:B:227:LYS:O	1:B:228:ILE:C	2.47	0.55
1:A:35:THR:HG23	1:A:42:LEU:HD12	1.87	0.55
1:A:35:THR:CG2	1:A:65:ALA:HA	2.26	0.55
1:A:199:ALA:HB1	1:A:204:LEU:HD21	1.89	0.55
1:B:226:THR:CG2	1:B:230:GLN:NE2	2.12	0.55
1:A:206:ARG:CZ	1:A:206:ARG:HB3	2.32	0.54
1:A:47:ARG:HA	1:A:50:GLN:NE2	2.22	0.54
1:B:124:VAL:HG12	1:B:124:VAL:O	2.06	0.54
1:B:50:GLN:OE1	1:B:100:VAL:HG23	2.07	0.54
1:B:108:LEU:HD12	1:B:108:LEU:O	2.07	0.54
1:A:283:ARG:HH11	1:A:283:ARG:CG	2.19	0.54
1:B:269:LYS:HE3	1:B:270:LEU:CG	2.31	0.54
1:B:281:ASN:C	1:B:282:PRO:C	2.76	0.54
1:A:233:ARG:HD2	1:A:234:TYR:N	2.23	0.53
1:B:14:ASP:O	1:B:15:ASP:C	2.50	0.53
1:A:3:LYS:HB2	1:A:27:GLU:O	2.08	0.53
1:A:251:ASP:O	1:A:252:PRO:C	2.52	0.53
1:B:30:LEU:O	1:B:31:LEU:C	2.51	0.53
1:B:168:ASN:O	1:B:171:ILE:HG22	2.08	0.53
1:A:74:LYS:HD3	1:A:76:MET:HE2	1.90	0.53
1:B:216:ARG:HG3	1:B:216:ARG:NH1	2.23	0.53
1:A:185:GLN:NE2	1:A:259:ARG:HH22	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:THR:HB	1:B:172:ASP:OD2	2.09	0.53
1:B:303:LEU:HD23	1:B:303:LEU:H	1.74	0.53
1:B:229:TYR:O	1:B:231:SER:N	2.41	0.53
1:B:201:PRO:CB	1:B:202:PRO:HD3	2.39	0.52
1:A:35:THR:HG23	1:A:42:LEU:HD11	1.91	0.52
1:A:230:GLN:CG	1:A:235:MET:HB3	2.38	0.52
1:B:215:ALA:O	1:B:218:MET:HB3	2.08	0.52
1:B:28:ILE:HD13	1:B:250:ILE:HG12	1.90	0.52
1:B:223:ASP:O	1:B:226:THR:N	2.42	0.52
1:A:160:ASN:OD1	1:A:161:ALA:N	2.42	0.52
1:A:314:PRO:O	1:A:315:GLN:CB	2.57	0.52
1:B:214:PRO:HB2	1:B:311:ILE:HD11	1.91	0.52
1:A:263:ASP:HB3	1:B:270:LEU:HD11	1.91	0.52
1:A:23:HIS:CD2	1:A:311:ILE:HD12	2.45	0.52
1:A:139:GLU:HG3	1:A:142:ILE:HG23	1.92	0.52
1:B:51:LEU:HD12	1:B:51:LEU:C	2.35	0.52
1:B:251:ASP:O	1:B:254:VAL:HG12	2.10	0.51
1:B:278:ASP:OD1	1:B:280:ARG:HB2	2.11	0.51
1:B:51:LEU:HD12	1:B:55:ILE:CD1	2.40	0.51
1:B:113:VAL:HG11	1:B:142:ILE:HB	1.93	0.51
1:B:223:ASP:C	1:B:226:THR:HB	2.34	0.51
1:B:74:LYS:HE3	1:B:76:MET:SD	2.51	0.51
1:A:240:VAL:HG23	1:A:240:VAL:O	2.10	0.51
1:B:35:THR:CG2	1:B:42:LEU:HD11	2.41	0.51
1:A:185:GLN:HE22	1:A:259:ARG:NH2	2.09	0.51
1:B:191:LEU:HA	1:B:194:THR:OG1	2.10	0.51
1:A:198:LEU:N	1:A:198:LEU:HD23	2.26	0.51
1:A:283:ARG:HG3	1:A:283:ARG:HH11	1.74	0.51
1:B:200:THR:CB	1:B:201:PRO:HD2	2.34	0.51
1:A:152:MET:HG3	1:A:242:ASP:HA	1.92	0.50
1:B:294:LYS:HB2	1:B:294:LYS:HZ1	1.75	0.50
1:B:14:ASP:HB2	1:B:242:ASP:CG	2.37	0.50
1:B:39:ASN:ND2	1:B:39:ASN:H	2.09	0.50
1:B:222:MET:O	1:B:226:THR:N	2.45	0.50
1:A:281:ASN:CB	1:A:282:PRO:HD3	2.40	0.50
1:B:131:ASN:N	3:B:959:HOH:O	2.25	0.50
1:A:109:ILE:O	1:A:113:VAL:HG23	2.11	0.50
1:A:75:ILE:CD1	1:A:75:ILE:N	2.70	0.50
1:A:206:ARG:HE	1:A:206:ARG:HA	1.75	0.50
1:B:55:ILE:HD13	1:B:55:ILE:H	1.74	0.50
1:B:119:LYS:HE3	1:B:144:ASP:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:CA	1:B:222:MET:HB2	2.40	0.50
1:B:206:ARG:CZ	1:B:206:ARG:HB3	2.40	0.49
1:B:226:THR:O	1:B:230:GLN:CD	2.54	0.49
1:A:152:MET:HE2	1:A:189:VAL:O	2.12	0.49
1:A:33:ILE:O	1:A:63:ILE:HA	2.13	0.49
1:B:230:GLN:O	1:B:233:ARG:O	2.29	0.49
1:B:283:ARG:N	1:B:283:ARG:C	2.64	0.49
1:B:300:PHE:O	1:B:303:LEU:HB2	2.12	0.49
1:A:257:THR:HA	1:A:291:VAL:O	2.12	0.49
1:B:28:ILE:CD1	1:B:250:ILE:HG12	2.43	0.49
1:B:100:VAL:O	1:B:101:ASP:C	2.55	0.49
1:A:139:GLU:HG3	1:A:139:GLU:O	2.13	0.49
1:B:34:THR:HG22	1:B:105:ALA:HB1	1.94	0.49
1:B:314:PRO:O	1:B:315:GLN:OXT	2.30	0.49
1:A:75:ILE:HD13	1:A:76:MET:N	2.23	0.48
1:A:97:LYS:O	1:A:99:LYS:HE2	2.12	0.48
1:B:298:GLU:OE1	1:B:298:GLU:HA	2.12	0.48
1:B:301:TRP:O	1:B:302:GLY:C	2.55	0.48
1:A:3:LYS:HE2	1:A:249:VAL:O	2.14	0.48
1:B:108:LEU:HD11	1:B:112:LEU:HD21	1.95	0.48
1:A:212:THR:HB	1:A:214:PRO:HD2	1.95	0.48
1:B:35:THR:HG22	1:B:42:LEU:HD11	1.95	0.48
1:B:196:GLN:NE2	1:B:293:VAL:O	2.46	0.48
1:A:35:THR:CG2	1:A:42:LEU:HD11	2.44	0.48
1:A:233:ARG:HA	1:A:233:ARG:HD3	1.57	0.48
1:B:219:LEU:C	1:B:222:MET:H	2.22	0.48
1:B:138:LEU:HA	1:B:138:LEU:HD23	1.32	0.48
1:B:46:THR:O	1:B:47:ARG:C	2.54	0.48
1:B:50:GLN:O	1:B:51:LEU:C	2.56	0.48
1:B:51:LEU:O	1:B:54:ASP:HB2	2.14	0.48
1:B:121:ILE:HG22	1:B:122:THR:H	1.78	0.47
1:A:181:ASN:ND2	3:A:923:HOH:O	2.46	0.47
1:A:200:THR:HB	1:A:201:PRO:HD2	1.95	0.47
1:A:227:LYS:O	1:A:228:ILE:C	2.57	0.47
1:B:11:PRO:CG	1:B:49:ALA:HB2	2.44	0.47
1:B:213:ASN:N	1:B:214:PRO:CD	2.77	0.47
1:B:246:VAL:O	1:B:247:ALA:C	2.57	0.47
1:A:201:PRO:HB2	1:A:202:PRO:CD	2.44	0.47
1:B:35:THR:HG23	1:B:42:LEU:HD12	1.96	0.47
1:B:305:LEU:O	1:B:309:GLU:HG3	2.15	0.47
1:B:311:ILE:HG13	1:B:312:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:HB2	3:A:911:HOH:O	2.13	0.47
1:B:4:LYS:HA	1:B:29:GLU:O	2.14	0.47
1:B:104:HIS:O	1:B:105:ALA:C	2.55	0.47
1:B:31:LEU:HD23	1:B:31:LEU:H	1.79	0.47
1:B:107:ASN:O	1:B:108:LEU:C	2.57	0.47
1:B:51:LEU:HD12	1:B:55:ILE:HG12	1.97	0.47
1:B:143:VAL:HA	1:B:184:TRP:CE3	2.50	0.47
1:B:283:ARG:N	1:B:283:ARG:CB	2.65	0.47
1:A:280:ARG:NH1	1:B:162:THR:CA	2.78	0.47
1:B:166:GLU:CD	1:B:168:ASN:H	2.22	0.47
1:A:9:CYS:HB2	1:A:15:ASP:OD2	2.15	0.47
1:B:35:THR:HG23	1:B:42:LEU:CD1	2.44	0.47
1:A:233:ARG:HD2	1:A:234:TYR:H	1.80	0.46
1:B:226:THR:HG22	1:B:227:LYS:HD3	1.96	0.46
1:A:201:PRO:HB2	1:A:202:PRO:HD3	1.97	0.46
1:B:16:ALA:O	1:B:19:ILE:HB	2.15	0.46
1:B:219:LEU:C	1:B:222:MET:HB2	2.40	0.46
1:A:88:GLY:HA2	1:A:224:TYR:CE2	2.51	0.46
1:B:182:GLU:OE1	1:B:182:GLU:HA	2.11	0.46
1:B:210:VAL:CG1	1:B:215:ALA:HB2	2.46	0.46
1:A:70:PRO:HG2	1:A:73:ARG:O	2.15	0.46
1:B:8:ASP:HB3	1:B:125:PRO:HA	1.97	0.46
1:B:182:GLU:HB2	1:B:184:TRP:NE1	2.31	0.46
1:B:214:PRO:HG2	1:B:311:ILE:HD11	1.96	0.46
1:B:216:ARG:O	1:B:217:PHE:C	2.59	0.46
1:B:269:LYS:CE	1:B:270:LEU:HG	2.35	0.46
1:B:76:MET:HG3	1:B:76:MET:O	2.16	0.45
1:B:269:LYS:HE2	1:B:269:LYS:HB3	1.71	0.45
1:B:2:ALA:C	1:B:27:GLU:O	2.58	0.45
1:A:262:VAL:HA	1:A:276:VAL:O	2.16	0.45
1:B:225:TYR:HA	1:B:228:ILE:HD12	1.99	0.45
1:B:302:GLY:O	1:B:305:LEU:N	2.49	0.45
1:A:25:ASN:CG	1:A:250:ILE:HD13	2.41	0.45
1:A:201:PRO:HD2	1:A:202:PRO:HD2	1.98	0.45
1:A:294:LYS:HB2	1:A:294:LYS:HE3	1.46	0.45
1:B:210:VAL:HG11	1:B:215:ALA:HB2	1.98	0.45
1:B:219:LEU:N	1:B:220:GLU:H	2.15	0.45
1:A:233:ARG:CD	1:A:234:TYR:N	2.79	0.45
1:A:281:ASN:ND2	1:B:232:ASN:ND2	2.65	0.45
1:A:213:ASN:N	1:A:214:PRO:CD	2.80	0.45
1:B:147:LYS:CB	1:B:147:LYS:NZ	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:O	1:A:223:ASP:HB2	2.17	0.45
1:B:200:THR:O	1:B:203:ILE:N	2.50	0.45
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.80	0.45
1:B:15:ASP:O	1:B:16:ALA:C	2.59	0.44
1:B:41:THR:O	1:B:42:LEU:C	2.59	0.44
1:B:313:ASP:HA	1:B:314:PRO:HD2	1.80	0.44
1:B:74:LYS:O	1:B:75:ILE:C	2.61	0.44
1:B:108:LEU:HD12	1:B:108:LEU:C	2.43	0.44
1:B:242:ASP:N	1:B:243:PRO:CD	2.80	0.44
1:A:230:GLN:CD	1:A:235:MET:HB3	2.42	0.44
1:B:100:VAL:C	1:B:101:ASP:O	2.57	0.44
1:B:303:LEU:O	1:B:304:VAL:C	2.58	0.44
1:A:201:PRO:CD	1:A:202:PRO:HD2	2.47	0.44
1:B:201:PRO:HA	1:B:204:LEU:HD12	1.99	0.44
1:B:282:PRO:C	1:B:282:PRO:N	2.64	0.44
1:A:10:ASP:HA	1:A:45:VAL:HG11	2.00	0.44
1:A:255:MET:HA	1:A:294:LYS:O	2.18	0.44
1:B:123:LEU:HD13	1:B:132:ILE:HD12	2.00	0.44
1:B:226:THR:O	1:B:230:GLN:NE2	2.51	0.44
1:A:111:ASP:O	1:A:112:LEU:C	2.61	0.44
1:B:222:MET:O	1:B:226:THR:CB	2.66	0.44
1:A:212:THR:O	1:A:216:ARG:HG2	2.18	0.43
1:B:219:LEU:HD23	1:B:222:MET:HG3	1.98	0.43
1:B:232:ASN:ND2	1:B:233:ARG:HB2	2.33	0.43
1:A:229:TYR:C	1:A:231:SER:N	2.75	0.43
1:B:281:ASN:C	1:B:281:ASN:HD22	2.24	0.43
1:A:213:ASN:HB2	1:A:313:ASP:OD1	2.18	0.43
1:B:123:LEU:HD23	1:B:123:LEU:HA	1.83	0.43
1:A:51:LEU:O	1:A:55:ILE:HD12	2.19	0.43
1:A:200:THR:HB	1:A:201:PRO:CD	2.48	0.43
1:A:251:ASP:HA	1:A:252:PRO:HD3	1.45	0.43
1:B:66:GLY:CA	1:B:105:ALA:HB3	2.48	0.43
1:B:160:ASN:CG	1:B:167:PHE:CD1	2.96	0.43
1:B:54:ASP:O	1:B:57:GLY:N	2.42	0.43
1:B:100:VAL:O	1:B:101:ASP:O	2.37	0.43
1:B:51:LEU:HD12	1:B:55:ILE:CG1	2.48	0.43
1:B:206:ARG:HA	1:B:209:GLU:HG3	2.01	0.43
1:B:226:THR:HG23	1:B:230:GLN:HE22	0.38	0.43
1:B:235:MET:SD	1:B:237:ALA:O	2.77	0.43
1:A:201:PRO:N	1:A:202:PRO:HD2	2.33	0.43
1:A:246:VAL:O	1:A:250:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ASN:CB	1:A:282:PRO:CD	2.94	0.42
1:B:17:VAL:O	1:B:18:ALA:C	2.62	0.42
1:B:116:HIS:O	1:B:145:ARG:NH1	2.52	0.42
1:B:259:ARG:HH12	1:B:290:GLN:NE2	2.17	0.42
1:B:97:LYS:HB3	1:B:97:LYS:HE2	1.53	0.42
1:B:185:GLN:HE22	1:B:259:ARG:HH22	0.69	0.42
1:B:6:ILE:HG13	1:B:121:ILE:HG21	2.01	0.42
1:B:193:LEU:HG	1:B:292:ALA:HB1	2.02	0.42
1:B:231:SER:O	1:B:232:ASN:C	2.63	0.42
1:A:280:ARG:HH12	1:B:162:THR:HA	1.84	0.42
1:B:160:ASN:OD1	1:B:166:GLU:HA	2.18	0.42
1:B:184:TRP:O	1:B:288:HIS:ND1	2.48	0.42
1:B:259:ARG:NH1	1:B:290:GLN:NE2	2.66	0.42
1:A:137:ARG:NH1	1:A:178:ILE:HG12	2.35	0.42
1:B:71:LEU:HD12	1:B:71:LEU:HA	1.84	0.42
1:A:269:LYS:HG2	1:A:270:LEU:CD2	2.48	0.42
1:A:154:GLY:HA3	1:A:275:THR:HG21	2.01	0.42
1:A:195:HIS:CD2	1:A:195:HIS:C	2.97	0.42
1:B:280:ARG:HB2	1:B:280:ARG:HE	1.73	0.42
1:A:71:LEU:HD12	1:A:71:LEU:HA	1.65	0.42
1:A:104:HIS:O	1:A:105:ALA:C	2.61	0.42
1:A:228:ILE:H	1:A:228:ILE:CD1	2.33	0.42
1:B:37:VAL:O	1:B:37:VAL:HG13	2.20	0.42
1:B:214:PRO:CB	1:B:311:ILE:HD11	2.50	0.41
1:B:11:PRO:HG2	1:B:45:VAL:O	2.20	0.41
1:B:205:GLN:O	1:B:208:LYS:N	2.53	0.41
1:B:214:PRO:CB	1:B:311:ILE:CD1	2.99	0.41
1:B:233:ARG:HA	1:B:233:ARG:HD2	1.25	0.41
1:A:303:LEU:HD23	1:A:303:LEU:HA	1.81	0.41
1:A:314:PRO:O	1:A:315:GLN:HB2	2.21	0.41
1:B:34:THR:HG21	1:B:105:ALA:HB1	2.00	0.41
1:A:168:ASN:O	1:A:171:ILE:HG22	2.21	0.41
1:A:216:ARG:NH1	1:A:216:ARG:HG3	2.36	0.41
1:A:281:ASN:HD21	1:B:232:ASN:ND2	2.18	0.41
1:A:218:MET:O	1:A:221:ILE:CG1	2.68	0.41
1:B:171:ILE:HG23	1:B:172:ASP:N	2.35	0.41
1:B:294:LYS:HB2	1:B:294:LYS:HZ2	1.79	0.41
1:A:76:MET:C	1:A:77:THR:OG1	2.64	0.40
1:B:216:ARG:HG2	1:B:216:ARG:H	1.58	0.40
1:B:11:PRO:HG3	1:B:49:ALA:HB2	2.02	0.40
1:B:203:ILE:C	1:B:205:GLN:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:HA	1:B:219:LEU:HD23	1.84	0.40
1:B:298:GLU:O	1:B:299:LYS:C	2.65	0.40
1:B:218:MET:O	1:B:219:LEU:C	2.64	0.40
1:A:76:MET:C	1:A:77:THR:HG1	2.29	0.40
1:A:160:ASN:OD1	1:A:166:GLU:HA	2.21	0.40
1:B:11:PRO:HG2	1:B:49:ALA:HB2	2.03	0.40
1:B:198:LEU:HD22	1:B:237:ALA:HB3	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	304/314 (97%)	283 (93%)	17 (6%)	4 (1%)	9	18
1	B	291/314 (93%)	235 (81%)	46 (16%)	10 (3%)	3	4
All	All	595/628 (95%)	518 (87%)	63 (11%)	14 (2%)	4	8

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ASN
1	B	3	LYS
1	B	228	ILE
1	B	197	ALA
1	B	230	GLN
1	A	253	SER
1	B	11	PRO
1	B	194	THR
1	B	314	PRO
1	A	230	GLN
1	B	13	LEU

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Mol	Chain	Res	Type
1	B	101	ASP
1	A	11	PRO
1	B	201	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	256/259 (99%)	209 (82%)	47 (18%)	1	3
1	B	247/259 (95%)	179 (72%)	68 (28%)	0	1
All	All	503/518 (97%)	388 (77%)	115 (23%)	1	1

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	13	LEU
1	A	27	GLU
1	A	28	ILE
1	A	30	LEU
1	A	35	THR
1	A	45	VAL
1	A	55	ILE
1	A	71	LEU
1	A	74	LYS
1	A	75	ILE
1	A	76	MET
1	A	77	THR
1	A	84	GLU
1	A	85	SER
1	A	95	GLU
1	A	99	LYS
1	A	101	ASP
1	A	103	ARG
1	A	119	LYS

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Mol	Chain	Res	Type
1	A	130	THR
1	A	138	LEU
1	A	141	ARG
1	A	142	ILE
1	A	143	VAL
1	A	144	ASP
1	A	147	LYS
1	A	152	MET
1	A	163	SER
1	A	170	ILE
1	A	182	GLU
1	A	184	TRP
1	A	206	ARG
1	A	211	ASP
1	A	216	ARG
1	A	227	LYS
1	A	231	SER
1	A	233	ARG
1	A	235	MET
1	A	242	ASP
1	A	258	GLU
1	A	269	LYS
1	A	280	ARG
1	A	283	ARG
1	A	285	GLU
1	A	294	LYS
1	A	313	ASP
1	B	3	LYS
1	B	7	LEU
1	B	27	GLU
1	B	28	ILE
1	B	30	LEU
1	B	31	LEU
1	B	33	ILE
1	B	34	THR
1	B	35	THR
1	B	39	ASN
1	B	41	THR
1	B	44	LYS
1	B	45	VAL
1	B	51	LEU
1	B	55	ILE

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Mol	Chain	Res	Type
1	B	58	ILE
1	B	69	LYS
1	B	71	LEU
1	B	74	LYS
1	B	75	ILE
1	B	76	MET
1	B	77	THR
1	B	97	LYS
1	B	99	LYS
1	B	101	ASP
1	B	103	ARG
1	B	109	ILE
1	B	110	ILE
1	B	112	LEU
1	B	114	MET
1	B	117	GLU
1	B	121	ILE
1	B	130	THR
1	B	137	ARG
1	B	138	LEU
1	B	143	VAL
1	B	144	ASP
1	B	147	LYS
1	B	152	MET
1	B	163	SER
1	B	183	SER
1	B	184	TRP
1	B	206	ARG
1	B	209	GLU
1	B	210	VAL
1	B	211	ASP
1	B	213	ASN
1	B	216	ARG
1	B	218	MET
1	B	221	ILE
1	B	222	MET
1	B	226	THR
1	B	227	LYS
1	B	229	TYR
1	B	232	ASN
1	B	233	ARG
1	B	235	MET

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Mol	Chain	Res	Type
1	B	255	MET
1	B	258	GLU
1	B	260	VAL
1	B	269	LYS
1	B	280	ARG
1	B	281	ASN
1	B	285	GLU
1	B	294	LYS
1	B	303	LEU
1	B	313	ASP
1	B	315	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	50	GLN
1	A	157	HIS
1	A	181	ASN
1	A	185	GLN
1	A	195	HIS
1	A	230	GLN
1	B	25	ASN
1	B	39	ASN
1	B	157	HIS
1	B	185	GLN
1	B	213	ASN
1	B	230	GLN
1	B	232	ASN
1	B	290	GLN

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](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	281:ASN	C	282:PRO	N	1.17

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.