



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:09 AM UTC

PDB ID : 1DBQ / pdb_00001dbq
Title : DNA-BINDING REGULATORY PROTEIN
Authors : Schumacher, M.A.; Choi, K.Y.; Lu, F.; Zalkin, H.; Brennan, R.G.
Deposited on : 1996-02-13
Resolution : 2.20 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

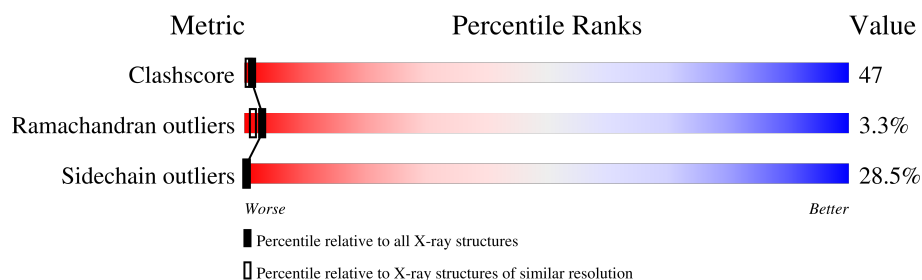
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	289	36% 37% 18% • •
1	B	289	31% 38% 21% 5% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4591 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 PURINE REPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2172	1372	378	403	19			
1	B	276	Total	C	N	O	S	0	0	0
			2172	1372	378	403	19			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is water.

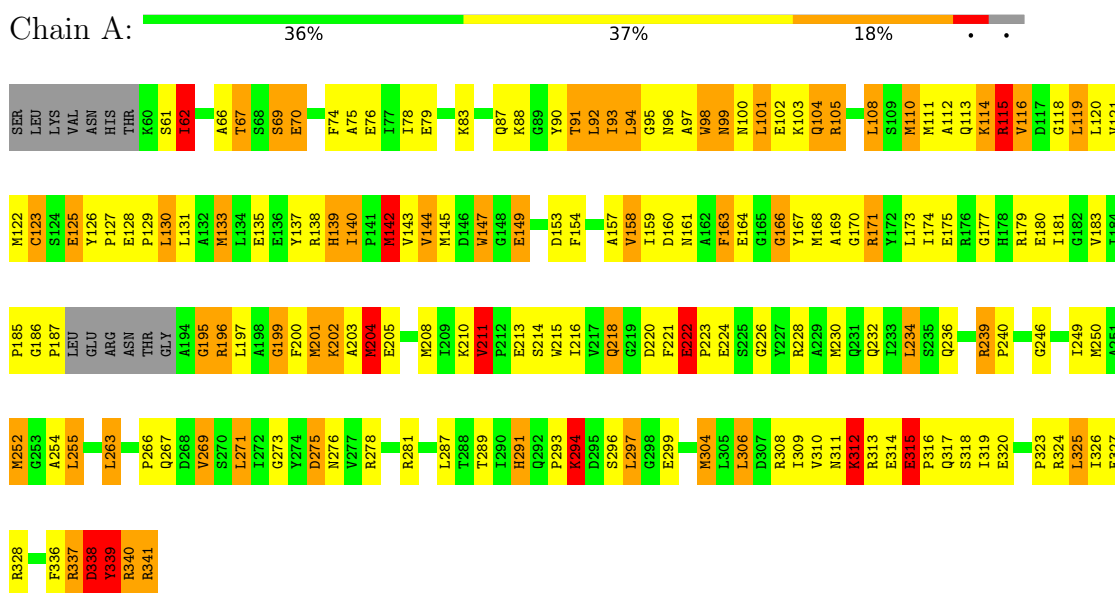
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	102	Total	O	0	0
			102	102		

3 Residue-property plots

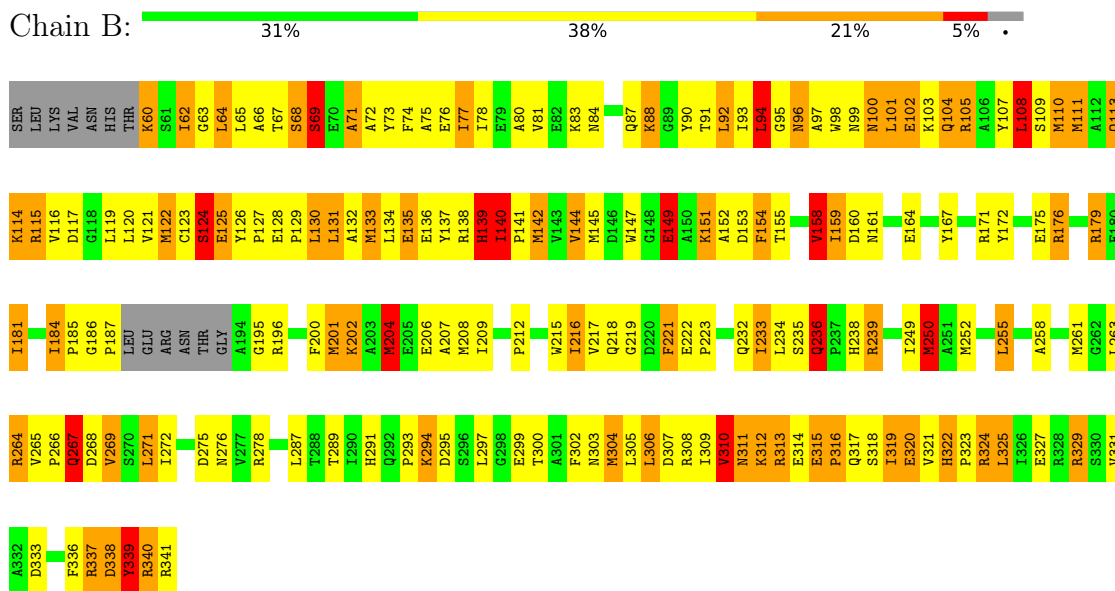
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: PURINE REPRESSOR



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	38.04Å 125.26Å 61.29Å 90.00° 100.17° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.156 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4591	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.42	12/2217 (0.5%)	1.67	48/2991 (1.6%)
1	B	1.30	7/2217 (0.3%)	1.61	41/2991 (1.4%)
All	All	1.36	19/4434 (0.4%)	1.64	89/5982 (1.5%)

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	1	0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	GLN	CA-C	-6.72	1.44	1.52
1	A	304	MET	SD-CE	-6.61	1.63	1.79
1	A	338	ASP	CA-C	-6.43	1.44	1.52
1	A	226	GLY	CA-C	6.28	1.59	1.51
1	B	111	MET	SD-CE	6.08	1.94	1.79
1	B	122	MET	SD-CE	5.99	1.94	1.79
1	A	211	VAL	N-CA	-5.98	1.41	1.46
1	A	142	MET	SD-CE	-5.83	1.65	1.79
1	B	216	ILE	CA-C	5.60	1.59	1.52
1	B	196	ARG	C-O	-5.56	1.17	1.24
1	A	166	GLY	CA-C	5.52	1.58	1.51
1	A	234	LEU	C-O	-5.52	1.17	1.24
1	A	337	ARG	CA-C	-5.40	1.46	1.52
1	A	273	GLY	C-O	5.38	1.29	1.24
1	A	203	ALA	CA-C	5.18	1.59	1.52
1	B	233	ILE	N-CA	-5.18	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	HIS	C-O	-5.11	1.17	1.24
1	B	239	ARG	N-CA	-5.07	1.41	1.45
1	A	133	MET	SD-CE	5.04	1.92	1.79

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	ILE	N-CA-CB	10.02	121.68	111.36
1	A	339	TYR	N-CA-CB	9.95	124.61	110.88
1	B	184	ILE	N-CA-C	-9.76	98.48	108.15
1	A	112	ALA	N-CA-C	-9.75	100.73	111.36
1	A	147	TRP	N-CA-C	-9.47	96.86	110.59
1	B	287	LEU	N-CA-C	9.17	123.28	109.25
1	B	160	ASP	N-CA-C	-9.16	95.43	110.17
1	A	339	TYR	CA-CB-CG	9.15	130.37	113.90
1	B	338	ASP	N-CA-CB	8.74	126.83	110.56
1	B	69	SER	N-CA-C	-8.52	101.95	111.07
1	A	144	VAL	CB-CA-C	8.45	121.54	111.32
1	B	181	ILE	N-CA-C	8.28	120.53	108.53
1	A	123	CYS	N-CA-C	8.01	124.95	113.02
1	B	337	ARG	N-CA-C	-7.72	103.76	113.02
1	B	338	ASP	CA-C-N	7.70	136.25	121.54
1	B	338	ASP	C-N-CA	7.70	136.25	121.54
1	B	142	MET	N-CA-C	7.67	118.37	108.24
1	A	287	LEU	N-CA-C	7.63	121.41	109.96
1	B	204	MET	N-CA-C	-7.58	102.96	111.07
1	B	267	GLN	N-CA-C	7.56	120.48	111.33
1	B	329	ARG	N-CA-C	7.32	121.92	112.41
1	A	338	ASP	N-CA-C	7.07	125.85	110.80
1	A	160	ASP	N-CA-C	-7.06	98.18	109.76
1	B	144	VAL	N-CA-CB	6.95	120.43	111.67
1	A	98	TRP	N-CA-C	6.88	125.44	110.80
1	A	147	TRP	CA-C-N	-6.87	107.06	122.04
1	A	147	TRP	C-N-CA	-6.87	107.06	122.04
1	B	195	GLY	N-CA-C	-6.75	97.18	113.18
1	A	338	ASP	N-CA-CB	6.75	121.90	110.49
1	B	236	GLN	O-C-N	6.64	126.50	121.85
1	B	304	MET	N-CA-C	-6.64	104.05	111.28
1	A	160	ASP	CA-C-N	-6.62	112.86	122.06
1	A	160	ASP	C-N-CA	-6.62	112.86	122.06
1	B	94	LEU	N-CA-C	6.62	119.37	109.25
1	B	204	MET	CG-SD-CE	-6.61	86.35	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	GLN	N-CA-C	6.56	120.23	110.52
1	A	196	ARG	N-CA-C	-6.43	103.78	111.69
1	A	183	VAL	N-CA-C	6.41	117.94	108.45
1	B	124	SER	N-CA-C	-6.41	104.22	111.07
1	A	139	HIS	N-CA-C	-6.28	105.10	112.89
1	B	108	LEU	N-CA-C	6.24	117.87	111.14
1	A	158	VAL	N-CA-CB	6.06	119.10	111.46
1	B	140	ILE	CB-CA-C	6.03	117.16	110.71
1	B	186	GLY	C-N-CD	-6.02	100.32	125.00
1	A	186	GLY	N-CA-C	-6.01	104.96	112.23
1	A	199	GLY	N-CA-C	-6.01	107.21	114.66
1	A	94	LEU	N-CA-C	5.99	119.40	109.46
1	B	184	ILE	CA-C-O	5.92	124.91	120.88
1	B	172	TYR	N-CA-C	-5.87	104.97	111.36
1	B	338	ASP	O-C-N	5.84	129.84	122.84
1	B	63	GLY	N-CA-C	-5.84	104.77	112.82
1	A	195	GLY	N-CA-C	-5.82	99.39	113.18
1	B	250	MET	N-CA-C	-5.77	105.08	111.36
1	A	67	THR	N-CA-C	-5.74	104.93	111.07
1	B	278	ARG	N-CA-C	5.73	118.27	111.33
1	A	115	ARG	N-CA-C	5.73	119.29	111.39
1	A	294	LYS	N-CA-C	-5.71	106.36	113.55
1	A	222	GLU	CA-C-N	5.70	125.17	119.24
1	A	222	GLU	C-N-CA	5.70	125.17	119.24
1	A	252	MET	N-CA-C	-5.70	105.07	111.28
1	B	71	ALA	N-CA-C	-5.67	97.96	107.32
1	A	315	GLU	CA-C-O	5.65	124.00	119.59
1	B	339	TYR	N-CA-CB	5.65	120.05	110.49
1	A	137	TYR	N-CA-C	5.58	119.18	112.93
1	A	336	PHE	CA-C-N	-5.57	115.02	122.42
1	A	336	PHE	C-N-CA	-5.57	115.02	122.42
1	A	163	PHE	N-CA-C	-5.54	105.24	111.28
1	B	91	THR	N-CA-C	-5.48	100.77	109.59
1	B	158	VAL	CA-C-N	-5.41	115.75	123.11
1	B	158	VAL	C-N-CA	-5.41	115.75	123.11
1	B	316	PRO	N-CA-C	5.40	119.05	111.33
1	B	339	TYR	CB-CA-C	5.39	121.15	110.42
1	B	258	ALA	N-CA-C	-5.33	104.52	111.02
1	A	293	PRO	N-CA-C	5.24	118.72	110.50
1	A	304	MET	N-CA-C	-5.23	105.66	111.36
1	B	139	HIS	CA-C-N	-5.18	118.86	122.59
1	B	139	HIS	C-N-CA	-5.18	118.86	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	VAL	N-CA-C	-5.17	98.55	107.24
1	A	291	HIS	CB-CA-C	-5.16	102.82	110.67
1	A	157	ALA	CA-C-N	-5.15	116.43	123.12
1	A	157	ALA	C-N-CA	-5.15	116.43	123.12
1	A	104	GLN	N-CA-C	-5.14	105.86	111.82
1	A	142	MET	N-CA-C	5.12	116.97	109.24
1	A	204	MET	CG-SD-CE	5.11	112.14	100.90
1	A	297	LEU	CA-C-N	5.08	125.58	119.94
1	A	297	LEU	C-N-CA	5.08	125.58	119.94
1	A	62	ILE	CB-CA-C	5.08	118.18	110.62
1	B	331	VAL	N-CA-C	5.06	115.19	108.11
1	A	239	ARG	N-CA-C	5.05	117.82	109.58

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	338	ASP	CA

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	2172	0	2142	167	0
1	B	2172	0	2142	241	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	142	0	0	6	0
3	B	102	0	0	9	0
All	All	4591	0	4284	405	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 47.

All (405) 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:77:ILE:HD12	1:B:294:LYS:HE3	1.26	1.11
1:A:110:MET:HE3	1:A:111:MET:HA	1.33	1.06
1:B:140:ILE:HD12	1:B:141:PRO:HD2	1.40	1.03
1:A:159:ILE:HB	1:A:320:GLU:HG2	1.38	1.01
1:B:76:GLU:HB2	1:B:294:LYS:HZ3	1.21	1.01
1:B:105:ARG:HB2	1:B:105:ARG:HH11	1.25	1.01
1:A:61:SER:HA	1:A:91:THR:HG22	1.44	0.99
1:B:115:ARG:HH11	1:B:115:ARG:HB3	1.26	0.99
1:B:92:LEU:HD13	1:B:94:LEU:HD22	1.43	0.99
1:B:234:LEU:HB3	1:B:261:MET:HE1	1.47	0.96
1:A:161:ASN:HB3	1:A:164:GLU:HG2	1.50	0.94
1:A:252:MET:HE1	1:B:252:MET:HE2	1.50	0.94
1:B:101:LEU:HD13	1:B:105:ARG:HH12	1.31	0.93
1:A:102:GLU:HG3	1:A:105:ARG:NH2	1.83	0.93
1:B:161:ASN:HB3	1:B:164:GLU:HG2	1.48	0.92
1:B:76:GLU:HB2	1:B:294:LYS:NZ	1.85	0.91
1:B:325:LEU:HD11	1:B:327:GLU:HG3	1.51	0.90
1:A:62:ILE:HG22	1:A:92:LEU:CD2	2.02	0.89
1:B:147:TRP:HA	1:B:158:VAL:HG13	1.55	0.89
1:A:135:GLU:HA	1:A:138:ARG:HD2	1.55	0.88
1:B:115:ARG:HB3	1:B:115:ARG:NH1	1.87	0.88
1:B:271:LEU:HD12	1:B:272:ILE:N	1.90	0.86
1:B:234:LEU:CB	1:B:261:MET:HE1	2.06	0.86
1:A:187:PRO:HD2	1:A:221:PHE:CE2	2.11	0.86
1:B:313:ARG:NH1	1:B:313:ARG:HB3	1.91	0.85
1:B:181:ILE:HD12	1:B:204:MET:HE1	1.60	0.84
1:A:110:MET:HE3	1:A:111:MET:CA	2.08	0.83
1:B:137:TYR:HA	1:B:139:HIS:NE2	1.94	0.82
1:B:100:ASN:O	1:B:104:GLN:HG3	1.78	0.82
1:B:77:ILE:HG22	1:B:122:MET:HE1	1.60	0.82
1:B:101:LEU:HD13	1:B:105:ARG:NH1	1.93	0.81
1:B:313:ARG:HB3	1:B:313:ARG:CZ	2.10	0.81
1:A:97:ALA:HB1	1:A:104:GLN:HG2	1.60	0.81
1:B:105:ARG:HA	1:B:133:MET:CE	2.11	0.81
1:B:123:CYS:HB2	1:B:126:TYR:CZ	2.17	0.80
1:B:67:THR:HG21	1:B:124:SER:OG	1.83	0.79
1:B:308:ARG:NH2	1:B:316:PRO:HA	1.98	0.78
1:A:110:MET:CE	1:A:114:LYS:HG3	2.13	0.78
1:B:147:TRP:CD2	1:B:158:VAL:HG11	2.19	0.78
1:B:140:ILE:HD12	1:B:141:PRO:CD	2.13	0.78
1:A:306:LEU:HD23	3:A:351:HOH:O	1.84	0.77
1:B:140:ILE:CD1	1:B:141:PRO:HD2	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:GLY:HA2	1:B:107:TYR:CE1	2.20	0.77
1:B:151:LYS:HD3	1:B:153:ASP:OD2	1.84	0.77
1:B:60:LYS:HD2	1:B:90:TYR:CE2	2.20	0.76
1:A:239:ARG:HB2	1:A:240:PRO:HD2	1.68	0.76
1:B:141:PRO:CG	1:B:309:ILE:HG22	2.16	0.76
1:B:105:ARG:HA	1:B:133:MET:HE3	1.67	0.76
1:B:141:PRO:HG2	1:B:309:ILE:HG22	1.66	0.75
1:A:62:ILE:HG22	1:A:92:LEU:HD23	1.67	0.75
1:A:135:GLU:O	1:A:138:ARG:HG3	1.86	0.75
1:B:100:ASN:OD1	1:B:102:GLU:HG2	1.84	0.75
1:B:161:ASN:CB	1:B:164:GLU:HG2	2.16	0.75
1:A:311:ASN:O	1:A:313:ARG:HG3	1.86	0.75
1:A:266:PRO:HA	1:A:269:VAL:O	1.87	0.75
1:A:101:LEU:HA	1:A:104:GLN:HE21	1.51	0.74
1:A:127:PRO:HB2	1:A:129:PRO:HD2	1.69	0.74
1:B:111:MET:O	1:B:116:VAL:HG22	1.88	0.74
1:B:304:MET:HE1	1:B:319:ILE:CD1	2.17	0.74
1:A:174:ILE:HD11	1:A:204:MET:CE	2.18	0.74
1:A:161:ASN:HB3	1:A:164:GLU:CG	2.16	0.73
1:B:307:ASP:OD1	1:B:311:ASN:HB2	1.89	0.73
1:B:159:ILE:HA	3:B:359:HOH:O	1.88	0.73
1:B:92:LEU:CD1	1:B:94:LEU:HD22	2.19	0.73
1:B:304:MET:HE1	1:B:319:ILE:HD12	1.70	0.72
1:B:139:HIS:H	1:B:139:HIS:CD2	2.05	0.72
1:A:102:GLU:HG3	1:A:105:ARG:HH21	1.51	0.72
1:A:291:HIS:HB2	1:A:326:ILE:HD11	1.73	0.71
1:B:76:GLU:HB3	1:B:295:ASP:OD1	1.90	0.71
1:A:101:LEU:HA	1:A:104:GLN:NE2	2.06	0.71
1:B:324:ARG:HB3	3:B:380:HOH:O	1.91	0.70
1:A:149:GLU:CD	1:A:149:GLU:H	1.98	0.70
1:A:185:PRO:HD2	1:A:218:GLN:HA	1.74	0.70
1:B:164:GLU:HG3	1:B:323:PRO:HG2	1.74	0.70
1:A:201:MET:N	1:A:201:MET:HE2	2.07	0.70
1:A:128:GLU:HB2	1:A:129:PRO:HD3	1.72	0.70
1:A:105:ARG:N	1:A:133:MET:HE1	2.07	0.69
1:B:105:ARG:HB2	1:B:105:ARG:NH1	2.04	0.69
1:B:147:TRP:CA	1:B:158:VAL:HG13	2.23	0.69
1:A:281:ARG:O	1:A:281:ARG:HD3	1.93	0.69
1:B:233:ILE:O	1:B:236:GLN:HG3	1.93	0.69
1:A:74:PHE:O	1:A:78:ILE:HD12	1.93	0.68
1:B:144:VAL:HG21	1:B:155:THR:HG22	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:VAL:HG22	1:B:269:VAL:HG23	1.74	0.68
1:A:62:ILE:HG22	1:A:92:LEU:HD21	1.74	0.68
1:A:100:ASN:O	1:A:104:GLN:HG3	1.93	0.68
1:B:144:VAL:CG2	1:B:155:THR:HA	2.24	0.68
1:B:147:TRP:NE1	1:B:158:VAL:HG21	2.08	0.67
1:B:310:VAL:HG22	1:B:311:ASN:N	2.10	0.67
1:B:125:GLU:HB3	1:B:127:PRO:HD3	1.75	0.67
1:B:77:ILE:HD12	1:B:294:LYS:CE	2.14	0.67
1:B:313:ARG:NH1	1:B:315:GLU:O	2.27	0.67
1:B:308:ARG:HH22	1:B:316:PRO:HA	1.60	0.67
1:B:200:PHE:HD2	1:B:201:MET:CE	2.06	0.66
1:A:214:SER:HB2	1:A:236:GLN:HE21	1.59	0.66
1:B:267:GLN:NE2	1:B:267:GLN:H	1.92	0.66
1:A:119:LEU:HD22	1:A:121:VAL:HG23	1.78	0.66
1:A:167:TYR:CE1	1:A:202:LYS:HE3	2.31	0.66
1:B:76:GLU:HB2	1:B:294:LYS:CE	2.26	0.66
1:B:126:TYR:O	1:B:131:LEU:HD22	1.96	0.65
1:B:105:ARG:HD3	1:B:133:MET:SD	2.36	0.65
1:A:74:PHE:HB3	1:A:78:ILE:CD1	2.27	0.65
1:A:324:ARG:NH1	3:A:422:HOH:O	2.29	0.65
1:B:60:LYS:HD2	1:B:90:TYR:HE2	1.59	0.65
1:A:135:GLU:HA	1:A:138:ARG:CD	2.26	0.65
1:A:105:ARG:HH11	1:A:105:ARG:CG	2.09	0.64
1:A:174:ILE:HD11	1:A:204:MET:HE3	1.79	0.64
1:A:164:GLU:O	1:A:168:MET:HG3	1.97	0.64
1:A:97:ALA:CB	1:A:104:GLN:HG2	2.27	0.64
1:A:74:PHE:HB3	1:A:78:ILE:HD11	1.80	0.64
1:B:339:TYR:HD1	1:B:340:ARG:HH11	1.46	0.63
1:B:149:GLU:CD	1:B:151:LYS:HG2	2.23	0.63
1:B:144:VAL:HG23	1:B:155:THR:HA	1.79	0.63
1:A:101:LEU:CA	1:A:104:GLN:HE21	2.11	0.63
1:A:105:ARG:O	1:A:105:ARG:HG2	1.98	0.62
1:A:149:GLU:N	1:A:149:GLU:OE1	2.30	0.62
1:A:75:ALA:O	1:A:79:GLU:HG3	2.00	0.62
1:A:159:ILE:HB	1:A:320:GLU:CG	2.23	0.62
1:B:159:ILE:N	1:B:159:ILE:HD12	2.14	0.62
1:B:139:HIS:ND1	1:B:140:ILE:HG22	2.15	0.61
1:A:115:ARG:NH1	1:A:115:ARG:HG3	2.16	0.61
1:B:107:TYR:O	1:B:111:MET:HG3	2.00	0.61
1:B:234:LEU:HD21	1:B:269:VAL:HG11	1.80	0.61
1:A:105:ARG:HH11	1:A:105:ARG:CB	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLU:OE2	1:B:151:LYS:HG2	2.01	0.61
1:B:159:ILE:O	1:B:320:GLU:HA	2.01	0.60
1:B:130:LEU:CD1	1:B:134:LEU:HD11	2.31	0.60
1:B:108:LEU:HD21	1:B:134:LEU:HD23	1.83	0.60
1:A:252:MET:HE1	1:B:252:MET:CE	2.30	0.60
1:B:127:PRO:HB2	1:B:129:PRO:HD2	1.82	0.60
1:A:276:ASN:OD1	1:A:328:ARG:NH2	2.34	0.60
1:A:304:MET:SD	1:A:319:ILE:HD11	2.41	0.60
1:B:200:PHE:HD2	1:B:201:MET:HE1	1.65	0.60
1:B:100:ASN:C	1:B:104:GLN:HE21	2.10	0.60
1:B:264:ARG:HB2	1:B:268:ASP:OD1	2.01	0.60
1:A:135:GLU:HG3	1:A:138:ARG:HD2	1.84	0.60
1:A:304:MET:O	1:A:308:ARG:HG3	2.02	0.59
1:A:337:ARG:O	1:A:338:ASP:HB2	2.01	0.59
1:B:110:MET:O	1:B:114:LYS:HG2	2.03	0.59
1:B:141:PRO:HG2	1:B:309:ILE:CG2	2.32	0.59
1:A:291:HIS:HB2	1:A:326:ILE:CD1	2.32	0.59
1:A:159:ILE:CB	1:A:320:GLU:HG2	2.23	0.59
1:A:339:TYR:O	1:A:340:ARG:HB3	2.03	0.59
1:B:271:LEU:HD12	1:B:271:LEU:C	2.28	0.58
1:B:304:MET:O	1:B:308:ARG:HB2	2.03	0.58
1:A:105:ARG:HH11	1:A:105:ARG:HG3	1.67	0.58
1:B:310:VAL:O	1:B:312:LYS:HG2	2.03	0.58
1:A:223:PRO:HD3	1:A:249:ILE:HG22	1.85	0.58
1:A:340:ARG:HG3	1:A:341:ARG:N	2.19	0.58
1:A:161:ASN:HB3	1:A:164:GLU:CD	2.28	0.58
1:B:202:LYS:O	1:B:206:GLU:HB3	2.03	0.58
1:A:223:PRO:HD3	1:A:249:ILE:CG2	2.35	0.57
1:B:185:PRO:HD2	1:B:217:VAL:O	2.03	0.57
1:B:130:LEU:HD13	1:B:134:LEU:CD1	2.35	0.57
1:A:66:ALA:O	1:A:96:ASN:HA	2.05	0.56
1:B:304:MET:SD	1:B:317:GLN:HB2	2.45	0.56
1:B:306:LEU:O	1:B:309:ILE:HG13	2.06	0.56
1:B:307:ASP:OD1	1:B:313:ARG:HG3	2.05	0.56
1:B:325:LEU:HD13	1:B:325:LEU:C	2.30	0.56
1:A:110:MET:SD	1:A:114:LYS:HE2	2.46	0.56
1:B:309:ILE:HD12	1:B:310:VAL:N	2.21	0.56
1:A:236:GLN:OE1	1:A:236:GLN:HA	2.04	0.56
1:B:339:TYR:O	1:B:340:ARG:HD2	2.05	0.56
1:B:73:TYR:O	1:B:294:LYS:NZ	2.39	0.55
1:A:105:ARG:CA	1:A:133:MET:HE1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ARG:HG3	1:A:197:LEU:N	2.21	0.55
1:A:90:TYR:HE2	1:A:306:LEU:HD11	1.70	0.55
1:A:115:ARG:HG3	1:A:115:ARG:HH11	1.71	0.55
1:B:76:GLU:HB2	1:B:294:LYS:HE2	1.87	0.55
1:B:306:LEU:O	1:B:310:VAL:HG12	2.06	0.55
1:B:161:ASN:HB2	1:B:323:PRO:HD2	1.88	0.55
1:B:100:ASN:C	1:B:104:GLN:HG3	2.31	0.55
1:B:140:ILE:HD12	1:B:140:ILE:C	2.32	0.55
1:A:196:ARG:NH1	1:A:246:GLY:O	2.40	0.54
1:A:337:ARG:O	1:A:337:ARG:HG3	2.07	0.54
1:A:170:GLY:HA2	1:A:200:PHE:CE1	2.43	0.54
1:A:201:MET:HE2	1:A:201:MET:CA	2.35	0.54
1:A:249:ILE:HB	3:A:439:HOH:O	2.07	0.54
1:A:97:ALA:HA	1:A:103:LYS:HD3	1.89	0.54
1:B:126:TYR:N	1:B:127:PRO:HD3	2.22	0.54
1:A:239:ARG:HB2	1:A:240:PRO:CD	2.37	0.53
1:B:202:LYS:HD3	3:B:394:HOH:O	2.08	0.53
1:A:115:ARG:HH11	1:A:115:ARG:CG	2.21	0.53
1:A:119:LEU:HD13	1:A:142:MET:HE3	1.89	0.53
1:B:119:LEU:HB2	1:B:142:MET:HB3	1.90	0.53
1:A:161:ASN:O	1:A:164:GLU:HG2	2.08	0.53
1:A:255:LEU:HD13	1:A:271:LEU:HD22	1.91	0.53
1:B:69:SER:HA	1:B:78:ILE:HD13	1.90	0.53
1:A:110:MET:CE	1:A:111:MET:HA	2.24	0.53
1:B:77:ILE:CG2	1:B:122:MET:HE1	2.37	0.53
1:B:101:LEU:CD1	1:B:105:ARG:HH12	2.12	0.53
1:A:111:MET:O	1:A:116:VAL:HG22	2.09	0.53
1:A:222:GLU:HB3	1:A:223:PRO:HD2	1.91	0.53
1:B:219:GLY:HA3	1:B:250:MET:SD	2.49	0.52
1:B:68:SER:HB3	1:B:71:ALA:HB2	1.89	0.52
1:B:77:ILE:O	1:B:80:ALA:HB3	2.09	0.52
1:B:187:PRO:HD2	1:B:221:PHE:CZ	2.44	0.52
1:A:326:ILE:HD12	1:A:326:ILE:N	2.24	0.52
1:B:119:LEU:CB	1:B:142:MET:HB3	2.40	0.52
1:B:123:CYS:HB2	1:B:126:TYR:CE2	2.45	0.52
1:B:87:GLN:NE2	3:B:370:HOH:O	2.36	0.52
1:B:87:GLN:HB3	1:B:88:LYS:HE3	1.91	0.52
1:B:300:THR:HG21	1:B:319:ILE:CG2	2.40	0.52
1:A:123:CYS:O	1:A:125:GLU:N	2.42	0.52
1:B:120:LEU:C	1:B:120:LEU:HD23	2.35	0.52
1:B:308:ARG:HG3	1:B:313:ARG:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:PHE:HA	1:A:195:GLY:O	2.10	0.51
1:A:281:ARG:HD3	1:A:281:ARG:C	2.35	0.51
1:A:70:GLU:OE1	1:A:70:GLU:HA	2.11	0.51
1:B:137:TYR:HA	1:B:139:HIS:HE2	1.72	0.51
1:A:98:TRP:O	1:A:99:ASN:HB2	2.11	0.51
1:A:313:ARG:NH1	1:A:313:ARG:HB2	2.26	0.51
1:B:73:TYR:CD2	1:B:74:PHE:CD1	2.99	0.51
1:A:110:MET:HE2	1:A:111:MET:HG2	1.93	0.50
1:A:110:MET:O	1:A:114:LYS:HG3	2.12	0.50
1:A:110:MET:SD	1:A:114:LYS:HG3	2.51	0.50
1:A:119:LEU:HD22	1:A:121:VAL:CG2	2.41	0.50
1:A:154:PHE:HA	1:A:316:PRO:HG3	1.93	0.50
1:A:118:GLY:HA2	1:A:140:ILE:CD1	2.41	0.50
1:B:121:VAL:HB	1:B:144:VAL:HG12	1.93	0.50
1:A:161:ASN:O	1:A:323:PRO:HG3	2.11	0.50
1:B:93:ILE:HD12	1:B:116:VAL:HG12	1.94	0.50
1:B:101:LEU:N	1:B:104:GLN:HE21	2.10	0.50
1:A:313:ARG:HB2	1:A:313:ARG:CZ	2.41	0.50
1:B:339:TYR:CD1	1:B:340:ARG:NH1	2.79	0.50
1:A:105:ARG:HA	1:A:133:MET:CE	2.42	0.49
1:B:101:LEU:HD21	1:B:129:PRO:HB2	1.94	0.49
1:B:158:VAL:C	1:B:159:ILE:HD12	2.37	0.49
1:B:161:ASN:ND2	1:B:321:VAL:O	2.45	0.49
1:B:201:MET:HE2	1:B:201:MET:N	2.27	0.49
1:A:102:GLU:HA	1:A:105:ARG:CZ	2.42	0.49
1:A:110:MET:HE2	1:A:111:MET:CG	2.42	0.49
1:A:325:LEU:C	1:A:326:ILE:HD12	2.37	0.49
1:B:88:LYS:HB3	1:B:90:TYR:CE1	2.48	0.49
1:B:187:PRO:HD2	1:B:221:PHE:CE2	2.47	0.49
1:B:64:LEU:HD12	1:B:64:LEU:C	2.37	0.49
1:A:249:ILE:O	1:A:252:MET:HB3	2.12	0.49
1:A:126:TYR:HD1	1:A:130:LEU:HD13	1.78	0.49
1:B:67:THR:O	1:B:68:SER:HB2	2.12	0.49
1:B:304:MET:CE	1:B:319:ILE:HD12	2.40	0.49
1:A:145:MET:HE2	1:A:147:TRP:CH2	2.47	0.49
1:B:158:VAL:HA	1:B:319:ILE:O	2.13	0.49
1:B:126:TYR:HB3	1:B:131:LEU:HD11	1.94	0.48
1:B:130:LEU:HD13	1:B:134:LEU:HD11	1.94	0.48
1:B:223:PRO:HD3	1:B:249:ILE:HG22	1.94	0.48
1:A:135:GLU:CG	1:A:138:ARG:HD2	2.43	0.48
1:B:76:GLU:H	1:B:294:LYS:HZ1	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LEU:O	1:B:105:ARG:HB2	2.14	0.48
1:B:266:PRO:HD3	3:B:407:HOH:O	2.13	0.48
1:A:90:TYR:N	1:A:90:TYR:CD1	2.81	0.48
1:A:174:ILE:HD11	1:A:204:MET:HE2	1.94	0.48
1:A:119:LEU:HD13	1:A:142:MET:CE	2.43	0.48
1:A:69:SER:N	1:A:96:ASN:OD1	2.40	0.47
1:A:220:ASP:O	1:A:221:PHE:HB2	2.13	0.47
1:A:110:MET:HE1	1:A:114:LYS:HG3	1.95	0.47
1:B:176:ARG:HH12	1:B:333:ASP:N	2.13	0.47
1:A:110:MET:HG3	1:A:111:MET:N	2.29	0.47
1:A:313:ARG:NH1	1:A:313:ARG:CB	2.77	0.47
1:B:73:TYR:HD2	1:B:74:PHE:CD1	2.32	0.47
1:B:137:TYR:HA	1:B:139:HIS:CE1	2.50	0.47
1:B:266:PRO:HD2	1:B:267:GLN:NE2	2.30	0.47
1:B:184:ILE:HG23	1:B:217:VAL:O	2.14	0.47
1:B:315:GLU:O	1:B:315:GLU:HG2	2.15	0.47
1:A:166:GLY:O	1:A:169:ALA:HB3	2.15	0.47
1:B:212:PRO:HD2	1:B:215:TRP:CE3	2.50	0.47
1:B:129:PRO:O	1:B:132:ALA:HB3	2.15	0.47
1:B:66:ALA:HB3	1:B:96:ASN:ND2	2.29	0.46
1:B:128:GLU:N	1:B:129:PRO:HD2	2.30	0.46
1:A:105:ARG:HH11	1:A:105:ARG:HB2	1.80	0.46
1:A:128:GLU:N	1:A:129:PRO:CD	2.78	0.46
1:B:64:LEU:HD22	1:B:81:VAL:HG11	1.97	0.46
1:B:144:VAL:HG23	1:B:155:THR:CA	2.45	0.46
1:B:294:LYS:O	1:B:297:LEU:HB2	2.16	0.46
1:B:147:TRP:CG	1:B:158:VAL:CG1	2.98	0.46
1:B:306:LEU:HD12	1:B:306:LEU:HA	1.48	0.46
1:B:310:VAL:C	1:B:312:LYS:H	2.24	0.46
1:A:159:ILE:HD12	1:A:320:GLU:HG3	1.97	0.46
1:A:275:ASP:O	1:A:276:ASN:HB3	2.15	0.46
1:B:135:GLU:HG2	1:B:138:ARG:HD3	1.97	0.46
1:B:276:ASN:HB3	1:B:291:HIS:HD2	1.80	0.46
1:A:315:GLU:HA	1:A:316:PRO:HD2	1.76	0.46
1:B:105:ARG:O	1:B:108:LEU:N	2.49	0.46
1:B:145:MET:HB3	1:B:147:TRP:CZ3	2.51	0.46
1:A:123:CYS:C	1:A:125:GLU:H	2.23	0.46
1:A:76:GLU:CD	1:A:294:LYS:HG3	2.40	0.46
1:A:153:ASP:HA	3:A:357:HOH:O	2.16	0.46
1:A:154:PHE:CD1	1:A:154:PHE:N	2.82	0.46
1:A:228:ARG:O	1:A:232:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLU:CB	1:A:129:PRO:HD3	2.40	0.45
1:B:100:ASN:CG	1:B:103:LYS:HB2	2.41	0.45
1:A:95:GLY:C	1:A:96:ASN:HD22	2.23	0.45
1:B:128:GLU:N	1:B:129:PRO:CD	2.79	0.45
1:B:136:GLU:O	1:B:139:HIS:NE2	2.46	0.45
1:A:126:TYR:CD1	1:A:130:LEU:HD13	2.52	0.45
1:B:149:GLU:OE1	1:B:151:LYS:HG2	2.16	0.45
1:B:159:ILE:N	1:B:159:ILE:CD1	2.80	0.45
1:B:294:LYS:HE2	1:B:294:LYS:HB3	1.47	0.45
1:A:224:GLU:O	1:A:224:GLU:HG2	2.11	0.45
1:A:312:LYS:H	1:A:312:LYS:HG2	1.19	0.45
1:A:311:ASN:O	1:A:313:ARG:N	2.50	0.45
1:B:126:TYR:N	1:B:127:PRO:CD	2.79	0.45
1:B:147:TRP:CD1	1:B:158:VAL:CG2	3.00	0.45
1:B:264:ARG:HB3	1:B:267:GLN:HB2	1.99	0.45
1:A:318:SER:C	1:A:319:ILE:HD13	2.42	0.45
1:B:302:PHE:CE2	1:B:306:LEU:CD2	3.00	0.45
1:A:177:GLY:HA3	1:A:337:ARG:HB2	1.98	0.45
1:B:114:LYS:N	1:B:114:LYS:CD	2.78	0.45
1:B:84:ASN:ND2	1:B:299:GLU:HA	2.31	0.45
1:B:113:GLN:C	1:B:115:ARG:H	2.23	0.45
1:B:73:TYR:CD2	1:B:73:TYR:C	2.95	0.44
1:B:142:MET:HA	1:B:305:LEU:HD11	1.97	0.44
1:B:73:TYR:CD2	1:B:74:PHE:N	2.85	0.44
1:B:261:MET:HE3	1:B:263:LEU:HD13	1.99	0.44
1:B:320:GLU:HG2	1:B:321:VAL:N	2.32	0.44
1:B:119:LEU:HD23	1:B:119:LEU:HA	1.68	0.44
1:A:108:LEU:HD12	1:A:108:LEU:HA	1.82	0.44
1:A:313:ARG:HH11	1:A:313:ARG:HB3	1.81	0.44
1:B:234:LEU:HD13	1:B:261:MET:CE	2.48	0.44
1:B:179:ARG:HB2	1:B:336:PHE:CE1	2.53	0.44
1:A:263:LEU:HD12	1:A:263:LEU:HA	1.74	0.44
1:B:117:ASP:O	1:B:309:ILE:HG21	2.18	0.44
1:B:147:TRP:CE2	1:B:158:VAL:HG11	2.51	0.44
1:B:264:ARG:HB2	1:B:268:ASP:CG	2.42	0.44
1:B:76:GLU:CB	1:B:294:LYS:HE2	2.48	0.43
1:B:130:LEU:HD11	1:B:134:LEU:HD11	2.00	0.43
1:B:147:TRP:CD1	1:B:158:VAL:HG21	2.53	0.43
1:A:171:ARG:HD2	1:A:171:ARG:HA	1.20	0.43
1:A:108:LEU:HD22	1:A:133:MET:HE3	2.00	0.43
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:GLY:CA	1:B:107:TYR:CD1	3.01	0.43
1:A:110:MET:HA	1:A:113:GLN:HB2	2.01	0.43
1:A:135:GLU:HA	1:A:138:ARG:CG	2.48	0.43
1:B:147:TRP:CG	1:B:158:VAL:HG11	2.54	0.43
1:B:101:LEU:CD2	1:B:129:PRO:HB2	2.48	0.43
1:B:114:LYS:HD2	1:B:114:LYS:HA	1.49	0.43
1:B:151:LYS:H	1:B:151:LYS:HG3	1.41	0.43
1:A:101:LEU:O	1:A:105:ARG:HB3	2.18	0.43
1:B:304:MET:HE3	1:B:304:MET:HB2	1.96	0.43
1:A:105:ARG:CB	1:A:105:ARG:NH1	2.80	0.43
1:B:137:TYR:O	1:B:140:ILE:HG23	2.19	0.43
1:B:276:ASN:HB2	1:B:291:HIS:HA	2.01	0.43
1:B:299:GLU:O	1:B:303:ASN:ND2	2.51	0.43
1:B:336:PHE:C	1:B:338:ASP:H	2.20	0.43
1:B:120:LEU:HD23	1:B:121:VAL:N	2.33	0.43
1:A:97:ALA:HB1	1:A:104:GLN:CG	2.42	0.43
1:A:173:LEU:HD23	1:A:173:LEU:HA	1.76	0.43
1:B:123:CYS:HB3	1:B:125:GLU:O	2.19	0.43
1:B:133:MET:O	1:B:137:TYR:HD1	2.02	0.43
1:A:164:GLU:HG3	1:A:323:PRO:HG2	2.00	0.42
1:B:60:LYS:HD3	1:B:60:LYS:HA	1.59	0.42
1:B:110:MET:HB3	1:B:110:MET:HE2	1.54	0.42
1:A:139:HIS:CE1	1:A:140:ILE:HG22	2.54	0.42
1:A:325:LEU:HD11	1:A:327:GLU:HG3	2.00	0.42
1:B:235:SER:C	1:B:236:GLN:HG2	2.44	0.42
1:A:119:LEU:HB2	1:A:140:ILE:HD11	2.01	0.42
1:B:151:LYS:O	1:B:153:ASP:N	2.52	0.42
1:B:154:PHE:HE1	3:B:409:HOH:O	2.01	0.42
1:A:110:MET:HE3	1:A:114:LYS:HG3	1.98	0.42
1:B:76:GLU:H	1:B:294:LYS:NZ	2.18	0.42
1:B:303:ASN:HD22	1:B:303:ASN:N	2.17	0.42
1:A:276:ASN:HA	1:A:289:THR:HG21	2.01	0.42
1:B:93:ILE:HD12	1:B:116:VAL:CG1	2.49	0.42
1:B:185:PRO:HD2	1:B:218:GLN:HA	2.01	0.42
1:B:269:VAL:HG13	3:B:379:HOH:O	2.19	0.42
1:A:230:MET:HG2	1:A:254:ALA:O	2.19	0.42
1:B:322:HIS:HA	1:B:323:PRO:HD2	1.69	0.42
1:A:211:VAL:HG22	1:A:216:ILE:HD11	2.00	0.42
1:A:313:ARG:CB	1:A:313:ARG:HH11	2.33	0.42
1:B:65:LEU:HD13	1:B:107:TYR:HB3	2.02	0.42
1:A:76:GLU:HB3	1:A:294:LYS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ILE:HB	1:B:320:GLU:HB2	2.02	0.42
1:B:261:MET:CE	1:B:263:LEU:HD13	2.50	0.42
1:A:163:PHE:CE2	1:A:199:GLY:HA2	2.55	0.41
1:B:267:GLN:H	1:B:267:GLN:HE21	1.65	0.41
1:B:308:ARG:HH21	1:B:313:ARG:HH22	1.68	0.41
1:B:131:LEU:HA	1:B:131:LEU:HD12	1.69	0.41
1:B:234:LEU:HA	1:B:234:LEU:HD23	1.82	0.41
1:B:171:ARG:O	1:B:175:GLU:HG3	2.20	0.41
1:B:204:MET:HE3	1:B:209:ILE:CG2	2.50	0.41
1:B:310:VAL:C	1:B:312:LYS:N	2.78	0.41
1:A:180:GLU:HB3	1:A:215:TRP:CZ3	2.56	0.41
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.85	0.41
1:B:95:GLY:HA2	1:B:107:TYR:CD1	2.53	0.41
1:B:105:ARG:HH11	1:B:105:ARG:CB	2.11	0.41
1:B:130:LEU:O	1:B:134:LEU:HG	2.21	0.41
1:B:171:ARG:NH1	3:B:435:HOH:O	2.29	0.41
1:B:271:LEU:HD12	1:B:272:ILE:H	1.78	0.41
1:B:101:LEU:HD12	3:B:357:HOH:O	2.20	0.41
1:A:232:GLN:HG2	3:A:468:HOH:O	2.21	0.41
1:B:102:GLU:HA	1:B:105:ARG:HB3	2.02	0.41
1:B:255:LEU:HD12	1:B:255:LEU:HA	1.85	0.41
1:B:313:ARG:HB3	1:B:313:ARG:HH11	1.82	0.41
1:B:207:ALA:O	1:B:208:MET:HB2	2.21	0.41
1:B:223:PRO:HD3	1:B:249:ILE:CG2	2.50	0.41
1:B:233:ILE:HA	1:B:236:GLN:OE1	2.21	0.41
1:B:62:ILE:HG12	1:B:305:LEU:HD23	2.02	0.40
1:B:167:TYR:OH	1:B:206:GLU:OE2	2.27	0.40
1:A:102:GLU:HA	1:A:105:ARG:NE	2.37	0.40
1:B:74:PHE:O	1:B:294:LYS:HE3	2.22	0.40
1:B:128:GLU:HB2	1:B:129:PRO:HD3	2.02	0.40
1:B:305:LEU:HA	1:B:305:LEU:HD12	1.77	0.40
1:A:197:LEU:HD11	1:A:201:MET:CE	2.51	0.40
1:A:93:ILE:HD13	1:B:93:ILE:HG12	2.03	0.40
1:A:179:ARG:HG2	3:A:446:HOH:O	2.21	0.40
1:B:276:ASN:HA	1:B:289:THR:HG21	2.03	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	272/289 (94%)	247 (91%)	21 (8%)	4 (2%)	8	6
1	B	272/289 (94%)	225 (83%)	33 (12%)	14 (5%)	1	0
All	All	544/578 (94%)	472 (87%)	54 (10%)	18 (3%)	3	1

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	275	ASP
1	A	312	LYS
1	A	340	ARG
1	B	68	SER
1	B	75	ALA
1	B	97	ALA
1	B	98	TRP
1	B	275	ASP
1	B	339	TYR
1	B	72	ALA
1	B	149	GLU
1	B	152	ALA
1	B	221	PHE
1	B	154	PHE
1	B	293	PRO
1	B	311	ASN
1	B	310	VAL

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	226/238 (95%)	165 (73%)	61 (27%)	0	0
1	B	226/238 (95%)	158 (70%)	68 (30%)	0	0
All	All	452/476 (95%)	323 (72%)	129 (28%)	0	0

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	A	67	THR
1	A	69	SER
1	A	70	GLU
1	A	83	LYS
1	A	87	GLN
1	A	88	LYS
1	A	91	THR
1	A	92	LEU
1	A	93	ILE
1	A	94	LEU
1	A	101	LEU
1	A	105	ARG
1	A	108	LEU
1	A	110	MET
1	A	114	LYS
1	A	115	ARG
1	A	116	VAL
1	A	119	LEU
1	A	120	LEU
1	A	122	MET
1	A	125	GLU
1	A	130	LEU
1	A	131	LEU
1	A	140	ILE
1	A	142	MET
1	A	144	VAL
1	A	149	GLU
1	A	158	VAL
1	A	171	ARG
1	A	175	GLU
1	A	181	ILE
1	A	201	MET

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Mol	Chain	Res	Type
1	A	202	LYS
1	A	204	MET
1	A	205	GLU
1	A	208	MET
1	A	210	LYS
1	A	211	VAL
1	A	213	GLU
1	A	222	GLU
1	A	250	MET
1	A	255	LEU
1	A	263	LEU
1	A	269	VAL
1	A	271	LEU
1	A	278	ARG
1	A	294	LYS
1	A	296	SER
1	A	299	GLU
1	A	306	LEU
1	A	309	ILE
1	A	310	VAL
1	A	312	LYS
1	A	314	GLU
1	A	315	GLU
1	A	317	GLN
1	A	325	LEU
1	A	338	ASP
1	A	339	TYR
1	A	341	ARG
1	B	60	LYS
1	B	62	ILE
1	B	64	LEU
1	B	69	SER
1	B	77	ILE
1	B	83	LYS
1	B	88	LYS
1	B	92	LEU
1	B	94	LEU
1	B	96	ASN
1	B	99	ASN
1	B	100	ASN
1	B	101	LEU
1	B	102	GLU

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Mol	Chain	Res	Type
1	B	104	GLN
1	B	105	ARG
1	B	108	LEU
1	B	109	SER
1	B	110	MET
1	B	113	GLN
1	B	114	LYS
1	B	115	ARG
1	B	124	SER
1	B	125	GLU
1	B	130	LEU
1	B	131	LEU
1	B	133	MET
1	B	135	GLU
1	B	139	HIS
1	B	140	ILE
1	B	149	GLU
1	B	151	LYS
1	B	158	VAL
1	B	159	ILE
1	B	176	ARG
1	B	179	ARG
1	B	201	MET
1	B	202	LYS
1	B	204	MET
1	B	216	ILE
1	B	222	GLU
1	B	232	GLN
1	B	236	GLN
1	B	239	ARG
1	B	250	MET
1	B	255	LEU
1	B	264	ARG
1	B	267	GLN
1	B	269	VAL
1	B	271	LEU
1	B	294	LYS
1	B	306	LEU
1	B	310	VAL
1	B	312	LYS
1	B	313	ARG
1	B	314	GLU

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Mol	Chain	Res	Type
1	B	315	GLU
1	B	318	SER
1	B	319	ILE
1	B	320	GLU
1	B	322	HIS
1	B	324	ARG
1	B	325	LEU
1	B	329	ARG
1	B	337	ARG
1	B	339	TYR
1	B	340	ARG
1	B	341	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	113	GLN
1	A	139	HIS
1	A	236	GLN
1	A	279	ASN
1	A	291	HIS
1	A	292	GLN
1	A	311	ASN
1	B	104	GLN
1	B	267	GLN
1	B	291	HIS
1	B	303	ASN
1	B	311	ASN
1	B	317	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 3 ligands modelled in this entry, 3 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

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.