



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:56 PM GMT

PDB ID : 1DBQ  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

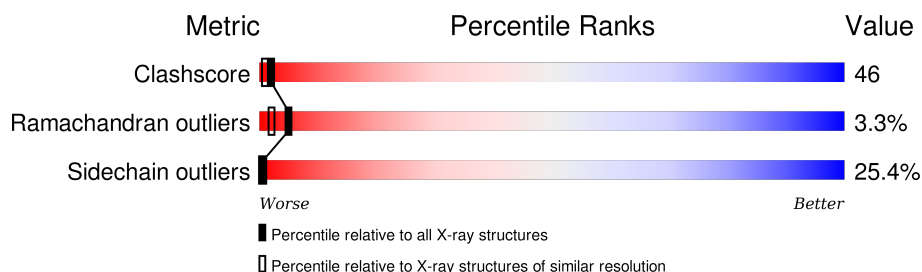
# 1 Overall quality at a glance

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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	289	 41% 39% 13% • •
1	B	289	 35% 42% 17% • •

## 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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

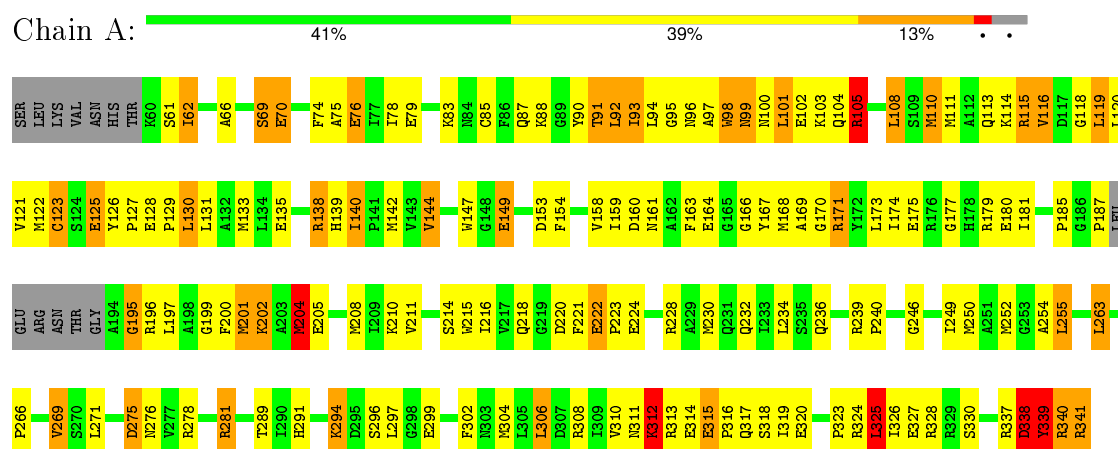
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	102	Total	O	0	0
			102	102		

### 3 Residue-property plots

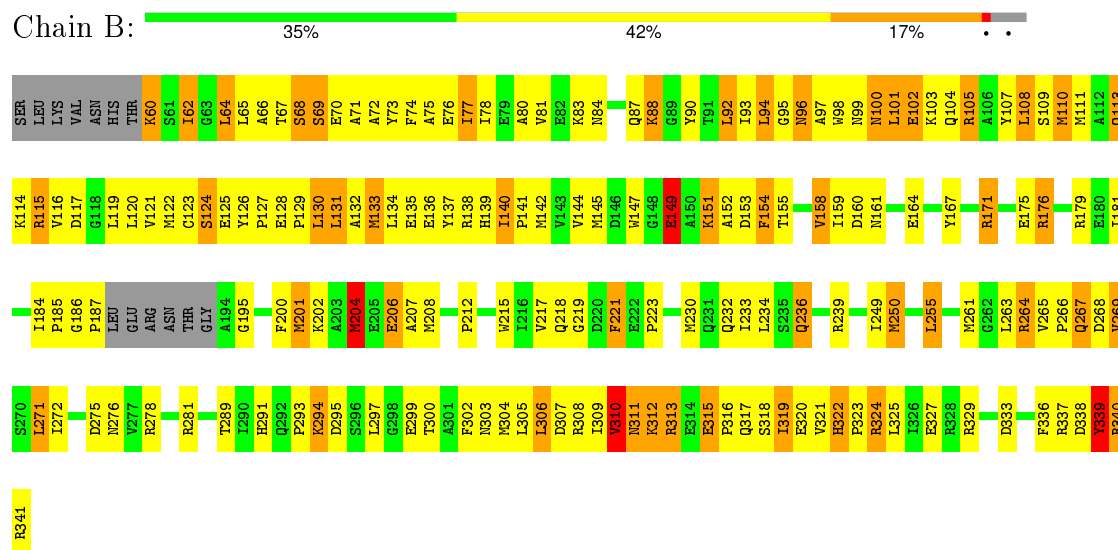
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

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 will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	33.0	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: 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	1.09	3/2217 (0.1%)	1.23	14/2991 (0.5%)
1	B	0.98	1/2217 (0.0%)	1.20	9/2991 (0.3%)
All	All	1.04	4/4434 (0.1%)	1.22	23/5982 (0.4%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	330	SER	CB-OG	6.19	1.50	1.42
1	A	76	GLU	CG-CD	6.03	1.60	1.51
1	B	206	GLU	CB-CG	-5.75	1.41	1.52
1	A	310	VAL	CB-CG2	-5.37	1.41	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	GLY	C-N-CD	-9.22	100.32	120.60
1	B	338	ASP	N-CA-CB	9.01	126.83	110.60
1	A	339	TYR	CA-CB-CG	8.93	130.37	113.40
1	B	204	MET	CG-SD-CE	-8.66	86.35	100.20
1	A	339	TYR	N-CA-CB	7.78	124.61	110.60
1	A	204	MET	CG-SD-CE	7.46	112.14	100.20
1	A	147	TRP	C-N-CA	-7.26	107.06	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	338	ASP	CA-C-N	-6.37	103.18	117.20
1	B	195	GLY	N-CA-C	-6.37	97.18	113.10
1	A	338	ASP	N-CA-CB	6.28	121.90	110.60
1	A	325	LEU	CA-CB-CG	5.90	128.87	115.30
1	B	338	ASP	C-N-CA	5.82	136.25	121.70
1	B	160	ASP	N-CA-C	-5.77	95.43	111.00
1	A	160	ASP	CB-CG-OD1	5.65	123.39	118.30
1	A	338	ASP	N-CA-C	5.50	125.85	111.00
1	A	195	GLY	N-CA-C	-5.49	99.39	113.10
1	B	339	TYR	CB-CA-C	5.38	121.15	110.40
1	A	98	TRP	N-CA-C	5.35	125.44	111.00
1	A	144	VAL	CB-CA-C	5.34	121.54	111.40
1	B	339	TYR	N-CA-CB	5.25	120.05	110.60
1	A	147	TRP	N-CA-C	-5.24	96.86	111.00
1	A	123	CYS	N-CA-C	5.17	124.95	111.00

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	166	0
1	B	2172	0	2142	235	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	400	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 46.

All (400) 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:B:140:ILE:HD12	1:B:141:PRO:HD2	1.40	1.03
1:A:110:MET:HE3	1:A:111:MET:HA	1.39	1.02
1:A:159:ILE:HB	1:A:320:GLU:HG2	1.38	1.01
1:B:105:ARG:HH11	1:B:105:ARG:HB2	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:A:161:ASN:HB3	1:A:164:GLU:HG2	1.50	0.94
1:B:101:LEU:HD13	1:B:105:ARG:HH12	1.31	0.93
1:B:234:LEU:HB3	1:B:261:MET:HE1	1.51	0.93
1:A:102:GLU:HG3	1:A:105:ARG:NH2	1.83	0.93
1:B:76:GLU:HB2	1:B:294:LYS:NZ	1.85	0.92
1:B:161:ASN:HB3	1:B:164:GLU:HG2	1.48	0.92
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:NH1	1:B:115:ARG:HB3	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: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:76:GLU:HB2	1:B:294:LYS:HZ3	1.41	0.82
1:B:101:LEU:HD13	1:B:105:ARG:NH1	1.93	0.81
1:B:313:ARG:CZ	1:B:313:ARG:HB3	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:105:ARG:HA	1:B:133:MET:HE3	1.63	0.80
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:B:147:TRP:CD2	1:B:158:VAL:HG11	2.19	0.78
1:A:110:MET:CE	1:A:114:LYS:HG3	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ILE:CD1	1:B:141:PRO:HD2	2.14	0.77
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: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: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:135:GLU:O	1:A:138:ARG:HG3	1.86	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: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: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:B:76:GLU:HB3	1:B:295:ASP:OD1	1.90	0.71
1:A:291:HIS:HB2	1:A:326:ILE:HD11	1.73	0.71
1:A:101:LEU:HA	1:A:104:GLN:NE2	2.06	0.71
1:A:110:MET:HE3	1:A:111:MET:CA	2.19	0.71
1:B:324:ARG:HB3	3:B:380:HOH:O	1.91	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:128:GLU:HB2	1:A:129:PRO:HD3	1.72	0.70
1:B:105:ARG:NH1	1:B:105:ARG:HB2	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:265:VAL:HG22	1:B:269:VAL:HG23	1.74	0.68
1:B:144:VAL:HG21	1:B:155:THR:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:76:GLU:HB2	1:B:294:LYS:CE	2.26	0.66
1:A:167:TYR:CE1	1:A:202:LYS:HE3	2.31	0.66
1:B:126:TYR:O	1:B:131:LEU:HD22	1.96	0.65
1:A:149:GLU:H	1:A:149:GLU:CD	1.98	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:CG	1:A:105:ARG:HH11	2.09	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:110:MET:CE	1:A:111:MET:HA	2.24	0.64
1:B:76:GLU:H	1:B:294:LYS:HZ1	1.44	0.64
1:A:74:PHE:HB3	1:A:78:ILE:HD11	1.80	0.64
1:A:110:MET:HE3	1:A:114:LYS:HG3	1.80	0.63
1:B:339:TYR:HD1	1:B:340:ARG:HH11	1.46	0.63
1:B:144:VAL:HG23	1:B:155:THR:HA	1.79	0.63
1:A:105:ARG:HA	1:A:133:MET:HE3	1.80	0.63
1:A:101:LEU:CA	1:A:104:GLN:HE21	2.11	0.63
1:A:201:MET:N	1:A:201:MET:HE2	2.14	0.63
1:A:110:MET:HE2	1:A:111:MET:CG	2.29	0.63
1:A:105:ARG:HG2	1:A:105:ARG:O	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:HD12	1:B:159:ILE:N	2.14	0.62
1:A:337:ARG:O	1:A:338:ASP:HB2	2.01	0.61
1:B:139:HIS:ND1	1:B:140:ILE:HG22	2.15	0.61
1:B:234:LEU:HD21	1:B:269:VAL:HG11	1.80	0.61
1:B:107:TYR:O	1:B:111:MET:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ARG:NH1	1:A:115:ARG:HG3	2.16	0.61
1:A:105:ARG:CB	1:A:105:ARG:HH11	2.13	0.61
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:B:127:PRO:HB2	1:B:129:PRO:HD2	1.82	0.60
1:A:304:MET:SD	1:A:319:ILE:HD11	2.41	0.60
1:A:276:ASN:OD1	1:A:328:ARG:NH2	2.34	0.60
1:A:85:CYS:HG	1:A:302:PHE:HE1	1.49	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:B:141:PRO:HG2	1:B:309:ILE:CG2	2.32	0.59
1:B:110:MET:O	1:B:114:LYS:HG2	2.03	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:149:GLU:CD	1:B:151:LYS:HG2	2.23	0.59
1:A:174:ILE:HD11	1:A:204:MET:HE3	1.84	0.59
1:B:304:MET:O	1:B:308:ARG:HB2	2.03	0.58
1:B:310:VAL:O	1:B:312:LYS:HG2	2.03	0.58
1:A:105:ARG:HG3	1:A:105:ARG:HH11	1.67	0.58
1:A:340:ARG:HG3	1:A:341:ARG:N	2.19	0.58
1:A:223:PRO:HD3	1:A:249:ILE:HG22	1.85	0.58
1:B:202:LYS:O	1:B:206:GLU:HB3	2.03	0.58
1:A:110:MET:HE2	1:A:111:MET:HG2	1.86	0.57
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:B:304:MET:SD	1:B:317:GLN:HB2	2.45	0.56
1:A:66:ALA:O	1:A:96:ASN:HA	2.05	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: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:HA	1:A:236:GLN:OE1	2.04	0.56
1:B:100:ASN:C	1:B:104:GLN:HE21	2.10	0.56
1:B:339:TYR:O	1:B:340:ARG:HD2	2.05	0.56
1:B:181:ILE:HD12	1:B:204:MET:HE1	1.86	0.55
1:A:196:ARG:HG3	1:A:197:LEU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TYR:HE2	1:A:306:LEU:HD11	1.70	0.55
1:A:115:ARG:HH11	1:A:115:ARG:HG3	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:A:119:LEU:HD13	1:A:142:MET:HE3	1.88	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:B:73:TYR:O	1:B:294:LYS:NZ	2.39	0.54
1:B:271:LEU:C	1:B:271:LEU:HD12	2.28	0.54
1:A:249:ILE:HB	3:A:439:HOH:O	2.07	0.54
1:A:170:GLY:HA2	1:A:200:PHE:CE1	2.43	0.54
1:B:126:TYR:N	1:B:127:PRO:HD3	2.22	0.54
1:A:97:ALA:HA	1:A:103:LYS:HD3	1.89	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:CG	1:A:115:ARG:HH11	2.21	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:B:69:SER:HA	1:B:78:ILE:HD13	1.90	0.53
1:A:255:LEU:HD13	1:A:271:LEU:HD22	1.91	0.53
1:A:161:ASN:HB3	1:A:164:GLU:CD	2.28	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:B:200:PHE:HD2	1:B:201:MET:HE2	1.72	0.53
1:A:174:ILE:HD11	1:A:204:MET:HE2	1.89	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:B:123:CYS:HB2	1:B:126:TYR:CE2	2.45	0.52
1:A:326:ILE:N	1:A:326:ILE:HD12	2.24	0.52
1:B:119:LEU:CB	1:B:142:MET:HB3	2.40	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:308:ARG:HG3	1:B:313:ARG:O	2.10	0.52
1:B:325:LEU:HD13	1:B:325:LEU:C	2.30	0.52
1:A:163:PHE:HA	1:A:195:GLY:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:MET:CE	1:B:319:ILE:HD12	2.40	0.51
1:B:137:TYR:HA	1:B:139:HIS:HE2	1.72	0.51
1:A:70:GLU:OE1	1:A:70:GLU:HA	2.11	0.51
1:A:313:ARG:NH1	1:A:313:ARG:HB2	2.26	0.51
1:A:98:TRP:O	1:A:99:ASN:HB2	2.11	0.51
1:A:224:GLU:O	1:A:224:GLU:HG2	2.11	0.51
1:B:73:TYR:CD2	1:B:74:PHE:CD1	2.99	0.51
1:A:110:MET:O	1:A:114:LYS:HG3	2.12	0.50
1:B:77:ILE:HG22	1:B:122:MET:CE	2.41	0.50
1:B:140:ILE:HD12	1:B:140:ILE:C	2.32	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:110:MET:HE2	1:A:111:MET:HG3	1.94	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:100:ASN:C	1:B:104:GLN:HG3	2.31	0.50
1:B:101:LEU:N	1:B:104:GLN:HE21	2.10	0.50
1:A:313:ARG:CZ	1:A:313:ARG:HB2	2.41	0.50
1:B:339:TYR:CD1	1:B:340:ARG:NH1	2.79	0.50
1:B:101:LEU:HD21	1:B:129:PRO:HB2	1.94	0.49
1:B:161:ASN:ND2	1:B:321:VAL:O	2.45	0.49
1:A:105:ARG:HA	1:A:133:MET:CE	2.42	0.49
1:A:102:GLU:HA	1:A:105:ARG:CZ	2.42	0.49
1:A:105:ARG:N	1:A:133:MET:HE1	2.27	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:A:197:LEU:HD11	1:A:201:MET:HE1	1.94	0.49
1:A:249:ILE:O	1:A:252:MET:HB3	2.12	0.49
1:B:67:THR:O	1:B:68:SER:HB2	2.12	0.49
1:A:126:TYR:HD1	1:A:130:LEU:HD13	1.78	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:B:76:GLU:N	1:B:294:LYS:HZ1	2.08	0.48
1:A:135:GLU:CG	1:A:138:ARG:HD2	2.43	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TYR:N	1:A:90:TYR:CD1	2.81	0.48
1:A:201:MET:CA	1:A:201:MET:HE2	2.44	0.48
1:A:220:ASP:O	1:A:221:PHE:HB2	2.13	0.47
1:A:119:LEU:HD13	1:A:142:MET:CE	2.43	0.47
1:A:69:SER:N	1:A:96:ASN:OD1	2.40	0.47
1:B:176:ARG:HH12	1:B:333:ASP:N	2.13	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: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:120:LEU:C	1:B:120:LEU:HD23	2.35	0.47
1:B:266:PRO:HD2	1:B:267:GLN:NE2	2.30	0.47
1:B:315:GLU:O	1:B:315:GLU:HG2	2.15	0.47
1:B:184:ILE:HG23	1:B:217:VAL:O	2.14	0.47
1:A:281:ARG:C	1:A:281:ARG:HD3	2.35	0.47
1:B:212:PRO:HD2	1:B:215:TRP:CE3	2.50	0.47
1:A:166:GLY:O	1:A:169:ALA:HB3	2.15	0.47
1:B:129:PRO:O	1:B:132:ALA:HB3	2.15	0.47
1:B:128:GLU:N	1:B:129:PRO:HD2	2.30	0.46
1:B:66:ALA:HB3	1:B:96:ASN:ND2	2.29	0.46
1:A:105:ARG:HB2	1:A:105:ARG:HH11	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:294:LYS:O	1:B:297:LEU:HB2	2.16	0.46
1:B:144:VAL:HG23	1:B:155:THR:CA	2.45	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:304:MET:HE3	1:B:319:ILE:HD12	1.97	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:B:234:LEU:CD1	1:B:261:MET:HE1	2.45	0.46
1:A:154:PHE:CD1	1:A:154:PHE:N	2.82	0.46
1:A:153:ASP:HA	3:A:357:HOH:O	2.16	0.46
1:B:181:ILE:HD12	1:B:204:MET:CE	2.46	0.46
1:A:228:ARG:O	1:A:232:GLN:HG2	2.16	0.46
1:A:128:GLU:CB	1:A:129:PRO:HD3	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:C	1:A:326:ILE:HD12	2.37	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:B:294:LYS:HB3	1:B:294:LYS:HE2	1.47	0.45
1:B:159:ILE:N	1:B:159:ILE:CD1	2.80	0.45
1:B:149:GLU:OE1	1:B:151:LYS:HG2	2.16	0.45
1:A:126:TYR:CD1	1:A:130:LEU:HD13	2.52	0.45
1:A:312:LYS:HG2	1:A:312:LYS:H	1.19	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:158:VAL:C	1:B:159:ILE:HD12	2.37	0.45
1:A:311:ASN:O	1:A:313:ARG:N	2.50	0.45
1:B:264:ARG:HB3	1:B:267:GLN:HB2	1.99	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:CD	1:B:114:LYS:N	2.78	0.45
1:B:84:ASN:ND2	1:B:299:GLU:HA	2.31	0.45
1:B:201:MET:HE2	1:B:201:MET:N	2.32	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:320:GLU:HG2	1:B:321:VAL:N	2.32	0.44
1:B:64:LEU:C	1:B:64:LEU:HD12	2.37	0.44
1:B:119:LEU:HA	1:B:119:LEU:HD23	1.68	0.44
1:B:234:LEU:HD13	1:B:261:MET:CE	2.48	0.44
1:A:313:ARG:HB3	1:A:313:ARG:HH11	1.81	0.44
1:A:108:LEU:HD12	1:A:108:LEU:HA	1.82	0.44
1:B:179:ARG:HB2	1:B:336:PHE:CE1	2.53	0.44
1:B:77:ILE:CG2	1:B:122:MET:HE2	2.48	0.44
1:B:117:ASP:O	1:B:309:ILE:HG21	2.18	0.44
1:A:263:LEU:HD12	1:A:263:LEU:HA	1.74	0.44
1:B:147:TRP:CE2	1:B:158:VAL:HG11	2.51	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:B:95:GLY:CA	1:B:107:TYR:CD1	3.01	0.43
1:A:297:LEU:HA	1:A:297:LEU:HD23	1.69	0.43
1:B:147:TRP:CG	1:B:158:VAL:HG11	2.54	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:101:LEU:CD2	1:B:129:PRO:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LYS:HA	1:B:114:LYS:HD2	1.49	0.43
1:B:151:LYS:HG3	1:B:151:LYS:H	1.41	0.43
1:A:101:LEU:O	1:A:105:ARG:HB3	2.18	0.43
1:B:137:TYR:O	1:B:140:ILE:HG23	2.19	0.43
1:A:105:ARG:NH1	1:A:105:ARG:CB	2.80	0.43
1:A:197:LEU:CD1	1:A:201:MET:HE1	2.49	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:120:LEU:HD23	1:B:121:VAL:N	2.33	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:97:ALA:HB1	1:A:104:GLN:CG	2.42	0.43
1:A:173:LEU:HA	1:A:173:LEU:HD23	1.76	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:A:325:LEU:HD11	1:A:327:GLU:HG3	2.00	0.42
1:A:139:HIS:CE1	1:A:140:ILE:HG22	2.54	0.42
1:B:151:LYS:O	1:B:153:ASP:N	2.52	0.42
1:A:119:LEU:HB2	1:A:140:ILE:HD11	2.01	0.42
1:B:154:PHE:HE1	3:B:409:HOH:O	2.01	0.42
1:B:303:ASN:N	1:B:303:ASN:HD22	2.17	0.42
1:B:269:VAL:HG13	3:B:379:HOH:O	2.19	0.42
1:B:93:ILE:HD12	1:B:116:VAL:CG1	2.49	0.42
1:A:276:ASN:HA	1:A:289:THR:HG21	2.01	0.42
1:B:185:PRO:HD2	1:B:218:GLN:HA	2.01	0.42
1:B:322:HIS:HA	1:B:323:PRO:HD2	1.69	0.42
1:A:230:MET:HG2	1:A:254:ALA:O	2.19	0.42
1:A:313:ARG:HH11	1:A:313:ARG:CB	2.33	0.42
1:A:211:VAL:HG22	1:A:216:ILE:HD11	2.00	0.42
1:B:65:LEU:HD13	1:B:107:TYR:HB3	2.02	0.42
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:76:GLU:HB3	1:A:294:LYS:HB2	2.02	0.42
1:A:76:GLU:CD	1:A:294:LYS:HG3	2.40	0.42
1:A:163:PHE:CE2	1:A:199:GLY:HA2	2.55	0.41
1:B:310:VAL:C	1:B:312:LYS:H	2.24	0.41
1:B:308:ARG:HH21	1:B:313:ARG:HH22	1.68	0.41
1:B:267:GLN:HE21	1:B:267:GLN:H	1.65	0.41
1:B:131:LEU:HD12	1:B:131:LEU:HA	1.69	0.41
1:B:110:MET:HE2	1:B:110:MET:HB3	1.69	0.41
1:B:234:LEU:HA	1:B:234:LEU:HD23	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLN:C	1:B:115:ARG:H	2.23	0.41
1:B:171:ARG:O	1:B:175:GLU:HG3	2.20	0.41
1:A:123:CYS:C	1:A:125:GLU:H	2.23	0.41
1:B:105:ARG:CB	1:B:105:ARG:HH11	2.11	0.41
1:B:130:LEU:O	1:B:134:LEU:HG	2.21	0.41
1:B:271:LEU:HD12	1:B:272:ILE:H	1.78	0.41
1:B:95:GLY:HA2	1:B:107:TYR:CD1	2.53	0.41
1:B:171:ARG:NH1	3:B:435:HOH:O	2.29	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:101:LEU:HD12	3:B:357:HOH:O	2.20	0.41
1:A:95:GLY:C	1:A:96:ASN:HD22	2.23	0.41
1:B:304:MET:HE1	1:B:319:ILE:CD1	2.50	0.41
1:B:100:ASN:CG	1:B:103:LYS:HB2	2.41	0.41
1:B:102:GLU:HA	1:B:105:ARG:HB3	2.02	0.41
1:B:313:ARG:HH11	1:B:313:ARG:HB3	1.82	0.41
1:A:232:GLN:HG2	3:A:468:HOH:O	2.21	0.41
1:B:255:LEU:HD12	1:B:255:LEU:HA	1.85	0.41
1:B:233:ILE:HA	1:B:236:GLN:OE1	2.21	0.41
1:B:223:PRO:HD3	1:B:249:ILE:CG2	2.50	0.41
1:B:207:ALA:O	1:B:208:MET:HB2	2.21	0.41
1:B:234:LEU:HD13	1:B:261:MET:HE1	2.02	0.40
1:B:200:PHE:HD2	1:B:201:MET:HE1	1.81	0.40
1:B:167:TYR:OH	1:B:206:GLU:OE2	2.27	0.40
1:B:62:ILE:HG12	1:B:305:LEU:HD23	2.02	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:A:102:GLU:HA	1:A:105:ARG:NE	2.37	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:318:SER:C	1:A:319:ILE:HD13	2.42	0.40
1:A:93:ILE:HD13	1:B:93:ILE:HG12	2.03	0.40
1:B:276:ASN:HA	1:B:289:THR:HG21	2.03	0.40
1:A:179:ARG:HG2	3:A:446:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	272/289 (94%)	247 (91%)	21 (8%)	4 (2%)	13	9
1	B	272/289 (94%)	225 (83%)	33 (12%)	14 (5%)	2	1
All	All	544/578 (94%)	472 (87%)	54 (10%)	18 (3%)	5	2

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/238 (95%)	171 (76%)	55 (24%)	1	0
1	B	226/238 (95%)	166 (74%)	60 (26%)	0	0
All	All	452/476 (95%)	337 (75%)	115 (25%)	1	0

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

Mol	Chain	Res	Type
1	A	62	ILE
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	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	138	ARG
1	A	140	ILE
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
1	A	202	LYS
1	A	204	MET

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Mol	Chain	Res	Type
1	A	205	GLU
1	A	208	MET
1	A	210	LYS
1	A	222	GLU
1	A	250	MET
1	A	255	LEU
1	A	263	LEU
1	A	269	VAL
1	A	278	ARG
1	A	281	ARG
1	A	294	LYS
1	A	296	SER
1	A	299	GLU
1	A	306	LEU
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	70	GLU
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
1	B	105	ARG
1	B	108	LEU
1	B	109	SER
1	B	110	MET
1	B	113	GLN

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Mol	Chain	Res	Type
1	B	115	ARG
1	B	124	SER
1	B	130	LEU
1	B	131	LEU
1	B	133	MET
1	B	140	ILE
1	B	149	GLU
1	B	151	LYS
1	B	158	VAL
1	B	171	ARG
1	B	176	ARG
1	B	201	MET
1	B	204	MET
1	B	230	MET
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	278	ARG
1	B	281	ARG
1	B	294	LYS
1	B	306	LEU
1	B	310	VAL
1	B	312	LYS
1	B	313	ARG
1	B	315	GLU
1	B	318	SER
1	B	319	ILE
1	B	322	HIS
1	B	324	ARG
1	B	329	ARG
1	B	337	ARG
1	B	339	TYR
1	B	340	ARG
1	B	341	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	113	GLN
1	A	139	HIS
1	A	231	GLN
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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates 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 ⓘ

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.